



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:32 AM UTC

PDB ID : 2GR9 / pdb_00002gr9
Title : Crystal structure of P5CR complexed with NADH
Authors : Meng, Z.; Lou, Z.; Liu, Z.; Rao, Z.
Deposited on : 2006-04-23
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

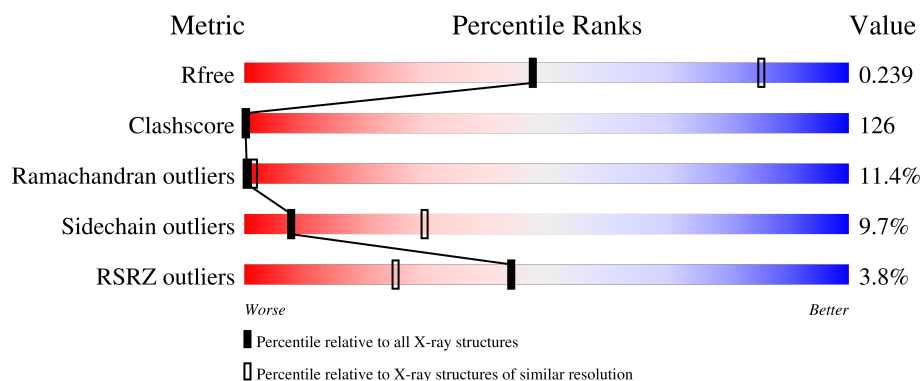
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	277	18% 59% 21% .
1	B	277	6% 17% 63% 19% .
1	C	277	9% 16% 67% 16% .
1	D	277	18% 66% 15% .
1	E	277	2% 14% 66% 20% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAI	A	1300	X	X	X	-
2	NAI	B	2300	X	-	X	-
2	NAI	C	3300	X	-	X	-
2	NAI	D	4300	X	-	X	-
2	NAI	E	5300	X	X	X	-
3	GLU	A	1301	-	-	X	-
3	GLU	B	2301	-	-	X	-
3	GLU	C	3301	-	-	X	-
3	GLU	D	4301	-	-	X	-
3	GLU	E	5301	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11077 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

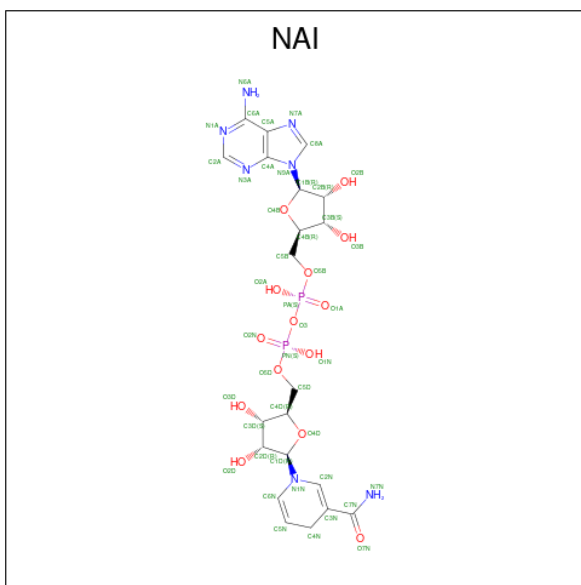
- Molecule 1 is a protein called Pyrroline-5-carboxylate reductase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	0	0
			2038	1279	363	383	13			
1	B	276	Total	C	N	O	S	0	0	0
			2023	1270	358	382	13			
1	C	277	Total	C	N	O	S	0	0	0
			2032	1276	360	383	13			
1	D	277	Total	C	N	O	S	0	0	0
			2038	1279	363	383	13			
1	E	277	Total	C	N	O	S	0	0	0
			2038	1279	363	383	13			

There are 10 discrepancies between the modelled and reference sequences:

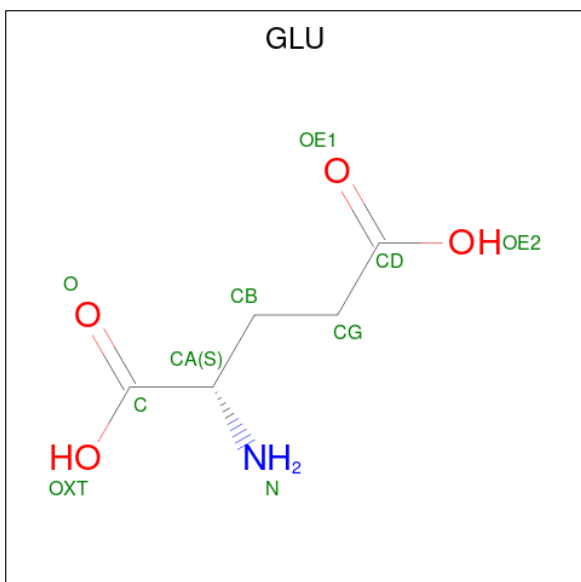
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ARG	-	cloning artifact	UNP P32322
A	0	GLY	-	cloning artifact	UNP P32322
B	-1	ARG	-	cloning artifact	UNP P32322
B	0	GLY	-	cloning artifact	UNP P32322
C	-1	ARG	-	cloning artifact	UNP P32322
C	0	GLY	-	cloning artifact	UNP P32322
D	-1	ARG	-	cloning artifact	UNP P32322
D	0	GLY	-	cloning artifact	UNP P32322
E	-1	ARG	-	cloning artifact	UNP P32322
E	0	GLY	-	cloning artifact	UNP P32322

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 21	N 6	O 14	P 2	0	0
2	B	1	Total 43	C 21	N 6	O 14	P 2	0	0
2	C	1	Total 43	C 21	N 6	O 14	P 2	0	0
2	D	1	Total 43	C 21	N 6	O 14	P 2	0	0
2	E	1	Total 43	C 21	N 6	O 14	P 2	0	0

- Molecule 3 is GLUTAMIC ACID (CCD ID: GLU) (formula: $C_5H_9NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	5	1	4		
3	B	1	Total	C	N	O	0	0
			10	5	1	4		
3	C	1	Total	C	N	O	0	0
			10	5	1	4		
3	D	1	Total	C	N	O	0	0
			10	5	1	4		
3	E	1	Total	C	N	O	0	0
			10	5	1	4		

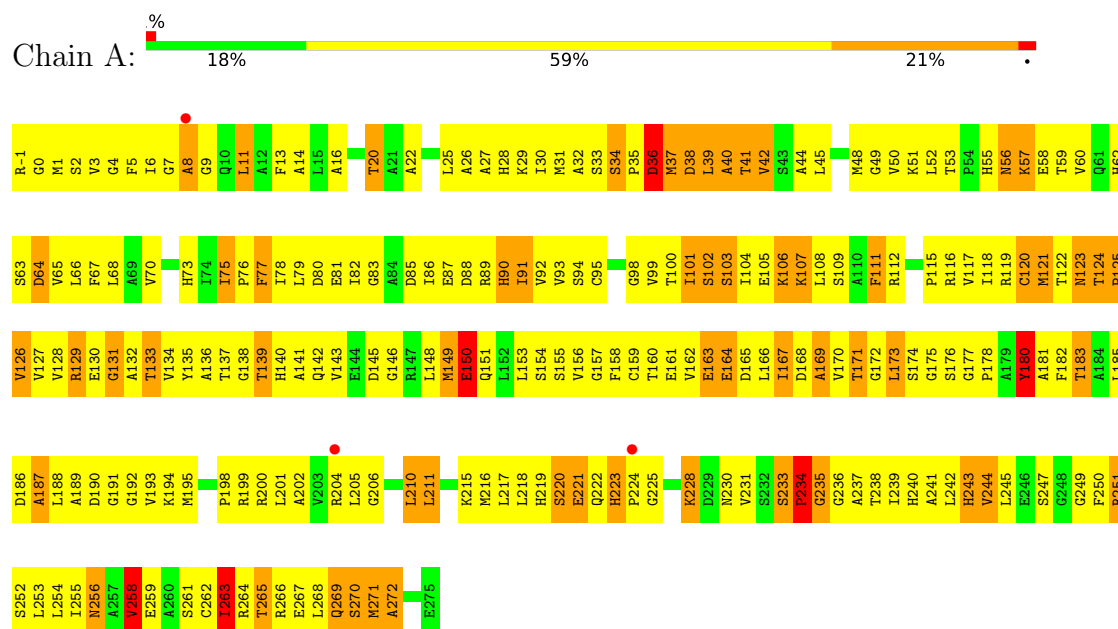
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	141	Total	O	0	0
			141	141		
4	B	93	Total	O	0	0
			93	93		
4	C	116	Total	O	0	0
			116	116		
4	D	155	Total	O	0	0
			155	155		
4	E	138	Total	O	0	0
			138	138		

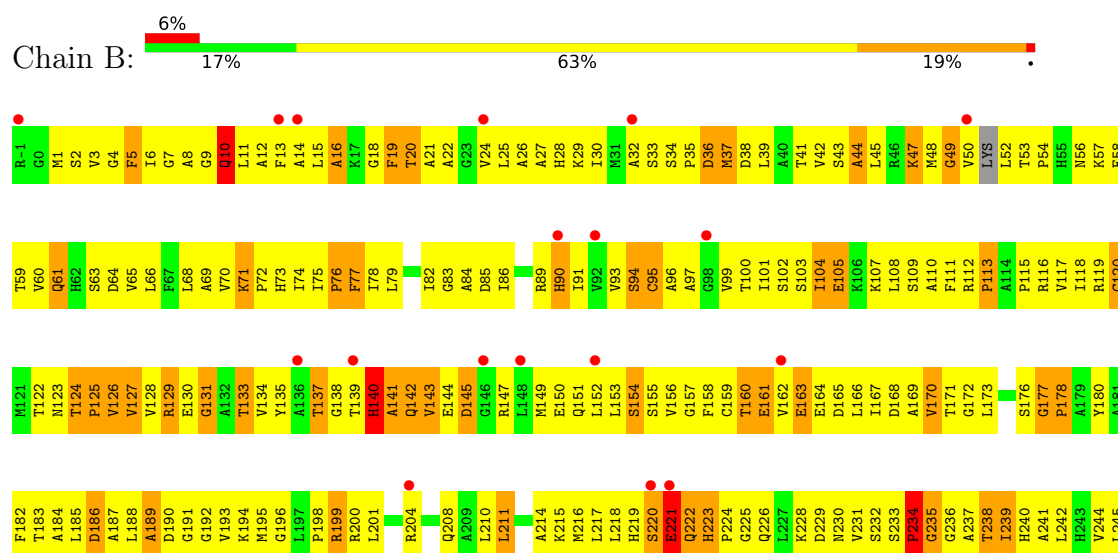
3 Residue-property plots

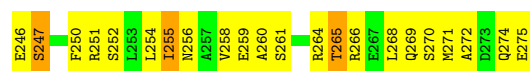
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Pyrroline-5-carboxylate reductase 1

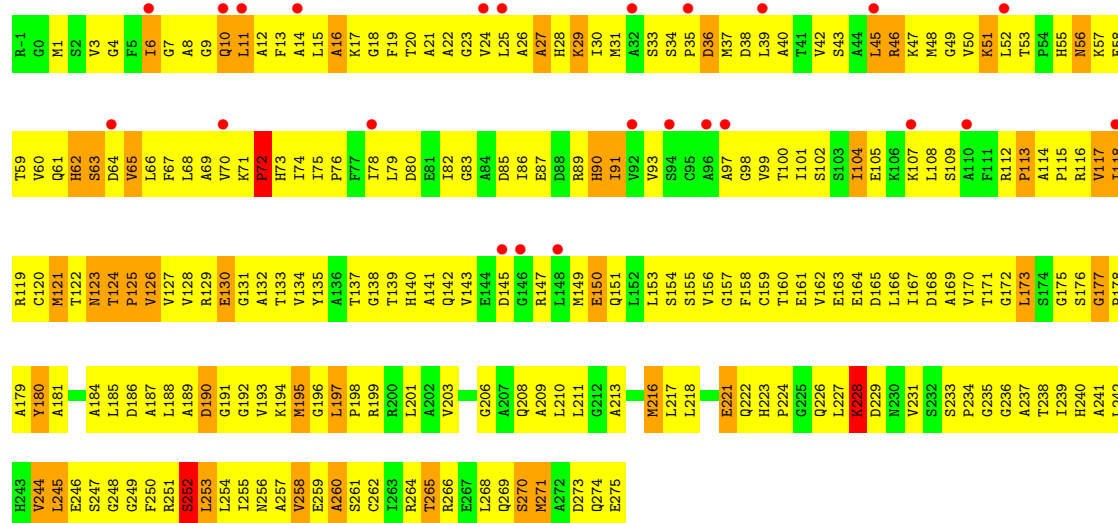


• Molecule 1: Pyrroline-5-carboxylate reductase 1

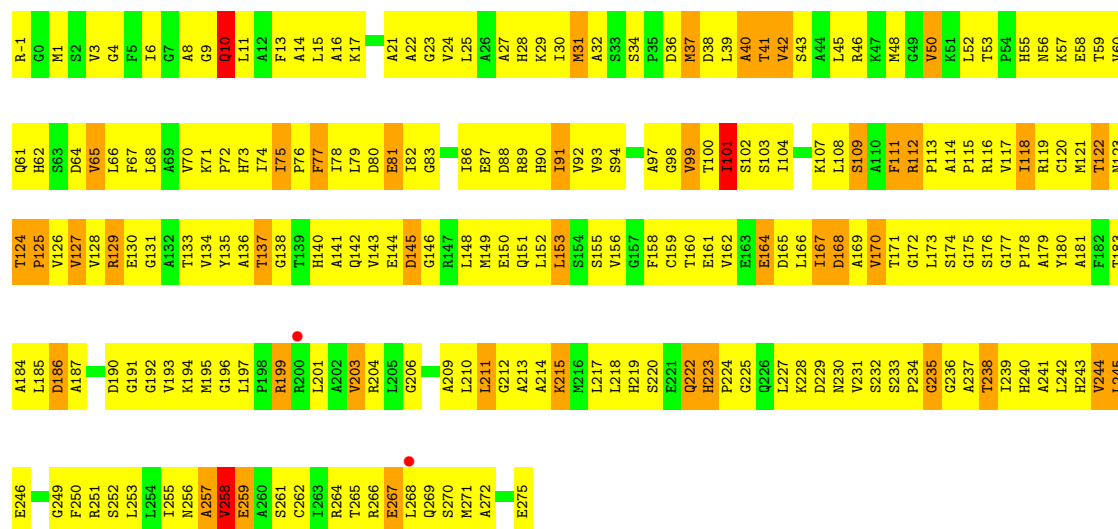




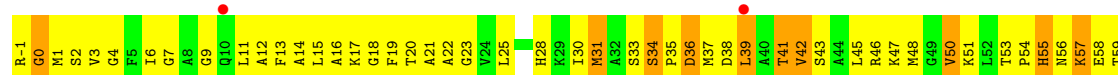
● Molecule 1: Pyrroline-5-carboxylate reductase 1



● Molecule 1: Pyrroline-5-carboxylate reductase 1



● Molecule 1: Pyrroline-5-carboxylate reductase 1



A241	Y180	G120	V60
L242	A181	M121	Q61
H243	F182	T122	H62
V244	T183	N123	S63
L245	A184	I124	D64
E246	L185	P125	V65
S247	D186	V126	L66
	A187	V127	F67
F250	L188	V128	L68
R251	A189	R129	A69
S252	D190	E130	V70
L253	G191	G131	K71
L254	G192	A132	P72
T255	V193	T133	H73
N256	K194	V134	I74
A257	M195	Y135	I75
V258	G196	A136	P76
E259	L197	T137	F77
A260	P198	G138	I78
S261	R199	T139	L79
C262	R200	H140	D80
T263	L201	A141	E81
R264	A202	G142	I82
T265	V203	V143	G83
R266		E144	A84
	G206	D145	D85
Q269	A207	G146	L86
		R147	E87
A272	A209	L148	D88
D273	L210	M149	R89
Q274	G211	E150	H90
E275	A213	Q151	I91
	A214	L152	V92
	K215	L153	G93
	H216	S154	S94
	L217	S155	C95
	L218	V156	A96
	H219	G157	A97
	S220	F158	G98
		C159	V99
	E221	T160	T100
	Q222	E161	I101
	H223	V162	S102
	P224	E163	S103
	G225	E164	I104
	Q226	D165	E105
	L227	L166	K106
	X228	L167	K107
	D229	D168	L108
	N230	A169	S109
	V231	V170	A110
	S232	T171	F111
	S233	G172	R112
	P234	L173	P113
	G235	S174	A114
	G236	G175	P115
	A237	S176	R116
	T238	G177	L117
	L239	P178	I118
	H240	A179	E119

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	208.18Å 122.64Å 120.71Å 90.00° 122.03° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 50.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.10) 97.2 (50.00-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.80Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.241 , 0.278 0.236 , 0.239	Depositor DCC
R_{free} test set	3139 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	61.4	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 102.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.017 for -1/2*h+1/2*k+1,1/2*h-1/2*k+1,1/2*h+1/2*k 0.026 for -1/2*h-1/2*k+1,-1/2*h-1/2*k-1,1/2*h-1/2*k	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11077	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAI

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.53	0/2069	1.09	20/2800 (0.7%)
1	B	0.47	0/2053	1.08	15/2779 (0.5%)
1	C	0.50	0/2063	1.10	15/2793 (0.5%)
1	D	0.55	1/2069 (0.0%)	1.08	11/2800 (0.4%)
1	E	0.70	2/2069 (0.1%)	1.25	22/2800 (0.8%)
All	All	0.56	3/10323 (0.0%)	1.12	83/13972 (0.6%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	129	ARG	C-N	18.38	1.59	1.33
1	E	128	VAL	C-N	-7.93	1.22	1.33
1	D	199	ARG	C-N	-7.34	1.24	1.33

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	128	VAL	O-C-N	19.16	146.53	122.57
1	E	128	VAL	CA-C-N	-13.71	99.30	122.89
1	E	128	VAL	C-N-CA	-13.71	99.30	122.89
1	E	39	LEU	N-CA-C	-11.42	98.73	112.89
1	D	245	LEU	N-CA-C	-10.81	99.50	111.07
1	E	129	ARG	O-C-N	-10.03	105.48	121.23
1	E	245	LEU	N-CA-C	-8.87	101.31	110.97
1	A	258	VAL	N-CA-C	-8.78	102.31	110.82
1	D	255	ILE	N-CA-C	-8.68	102.26	110.42
1	D	101	ILE	N-CA-C	-8.63	102.00	110.72
1	C	221	GLU	N-CA-C	-8.48	103.37	114.31
1	B	21	ALA	N-CA-C	-8.33	103.02	113.01
1	E	87	GLU	N-CA-C	8.22	120.95	107.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	271	MET	N-CA-C	-8.20	104.41	114.75
1	B	110	ALA	N-CA-C	-8.15	104.20	114.56
1	A	64	ASP	N-CA-C	-8.07	103.56	113.41
1	B	49	GLY	N-CA-C	-7.95	101.28	114.48
1	E	145	ASP	N-CA-C	-7.84	103.70	113.18
1	A	0	GLY	N-CA-C	-7.30	103.56	115.46
1	C	180	TYR	N-CA-C	-7.27	102.96	111.03
1	D	108	LEU	N-CA-C	-7.26	104.42	113.28
1	B	126	VAL	N-CA-C	-7.22	103.42	110.72
1	C	126	VAL	N-CA-C	-7.15	102.56	112.50
1	E	64	ASP	N-CA-C	-7.10	104.24	113.12
1	E	129	ARG	CA-C-N	6.99	134.90	121.54
1	E	129	ARG	C-N-CA	6.99	134.90	121.54
1	E	154	SER	N-CA-C	-6.94	104.81	113.28
1	A	90	HIS	N-CA-C	6.87	120.65	110.48
1	B	104	ILE	N-CA-C	-6.86	106.81	113.53
1	E	272	ALA	N-CA-C	-6.83	104.69	113.16
1	C	228	LYS	N-CA-C	-6.79	103.81	111.07
1	C	80	ASP	N-CA-C	-6.75	104.86	113.23
1	B	272	ALA	N-CA-C	-6.71	104.57	112.89
1	E	0	GLY	N-CA-C	-6.55	104.39	115.80
1	B	103	SER	N-CA-C	-6.41	105.62	113.50
1	C	260	ALA	N-CA-C	-6.34	104.25	112.23
1	A	180	TYR	N-CA-C	-6.33	104.48	111.82
1	C	186	ASP	N-CA-C	-6.32	105.57	113.28
1	C	29	LYS	N-CA-C	-6.22	105.67	113.20
1	D	109	SER	N-CA-C	-6.14	104.64	111.71
1	D	222	GLN	N-CA-C	6.12	117.83	111.03
1	A	101	ILE	N-CA-C	-6.08	104.59	110.42
1	B	255	ILE	CB-CA-C	-6.07	104.11	111.88
1	A	251	ARG	N-CA-C	-6.05	104.31	111.03
1	C	245	LEU	N-CA-C	-6.02	104.06	111.40
1	A	221	GLU	CB-CA-C	6.01	122.37	110.42
1	A	271	MET	N-CA-C	-5.98	105.55	114.64
1	C	6	ILE	N-CA-C	-5.96	104.50	111.00
1	B	133	THR	N-CA-C	5.94	118.20	109.24
1	A	58	GLU	N-CA-C	-5.92	104.90	111.71
1	E	55	HIS	N-CA-C	5.88	118.11	108.52
1	B	131	GLY	N-CA-C	-5.87	103.52	112.51
1	D	112	ARG	CA-C-N	5.85	125.54	119.05
1	D	112	ARG	C-N-CA	5.85	125.54	119.05
1	E	198	PRO	N-CA-C	-5.84	102.10	111.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	130	GLU	N-CA-C	5.83	117.40	109.11
1	B	145	ASP	N-CA-C	-5.80	106.24	113.38
1	A	57	LYS	N-CA-C	-5.72	105.39	112.72
1	A	63	SER	N-CA-C	5.72	118.80	109.59
1	A	233	SER	CA-C-N	5.72	126.99	119.84
1	A	233	SER	C-N-CA	5.72	126.99	119.84
1	A	245	LEU	N-CA-C	-5.71	104.97	111.07
1	D	186	ASP	N-CA-C	-5.61	103.97	112.04
1	D	91	ILE	N-CA-C	-5.56	99.63	107.75
1	E	180	TYR	N-CA-C	-5.55	104.87	111.03
1	A	169	ALA	N-CA-C	-5.43	105.01	111.03
1	C	117	VAL	N-CA-C	5.39	115.88	108.12
1	A	81	GLU	N-CA-C	-5.39	107.72	114.56
1	E	63	SER	N-CA-C	5.38	118.99	109.96
1	D	241	ALA	N-CA-C	-5.37	105.12	110.97
1	C	191	GLY	N-CA-C	-5.36	100.49	113.18
1	A	133	THR	N-CA-C	5.33	118.17	109.59
1	B	221	GLU	CB-CA-C	5.33	121.02	110.42
1	E	101	ILE	N-CA-C	-5.29	104.47	111.09
1	A	131	GLY	N-CA-C	-5.25	105.83	112.54
1	B	255	ILE	N-CA-C	-5.23	104.86	110.36
1	E	155	SER	N-CA-C	-5.23	106.86	113.18
1	A	272	ALA	N-CA-C	-5.22	106.30	113.30
1	B	44	ALA	N-CA-C	-5.21	106.83	114.39
1	B	265	THR	N-CA-C	-5.15	105.74	112.23
1	E	196	GLY	N-CA-C	5.12	122.96	115.08
1	E	135	TYR	N-CA-C	5.02	117.60	109.06
1	C	252	SER	N-CA-C	-5.01	100.12	110.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2038	0	2084	515	6

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2023	0	2059	516	5
1	C	2032	0	2072	554	2
1	D	2038	0	2084	462	2
1	E	2038	0	2084	519	1
2	A	43	0	23	26	0
2	B	43	0	24	68	5
2	C	43	0	23	38	4
2	D	43	0	24	40	0
2	E	43	0	21	32	1
3	A	10	0	5	8	0
3	B	10	0	5	17	0
3	C	10	0	5	12	0
3	D	10	0	5	21	0
3	E	10	0	5	11	0
4	A	141	0	0	264	6
4	B	93	0	0	173	3
4	C	116	0	0	263	4
4	D	155	0	0	251	2
4	E	138	0	0	297	1
All	All	11077	0	10523	2646	22

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 126.

All (2646) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1300:NAI:C1D	2:A:1300:NAI:N1N	1.68	1.55
2:E:5300:NAI:O3	2:E:5300:NAI:PN	1.13	1.50
1:B:129:ARG:CZ	2:B:2300:NAI:H2N	1.48	1.40
2:E:5300:NAI:O5B	2:E:5300:NAI:C5B	1.71	1.36
2:D:4300:NAI:H1D	3:D:4301:GLU:N	1.41	1.36
1:E:199:ARG:HG3	4:E:5320:HOH:O	1.21	1.35
1:B:129:ARG:HH22	3:B:2301:GLU:CB	1.40	1.35
1:E:251:ARG:HB3	4:E:5348:HOH:O	1.27	1.34
1:A:42:VAL:HG23	4:A:1349:HOH:O	1.19	1.33
1:E:111:PHE:HB3	4:E:5422:HOH:O	1.26	1.32
1:D:265:THR:HB	4:D:4360:HOH:O	1.23	1.31
1:E:150:GLU:HB3	4:E:5327:HOH:O	1.15	1.31
1:B:129:ARG:NH1	2:B:2300:NAI:H2N	1.42	1.31
1:A:141:ALA:HA	4:A:1390:HOH:O	1.25	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:38:ASP:HA	4:E:5427:HOH:O	1.27	1.30
1:B:129:ARG:NH2	2:B:2300:NAI:O7N	1.65	1.29
1:B:37:MET:HB2	4:B:2393:HOH:O	1.12	1.28
1:D:214:ALA:HA	4:D:4323:HOH:O	1.29	1.28
1:A:82:ILE:HA	4:A:1437:HOH:O	1.30	1.28
1:C:259:GLU:HB3	4:C:3381:HOH:O	1.33	1.28
1:A:11:LEU:HB2	4:A:1389:HOH:O	1.30	1.27
1:B:99:VAL:HG21	4:B:2309:HOH:O	1.33	1.26
1:A:258:VAL:HA	4:A:1302:HOH:O	1.19	1.26
1:E:91:ILE:HB	4:E:5344:HOH:O	1.30	1.26
1:E:185:LEU:HG	4:E:5383:HOH:O	1.29	1.26
1:C:180:TYR:HB2	4:C:3336:HOH:O	1.28	1.26
1:E:188:LEU:HD23	4:E:5343:HOH:O	1.12	1.25
2:A:1300:NAI:C2N	3:A:1301:GLU:HB3	1.65	1.24
1:B:238:THR:HG22	4:B:2352:HOH:O	1.37	1.24
2:B:2300:NAI:C2N	3:B:2301:GLU:HB3	1.65	1.24
1:C:31:MET:HE2	4:C:3362:HOH:O	1.32	1.24
2:C:3300:NAI:C2N	3:C:3301:GLU:HB3	1.65	1.24
1:E:134:VAL:HG13	4:E:5413:HOH:O	1.36	1.24
1:A:182:PHE:HA	4:A:1419:HOH:O	1.38	1.24
1:D:126:VAL:HA	4:D:4331:HOH:O	1.11	1.24
1:D:227:LEU:HB2	4:D:4363:HOH:O	1.28	1.24
1:A:157:GLY:O	2:A:1300:NAI:H42N	1.32	1.23
2:E:5300:NAI:O5D	3:E:5301:GLU:O	1.54	1.22
1:A:272:ALA:HB3	4:A:1407:HOH:O	1.35	1.22
1:B:158:PHE:CZ	2:B:2300:NAI:H4B	1.73	1.22
2:E:5300:NAI:O1N	3:E:5301:GLU:HA	1.38	1.22
1:E:179:ALA:HA	4:E:5369:HOH:O	1.38	1.22
1:E:163:GLU:HG3	4:E:5399:HOH:O	1.39	1.22
1:D:186:ASP:HA	4:D:4361:HOH:O	1.34	1.21
1:B:129:ARG:NH2	3:B:2301:GLU:CB	2.02	1.21
1:B:129:ARG:NH2	2:B:2300:NAI:H2N	1.55	1.20
1:C:122:THR:HB	4:C:3317:HOH:O	1.41	1.20
1:D:240:HIS:HA	4:D:4320:HOH:O	1.37	1.20
1:C:29:LYS:HG3	4:C:3344:HOH:O	1.39	1.19
1:A:199:ARG:HA	4:A:1369:HOH:O	1.38	1.19
1:A:171:THR:HA	4:A:1402:HOH:O	1.36	1.19
1:D:231:VAL:HG12	4:D:4401:HOH:O	1.37	1.19
1:C:180:TYR:HA	4:C:3302:HOH:O	1.43	1.18
1:C:257:ALA:HA	4:C:3378:HOH:O	1.39	1.18
1:C:261:SER:HA	4:C:3354:HOH:O	1.40	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:251:ARG:HG2	4:E:5317:HOH:O	1.43	1.17
1:A:191:GLY:HA2	4:A:1420:HOH:O	1.44	1.17
1:B:129:ARG:HH22	3:B:2301:GLU:HB3	1.00	1.17
1:D:167:ILE:HG22	4:D:4440:HOH:O	1.40	1.17
1:A:217:LEU:HB3	4:A:1312:HOH:O	1.43	1.16
1:C:122:THR:HB	4:C:3331:HOH:O	1.37	1.16
1:D:99:VAL:HA	4:D:4445:HOH:O	1.41	1.16
1:B:129:ARG:CZ	2:B:2300:NAI:O7N	1.92	1.16
1:E:176:SER:HA	4:E:5333:HOH:O	1.44	1.16
1:B:119:ARG:HG3	4:B:2333:HOH:O	1.42	1.16
1:D:122:THR:HG23	1:D:133:THR:HB	1.25	1.16
1:D:217:LEU:HD13	4:D:4372:HOH:O	1.45	1.16
1:E:158:PHE:HA	4:E:5425:HOH:O	1.43	1.15
1:E:229:ASP:HA	4:E:5337:HOH:O	1.46	1.15
1:A:254:LEU:HB3	4:A:1360:HOH:O	1.47	1.15
1:B:129:ARG:NH2	2:B:2300:NAI:C2N	2.09	1.15
1:C:157:GLY:O	2:C:3300:NAI:H42N	1.45	1.15
1:D:119:ARG:HD2	4:D:4422:HOH:O	1.47	1.15
1:D:239:ILE:HG13	4:D:4429:HOH:O	1.45	1.15
1:E:80:ASP:HB2	4:E:5336:HOH:O	1.47	1.14
1:D:180:TYR:HA	4:D:4308:HOH:O	1.45	1.14
1:C:158:PHE:CZ	2:C:3300:NAI:O3B	1.99	1.14
1:C:255:ILE:HB	4:C:3364:HOH:O	1.48	1.14
1:E:238:THR:HG21	4:E:5321:HOH:O	1.45	1.14
1:A:162:VAL:HA	4:A:1355:HOH:O	1.46	1.14
1:D:267:GLU:HB2	4:D:4338:HOH:O	1.46	1.14
1:D:251:ARG:HB2	4:D:4342:HOH:O	1.46	1.13
1:A:40:ALA:HB3	4:A:1336:HOH:O	1.49	1.12
1:A:86:ILE:HD12	1:A:108:LEU:HD11	1.28	1.13
1:E:194:LYS:HA	4:E:5303:HOH:O	1.48	1.12
1:C:244:VAL:HA	4:C:3321:HOH:O	1.44	1.12
1:D:224:PRO:HD2	4:D:4355:HOH:O	1.47	1.12
1:B:129:ARG:CZ	2:B:2300:NAI:C2N	2.27	1.12
1:A:105:GLU:HB2	4:A:1344:HOH:O	1.43	1.12
1:B:228:LYS:HA	4:B:2364:HOH:O	1.50	1.12
1:C:48:MET:HB2	4:C:3371:HOH:O	1.49	1.12
1:C:126:VAL:HA	4:C:3307:HOH:O	1.46	1.12
2:E:5300:NAI:PN	3:E:5301:GLU:O	2.07	1.12
1:B:259:GLU:HB3	4:B:2381:HOH:O	1.46	1.11
1:B:228:LYS:HE3	4:B:2386:HOH:O	1.48	1.11
4:A:1352:HOH:O	1:C:194:LYS:HG3	1.48	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:GLU:HA	4:A:1366:HOH:O	1.51	1.10
1:C:75:ILE:HD12	4:C:3415:HOH:O	1.51	1.09
2:D:4300:NAI:H4N	3:D:4301:GLU:O	1.50	1.09
2:E:5300:NAI:H8A	2:E:5300:NAI:O2B	1.36	1.09
1:D:135:TYR:HE1	4:D:4398:HOH:O	1.36	1.09
1:C:218:LEU:HD13	2:C:3300:NAI:C5D	1.83	1.09
1:E:262:CYS:SG	4:E:5342:HOH:O	2.09	1.09
1:A:210:LEU:HD21	4:A:1380:HOH:O	1.52	1.08
1:E:134:VAL:HB	4:E:5407:HOH:O	1.50	1.08
1:A:218:LEU:HD22	2:A:1300:NAI:H52A	1.31	1.07
1:A:1:MET:HB3	4:A:1427:HOH:O	1.53	1.07
1:D:124:THR:HG23	4:D:4375:HOH:O	1.53	1.07
1:D:218:LEU:HD22	2:D:4300:NAI:H52A	1.29	1.07
2:D:4300:NAI:N1N	3:D:4301:GLU:N	2.01	1.07
1:D:91:ILE:HA	4:D:4455:HOH:O	1.55	1.06
1:D:229:ASP:HB2	4:D:4393:HOH:O	1.55	1.06
2:D:4300:NAI:C4N	3:D:4301:GLU:O	2.02	1.06
1:A:182:PHE:CE1	4:A:1324:HOH:O	2.08	1.06
1:B:142:GLN:HG2	1:B:143:VAL:H	1.14	1.06
1:D:185:LEU:HG	4:D:4330:HOH:O	1.52	1.06
1:D:37:MET:HG2	4:D:4306:HOH:O	1.51	1.06
1:C:129:ARG:HH12	3:C:3301:GLU:HG3	1.17	1.06
2:D:4300:NAI:C2N	3:D:4301:GLU:CA	2.34	1.06
1:B:29:LYS:HB3	4:B:2332:HOH:O	1.56	1.05
1:C:60:VAL:HG23	4:C:3383:HOH:O	1.51	1.05
1:C:218:LEU:HD22	2:C:3300:NAI:PA	1.96	1.05
2:D:4300:NAI:C1D	3:D:4301:GLU:N	2.20	1.05
2:A:1300:NAI:C6N	3:A:1301:GLU:OXT	2.04	1.05
1:A:133:THR:HG21	1:A:153:LEU:HD13	1.37	1.04
1:B:129:ARG:NH2	2:B:2300:NAI:C7N	2.19	1.04
1:B:154:SER:O	2:B:2300:NAI:N7N	1.91	1.04
1:D:195:MET:HE3	4:D:4366:HOH:O	1.57	1.04
1:D:64:ASP:HB3	4:D:4353:HOH:O	1.55	1.04
1:D:78:ILE:HD11	4:D:4446:HOH:O	1.55	1.04
1:A:95:CYS:HB2	4:A:1337:HOH:O	1.56	1.04
1:C:218:LEU:HD13	2:C:3300:NAI:H52N	1.40	1.04
2:E:5300:NAI:C5B	2:E:5300:NAI:PA	2.45	1.04
1:B:129:ARG:NE	2:B:2300:NAI:O7N	1.89	1.04
1:D:141:ALA:HB2	4:D:4364:HOH:O	1.58	1.04
1:A:95:CYS:CB	4:A:1337:HOH:O	2.07	1.03
1:A:183:THR:HA	4:A:1354:HOH:O	1.58	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ARG:NH2	3:B:2301:GLU:HB3	1.64	1.03
1:B:259:GLU:HA	4:B:2307:HOH:O	1.58	1.03
1:B:219:HIS:CE1	2:B:2300:NAI:O5D	2.12	1.03
1:C:29:LYS:CD	4:C:3404:HOH:O	2.06	1.03
1:B:189:ALA:C	4:B:2302:HOH:O	2.00	1.03
1:E:122:THR:HB	1:E:133:THR:HG22	1.41	1.03
1:A:178:PRO:HD2	4:A:1436:HOH:O	1.59	1.02
1:C:70:VAL:HB	4:C:3407:HOH:O	1.58	1.02
1:D:107:LYS:HD2	4:D:4370:HOH:O	1.59	1.02
1:B:176:SER:HB2	4:B:2324:HOH:O	1.55	1.02
1:B:158:PHE:CE1	2:B:2300:NAI:H4B	1.93	1.02
1:B:158:PHE:CE2	2:B:2300:NAI:O3B	2.12	1.01
1:D:30:ILE:HB	4:D:4425:HOH:O	1.62	1.00
1:C:237:ALA:HA	4:C:3411:HOH:O	1.59	1.00
1:E:187:ALA:HB2	4:E:5363:HOH:O	1.58	1.00
1:A:112:ARG:CD	4:A:1392:HOH:O	2.08	1.00
1:B:75:ILE:HB	1:B:76:PRO:HD3	1.40	1.00
2:A:1300:NAI:H5N	4:A:1412:HOH:O	1.61	1.00
2:C:3300:NAI:C6N	3:C:3301:GLU:OXT	2.10	1.00
1:A:16:ALA:HB3	4:A:1387:HOH:O	1.62	1.00
2:E:5300:NAI:O2B	2:E:5300:NAI:C8A	2.08	0.99
2:D:4300:NAI:C3N	3:D:4301:GLU:O	2.10	0.99
2:B:2300:NAI:C6N	3:B:2301:GLU:OXT	2.10	0.99
1:A:161:GLU:HB3	4:A:1364:HOH:O	1.61	0.99
1:B:71:LYS:HB3	1:B:72:PRO:HD2	1.43	0.99
1:C:168:ASP:HA	4:C:3380:HOH:O	1.61	0.99
1:E:112:ARG:HG3	4:E:5328:HOH:O	1.61	0.99
2:D:4300:NAI:C2N	3:D:4301:GLU:HA	1.92	0.99
1:C:22:ALA:HB3	4:C:3369:HOH:O	1.61	0.99
1:C:129:ARG:HD2	2:C:3300:NAI:O7N	1.62	0.99
1:C:213:ALA:HB2	4:C:3386:HOH:O	1.63	0.99
1:B:155:SER:HA	2:B:2300:NAI:H72N	1.25	0.98
1:E:185:LEU:HA	4:E:5323:HOH:O	1.61	0.98
1:C:129:ARG:NH1	3:C:3301:GLU:HG3	1.76	0.98
1:B:195:MET:HE2	1:B:195:MET:HA	1.44	0.98
1:D:178:PRO:HB2	4:D:4454:HOH:O	1.62	0.98
1:A:98:GLY:HA2	4:A:1328:HOH:O	1.62	0.98
1:E:17:LYS:HB2	4:E:5306:HOH:O	1.61	0.98
1:A:234:PRO:HB3	1:C:196:GLY:O	1.62	0.98
1:C:151:GLN:HA	4:C:3319:HOH:O	1.64	0.98
1:B:129:ARG:NH1	2:B:2300:NAI:C2N	2.27	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:THR:HA	4:B:2305:HOH:O	1.61	0.97
1:D:122:THR:CG2	1:D:133:THR:HB	1.93	0.97
1:B:158:PHE:CZ	2:B:2300:NAI:O3B	2.18	0.97
1:D:194:LYS:HB3	4:D:4366:HOH:O	1.64	0.96
1:D:174:SER:C	4:D:4315:HOH:O	2.07	0.96
2:E:5300:NAI:H51N	4:E:5404:HOH:O	1.63	0.96
1:C:176:SER:HA	4:C:3330:HOH:O	1.66	0.96
1:E:9:GLY:H	1:E:41:THR:HG21	1.28	0.96
1:E:188:LEU:HA	4:E:5343:HOH:O	1.65	0.96
1:B:218:LEU:HD22	2:B:2300:NAI:PA	2.04	0.96
1:C:48:MET:CB	4:C:3371:HOH:O	2.06	0.96
1:D:122:THR:HG23	1:D:133:THR:CB	1.96	0.96
1:B:45:LEU:HD11	4:B:2314:HOH:O	1.62	0.96
1:C:112:ARG:HH11	1:C:113:PRO:HD2	1.27	0.96
1:E:163:GLU:CG	4:E:5399:HOH:O	2.02	0.96
1:C:108:LEU:HB3	4:C:3358:HOH:O	1.65	0.96
1:B:33:SER:HB2	1:B:59:THR:OG1	1.66	0.95
1:B:218:LEU:HD13	2:B:2300:NAI:H52N	1.46	0.95
1:C:49:GLY:C	4:C:3363:HOH:O	2.09	0.95
1:D:219:HIS:HE1	2:D:4300:NAI:C5D	1.79	0.95
1:E:17:LYS:CB	4:E:5306:HOH:O	2.14	0.95
1:A:13:PHE:HA	4:A:1387:HOH:O	1.64	0.95
1:D:165:ASP:HB2	4:D:4368:HOH:O	1.67	0.95
1:A:182:PHE:CA	4:A:1419:HOH:O	2.01	0.95
1:E:188:LEU:HD12	4:E:5439:HOH:O	1.65	0.95
1:D:62:HIS:C	4:D:4448:HOH:O	2.08	0.95
1:E:47:LYS:HE2	4:E:5338:HOH:O	1.65	0.95
1:E:63:SER:C	4:E:5417:HOH:O	2.08	0.95
1:B:9:GLY:H	1:B:12:ALA:HB3	1.28	0.95
1:B:153:LEU:C	4:B:2392:HOH:O	2.10	0.95
1:E:225:GLY:CA	4:E:5353:HOH:O	2.14	0.95
1:C:178:PRO:HB2	4:C:3396:HOH:O	1.65	0.94
1:C:29:LYS:HD3	4:C:3404:HOH:O	1.65	0.94
1:C:122:THR:CB	4:C:3317:HOH:O	2.03	0.94
1:D:180:TYR:CA	4:D:4308:HOH:O	2.09	0.94
1:C:101:ILE:HG12	4:C:3394:HOH:O	1.66	0.94
1:D:118:ILE:HB	4:D:4408:HOH:O	1.67	0.94
1:B:14:ALA:HA	1:B:127:VAL:HG22	1.49	0.94
1:E:101:ILE:HG13	4:E:5418:HOH:O	1.66	0.94
1:C:195:MET:HA	1:C:195:MET:HE3	1.48	0.94
1:C:213:ALA:N	4:C:3386:HOH:O	2.01	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:ARG:HD2	4:C:3303:HOH:O	1.68	0.94
1:D:-1:ARG:HG3	4:D:4424:HOH:O	1.68	0.94
1:E:132:ALA:HB3	4:E:5335:HOH:O	1.67	0.94
1:C:89:ARG:HD2	1:C:90:HIS:N	1.83	0.94
1:B:155:SER:CA	2:B:2300:NAI:H72N	1.81	0.94
1:C:122:THR:HB	1:C:133:THR:HG22	1.48	0.94
1:C:179:ALA:N	4:C:3396:HOH:O	2.01	0.94
1:B:89:ARG:NH2	4:B:2325:HOH:O	2.00	0.93
1:B:236:GLY:HA2	1:B:239:ILE:HG22	1.49	0.93
1:E:132:ALA:HB1	4:E:5391:HOH:O	1.67	0.93
1:A:9:GLY:H	1:A:41:THR:HG21	1.33	0.93
1:A:250:PHE:N	4:A:1314:HOH:O	2.02	0.93
4:C:3375:HOH:O	1:D:199:ARG:HD3	1.67	0.93
1:A:186:ASP:N	4:A:1370:HOH:O	2.01	0.93
1:C:237:ALA:CB	4:C:3411:HOH:O	2.16	0.93
1:A:121:MET:HB2	4:A:1327:HOH:O	1.68	0.92
1:C:167:ILE:CG2	4:C:3345:HOH:O	2.16	0.92
1:D:98:GLY:N	4:D:4333:HOH:O	2.01	0.92
1:A:210:LEU:HG	4:A:1421:HOH:O	1.68	0.92
1:E:-1:ARG:CD	4:E:5319:HOH:O	2.17	0.92
1:E:63:SER:N	4:E:5372:HOH:O	2.00	0.92
1:A:95:CYS:N	4:A:1337:HOH:O	2.03	0.92
1:A:266:ARG:CD	4:A:1331:HOH:O	2.16	0.92
1:E:3:VAL:N	4:E:5387:HOH:O	2.01	0.92
1:B:247:SER:HA	4:B:2350:HOH:O	1.70	0.92
1:A:222:GLN:HG2	4:A:1441:HOH:O	1.69	0.92
1:C:4:GLY:N	4:C:3356:HOH:O	2.02	0.92
1:C:108:LEU:HD23	4:C:3329:HOH:O	1.70	0.92
1:E:69:ALA:HB3	4:E:5379:HOH:O	1.70	0.92
1:E:107:LYS:N	4:E:5384:HOH:O	2.01	0.92
1:B:153:LEU:CA	4:B:2392:HOH:O	2.16	0.92
1:C:7:GLY:N	4:C:3322:HOH:O	2.03	0.92
1:E:241:ALA:O	1:E:244:VAL:HG12	1.69	0.92
1:B:29:LYS:HE2	4:B:2332:HOH:O	1.68	0.91
1:C:45:LEU:HA	4:C:3371:HOH:O	1.71	0.91
1:C:129:ARG:HH12	3:C:3301:GLU:CG	1.83	0.91
1:B:5:PHE:HZ	1:B:15:LEU:HB2	1.34	0.91
1:C:171:THR:O	1:C:175:GLY:HA3	1.71	0.91
1:E:130:GLU:N	4:E:5401:HOH:O	2.02	0.91
1:C:259:GLU:N	4:C:3391:HOH:O	2.03	0.91
1:C:266:ARG:CD	4:C:3303:HOH:O	2.19	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:GLY:HA2	4:D:4397:HOH:O	1.68	0.91
1:A:119:ARG:CG	4:A:1372:HOH:O	2.18	0.90
1:A:119:ARG:NH2	4:A:1328:HOH:O	2.03	0.90
1:D:219:HIS:CE1	2:D:4300:NAI:O5D	2.24	0.90
1:E:122:THR:HB	4:E:5385:HOH:O	1.70	0.90
1:B:176:SER:CB	4:B:2324:HOH:O	2.14	0.90
2:B:2300:NAI:C3N	3:B:2301:GLU:HB3	2.00	0.90
1:E:215:LYS:CE	4:E:5430:HOH:O	2.18	0.90
1:E:185:LEU:HD23	4:E:5323:HOH:O	1.71	0.90
1:A:29:LYS:NZ	4:A:1400:HOH:O	2.04	0.90
2:E:5300:NAI:O1N	3:E:5301:GLU:CA	2.18	0.90
2:C:3300:NAI:C3N	3:C:3301:GLU:HB3	2.00	0.90
1:B:218:LEU:HD13	2:B:2300:NAI:C5D	2.01	0.90
1:D:78:ILE:CD1	4:D:4446:HOH:O	2.14	0.90
1:B:129:ARG:NH2	3:B:2301:GLU:HB2	1.86	0.90
1:B:129:ARG:HH12	2:B:2300:NAI:H2N	1.30	0.90
1:D:141:ALA:HA	4:D:4386:HOH:O	1.69	0.90
4:B:2308:HOH:O	1:D:239:ILE:CG2	2.18	0.89
1:C:105:GLU:HG2	4:C:3315:HOH:O	1.71	0.89
1:C:247:SER:C	4:C:3402:HOH:O	2.15	0.89
1:D:87:GLU:HB3	4:D:4322:HOH:O	1.71	0.89
1:A:7:GLY:N	4:A:1305:HOH:O	2.05	0.89
1:A:88:ASP:HB2	1:A:112:ARG:HH21	1.38	0.89
1:A:239:ILE:HG12	4:C:3309:HOH:O	1.73	0.89
1:E:122:THR:HG22	1:E:133:THR:HB	1.54	0.89
1:E:246:GLU:HB3	4:E:5312:HOH:O	1.70	0.89
1:A:256:ASN:N	4:A:1335:HOH:O	2.06	0.89
1:D:178:PRO:C	4:D:4454:HOH:O	2.16	0.89
1:C:236:GLY:C	4:C:3398:HOH:O	2.14	0.89
1:A:122:THR:C	4:A:1428:HOH:O	2.14	0.89
1:C:237:ALA:N	4:C:3398:HOH:O	2.06	0.89
1:C:266:ARG:HA	4:C:3340:HOH:O	1.72	0.89
1:C:129:ARG:CZ	2:C:3300:NAI:H2N	2.02	0.89
1:E:65:VAL:HA	4:E:5344:HOH:O	1.72	0.89
1:E:162:VAL:HG13	1:E:166:LEU:HD12	1.55	0.89
1:C:133:THR:HG22	4:C:3317:HOH:O	1.71	0.88
1:C:203:VAL:HA	4:C:3355:HOH:O	1.73	0.88
1:B:73:HIS:CD2	4:B:2320:HOH:O	2.26	0.88
1:B:129:ARG:NH1	2:B:2300:NAI:O2D	2.07	0.88
1:D:53:THR:HB	4:D:4404:HOH:O	1.73	0.88
1:A:102:SER:HB2	4:A:1358:HOH:O	1.72	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:187:ALA:HA	4:E:5381:HOH:O	1.70	0.88
1:B:73:HIS:HD2	4:B:2320:HOH:O	1.56	0.88
2:D:4300:NAI:C4N	3:D:4301:GLU:C	2.45	0.88
1:E:122:THR:CB	4:E:5385:HOH:O	2.21	0.88
1:A:154:SER:O	2:A:1300:NAI:N7N	2.05	0.88
1:B:50:VAL:HB	4:B:2385:HOH:O	1.73	0.88
1:C:160:THR:CG2	4:C:3323:HOH:O	2.22	0.88
2:E:5300:NAI:O3	2:E:5300:NAI:O5D	1.92	0.88
1:C:192:GLY:CA	4:C:3367:HOH:O	2.20	0.88
1:D:257:ALA:C	4:D:4349:HOH:O	2.17	0.87
1:E:200:ARG:HG3	4:E:5416:HOH:O	1.74	0.87
1:B:95:CYS:HA	4:B:2349:HOH:O	1.73	0.87
1:B:129:ARG:NH2	2:B:2300:NAI:C3N	2.36	0.87
1:E:123:ASN:ND2	4:E:5335:HOH:O	2.07	0.87
2:E:5300:NAI:C5D	3:E:5301:GLU:O	2.22	0.87
1:A:112:ARG:NE	4:A:1392:HOH:O	2.08	0.87
1:C:112:ARG:HG3	1:C:113:PRO:HD2	1.54	0.87
1:A:124:THR:O	1:A:127:VAL:HG23	1.75	0.87
1:B:122:THR:HG22	1:B:133:THR:CB	2.04	0.87
1:D:64:ASP:CB	4:D:4353:HOH:O	2.15	0.87
1:D:272:ALA:HB1	4:D:4328:HOH:O	1.71	0.87
1:B:158:PHE:CZ	2:B:2300:NAI:C4B	2.57	0.87
1:B:12:ALA:HB3	4:B:2314:HOH:O	1.75	0.87
1:B:190:ASP:N	4:B:2302:HOH:O	2.06	0.86
1:A:161:GLU:CD	4:A:1364:HOH:O	2.16	0.86
1:C:33:SER:HB2	1:C:59:THR:OG1	1.75	0.86
1:D:228:LYS:C	4:D:4310:HOH:O	2.16	0.86
1:B:236:GLY:HA3	4:B:2318:HOH:O	1.75	0.86
1:A:102:SER:N	4:A:1358:HOH:O	2.08	0.86
1:B:228:LYS:CE	4:B:2386:HOH:O	2.12	0.86
1:C:28:HIS:HA	1:C:51:LYS:HE3	1.58	0.86
1:C:155:SER:HA	2:C:3300:NAI:H72N	1.37	0.86
1:B:73:HIS:CE1	4:B:2390:HOH:O	2.28	0.86
1:D:224:PRO:CD	4:D:4355:HOH:O	2.14	0.86
1:D:30:ILE:HB	1:D:50:VAL:HG22	1.55	0.86
1:C:69:ALA:N	4:C:3322:HOH:O	2.07	0.86
1:B:228:LYS:CA	4:B:2364:HOH:O	2.12	0.86
1:E:73:HIS:HB2	4:E:5415:HOH:O	1.75	0.86
1:E:88:ASP:N	4:E:5318:HOH:O	2.03	0.86
1:A:259:GLU:CA	4:A:1366:HOH:O	2.17	0.86
1:E:53:THR:HG22	1:E:55:HIS:H	1.38	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:SER:CB	4:A:1358:HOH:O	2.24	0.85
1:B:129:ARG:HH22	3:B:2301:GLU:CG	1.89	0.85
1:D:57:LYS:CE	4:D:4376:HOH:O	2.21	0.85
1:E:115:PRO:HA	4:E:5436:HOH:O	1.76	0.85
1:C:251:ARG:HA	4:C:3359:HOH:O	1.76	0.85
1:B:193:VAL:HG12	1:D:239:ILE:HD13	1.58	0.85
1:E:53:THR:HG21	4:E:5332:HOH:O	1.75	0.85
1:B:10:GLN:NE2	4:B:2354:HOH:O	2.08	0.85
1:B:185:LEU:HD21	1:B:210:LEU:HD12	1.58	0.85
1:E:94:SER:C	4:E:5423:HOH:O	2.20	0.85
1:E:174:SER:HB2	4:E:5335:HOH:O	1.76	0.85
1:E:55:HIS:HB2	4:E:5332:HOH:O	1.75	0.85
1:E:111:PHE:HE1	4:E:5326:HOH:O	1.58	0.85
1:A:138:GLY:HA3	4:A:1310:HOH:O	1.75	0.85
1:D:39:LEU:HD23	4:D:4405:HOH:O	1.77	0.85
1:D:219:HIS:CE1	2:D:4300:NAI:C5D	2.59	0.85
1:C:53:THR:HG21	1:C:58:GLU:HB2	1.58	0.85
1:C:123:ASN:HD21	1:C:132:ALA:HB3	1.42	0.85
1:C:237:ALA:CA	4:C:3411:HOH:O	2.21	0.85
1:B:155:SER:HA	2:B:2300:NAI:N7N	1.90	0.85
1:A:266:ARG:CZ	4:A:1440:HOH:O	2.24	0.84
1:B:95:CYS:N	4:B:2349:HOH:O	2.09	0.84
1:B:241:ALA:HA	4:B:2329:HOH:O	1.75	0.84
1:E:231:VAL:HG12	4:E:5321:HOH:O	1.77	0.84
1:E:183:THR:CB	4:E:5370:HOH:O	2.24	0.84
1:A:181:ALA:C	4:A:1419:HOH:O	2.20	0.84
1:A:259:GLU:O	1:A:263:ILE:HD13	1.76	0.84
1:C:192:GLY:C	4:C:3367:HOH:O	2.19	0.84
1:E:96:ALA:N	4:E:5423:HOH:O	2.07	0.84
1:A:118:ILE:HG22	1:A:137:THR:HA	1.60	0.84
1:A:119:ARG:HG3	4:A:1372:HOH:O	1.77	0.84
1:B:129:ARG:HH22	2:B:2300:NAI:C2N	1.86	0.84
1:B:160:THR:CG2	4:B:2360:HOH:O	2.26	0.84
1:E:183:THR:HG22	4:E:5370:HOH:O	1.76	0.84
1:A:210:LEU:CD2	4:A:1380:HOH:O	2.16	0.84
1:B:74:ILE:HG13	4:B:2309:HOH:O	1.77	0.84
1:C:162:VAL:HB	1:C:166:LEU:HD12	1.57	0.84
1:E:188:LEU:CA	4:E:5343:HOH:O	2.21	0.84
1:B:138:GLY:HA3	4:B:2370:HOH:O	1.77	0.84
2:D:4300:NAI:C3N	3:D:4301:GLU:C	2.50	0.84
1:E:199:ARG:C	4:E:5320:HOH:O	2.21	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:243:HIS:CE1	4:E:5357:HOH:O	2.30	0.84
1:C:247:SER:HA	4:C:3402:HOH:O	1.76	0.84
1:D:53:THR:HG22	1:D:55:HIS:H	1.41	0.84
1:D:118:ILE:HG23	1:D:137:THR:HA	1.60	0.84
1:B:45:LEU:HB2	1:B:52:LEU:HD21	1.58	0.84
1:B:129:ARG:HH22	2:B:2300:NAI:H2N	1.43	0.84
1:C:194:LYS:HA	4:C:3309:HOH:O	1.77	0.84
1:A:-1:ARG:CG	4:A:1332:HOH:O	2.26	0.83
1:D:121:MET:HE3	1:D:171:THR:HA	1.60	0.83
1:E:182:PHE:HB2	4:E:5369:HOH:O	1.77	0.83
1:A:28:HIS:ND1	4:A:1382:HOH:O	2.10	0.83
1:D:9:GLY:N	1:D:41:THR:HG21	1.93	0.83
1:D:228:LYS:HE2	4:D:4414:HOH:O	1.78	0.83
1:A:255:ILE:HG22	4:A:1335:HOH:O	1.79	0.83
1:B:11:LEU:HD23	4:B:2343:HOH:O	1.78	0.83
1:B:160:THR:HG23	4:B:2360:HOH:O	1.79	0.83
1:B:250:PHE:HB2	4:B:2353:HOH:O	1.77	0.83
1:C:171:THR:CA	4:C:3351:HOH:O	2.26	0.83
1:D:126:VAL:HG13	1:D:156:VAL:HG11	1.60	0.83
1:C:199:ARG:CD	4:C:3392:HOH:O	2.27	0.83
1:C:133:THR:CG2	4:C:3317:HOH:O	2.25	0.83
1:E:212:GLY:HA2	4:E:5314:HOH:O	1.76	0.83
1:B:245:LEU:HA	4:B:2353:HOH:O	1.79	0.83
1:C:89:ARG:HD2	1:C:90:HIS:H	1.39	0.83
1:C:213:ALA:CA	4:C:3386:HOH:O	2.27	0.83
1:D:136:ALA:HA	4:D:4394:HOH:O	1.78	0.83
1:A:194:LYS:NZ	4:A:1381:HOH:O	2.12	0.82
1:C:171:THR:N	4:C:3351:HOH:O	2.11	0.82
1:E:-1:ARG:HD3	4:E:5319:HOH:O	1.76	0.82
1:A:149:MET:HE2	1:A:153:LEU:HG	1.59	0.82
1:B:79:LEU:HD11	1:B:104:ILE:HG12	1.61	0.82
1:D:251:ARG:NH1	4:D:4427:HOH:O	2.12	0.82
1:D:123:ASN:HB3	4:D:4309:HOH:O	1.78	0.82
1:D:211:LEU:HD12	4:D:4406:HOH:O	1.79	0.82
1:E:274:GLN:HG3	1:E:275:GLU:H	1.41	0.82
1:A:120:CYS:HA	4:A:1368:HOH:O	1.79	0.82
1:D:266:ARG:NH2	4:D:4378:HOH:O	2.05	0.82
1:E:31:MET:HG2	1:E:51:LYS:HB2	1.61	0.82
1:D:107:LYS:CD	4:D:4370:HOH:O	2.22	0.82
1:E:195:MET:HA	1:E:195:MET:HE3	1.61	0.82
1:E:262:CYS:SG	4:E:5375:HOH:O	2.38	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:GLU:HG3	4:D:4383:HOH:O	1.80	0.82
1:B:164:GLU:HG3	1:B:167:ILE:HD12	1.62	0.82
1:C:131:GLY:HA3	4:C:3307:HOH:O	1.78	0.82
1:A:258:VAL:CG2	4:A:1302:HOH:O	2.27	0.81
1:C:7:GLY:CA	4:C:3322:HOH:O	2.25	0.81
1:C:134:VAL:HB	4:C:3327:HOH:O	1.80	0.81
1:C:258:VAL:HG12	1:C:258:VAL:O	1.79	0.81
1:D:223:HIS:N	4:D:4384:HOH:O	2.01	0.81
2:A:1300:NAI:H51N	4:A:1431:HOH:O	1.78	0.81
1:B:82:ILE:HA	4:B:2376:HOH:O	1.78	0.81
1:B:82:ILE:HG22	1:B:86:ILE:HD11	1.61	0.81
1:D:272:ALA:HA	4:D:4400:HOH:O	1.80	0.81
1:A:9:GLY:N	1:A:41:THR:HG21	1.94	0.81
1:A:266:ARG:NH1	4:A:1308:HOH:O	2.14	0.81
1:B:7:GLY:O	1:B:12:ALA:HB2	1.80	0.81
1:C:7:GLY:HA3	4:C:3322:HOH:O	1.80	0.81
1:C:247:SER:CA	4:C:3402:HOH:O	2.27	0.81
1:D:158:PHE:CZ	2:D:4300:NAI:O3B	2.33	0.81
1:A:185:LEU:C	4:A:1370:HOH:O	2.21	0.81
1:C:86:ILE:C	4:C:3382:HOH:O	2.24	0.81
1:D:31:MET:HG2	1:D:59:THR:HA	1.62	0.81
1:D:121:MET:HG2	4:D:4324:HOH:O	1.79	0.81
1:B:6:ILE:HD12	1:B:56:ASN:O	1.81	0.81
1:B:122:THR:HG22	1:B:133:THR:HB	1.59	0.81
1:C:240:HIS:HB2	4:C:3398:HOH:O	1.80	0.81
1:A:239:ILE:HG21	4:C:3309:HOH:O	1.81	0.81
1:A:202:ALA:HB3	4:A:1369:HOH:O	1.80	0.81
1:B:63:SER:HB2	1:B:89:ARG:HH12	1.45	0.81
1:D:133:THR:O	1:D:159:CYS:HA	1.81	0.81
1:E:153:LEU:HB2	4:E:5432:HOH:O	1.80	0.81
2:A:1300:NAI:N1N	3:A:1301:GLU:OXT	2.14	0.81
1:D:211:LEU:HD12	1:D:211:LEU:O	1.80	0.81
1:D:223:HIS:C	4:D:4372:HOH:O	2.24	0.81
1:C:262:CYS:SG	4:C:3320:HOH:O	2.39	0.80
1:C:184:ALA:C	4:C:3352:HOH:O	2.24	0.80
1:B:142:GLN:HG2	1:B:143:VAL:N	1.94	0.80
1:E:138:GLY:HA2	4:E:5418:HOH:O	1.79	0.80
1:E:183:THR:HB	4:E:5370:HOH:O	1.80	0.80
1:B:5:PHE:CZ	1:B:15:LEU:HB2	2.16	0.80
1:A:123:ASN:HD21	1:A:132:ALA:H	1.30	0.80
1:B:251:ARG:HD3	4:B:2330:HOH:O	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:VAL:HG21	1:D:82:ILE:HG23	1.63	0.80
1:E:60:VAL:HG21	1:E:82:ILE:HD12	1.63	0.80
1:B:178:PRO:C	4:B:2373:HOH:O	2.25	0.80
1:C:87:GLU:HG3	4:C:3382:HOH:O	1.80	0.80
1:C:218:LEU:CD1	2:C:3300:NAI:C5D	2.59	0.80
1:D:91:ILE:CA	4:D:4455:HOH:O	2.19	0.80
1:E:215:LYS:HE2	4:E:5430:HOH:O	1.77	0.80
4:B:2308:HOH:O	1:D:239:ILE:HG23	1.82	0.80
1:C:158:PHE:CE1	2:C:3300:NAI:H4B	2.17	0.80
1:C:236:GLY:CA	4:C:3398:HOH:O	2.30	0.80
1:D:124:THR:CB	4:D:4375:HOH:O	2.30	0.80
2:A:1300:NAI:C1D	2:A:1300:NAI:C2N	2.60	0.80
1:C:218:LEU:CD1	2:C:3300:NAI:H52N	2.12	0.80
1:D:88:ASP:CA	4:D:4432:HOH:O	2.29	0.80
1:D:219:HIS:HE1	2:D:4300:NAI:H51N	1.45	0.80
1:C:226:GLN:HG2	4:C:3366:HOH:O	1.82	0.79
1:E:9:GLY:N	1:E:41:THR:HG21	1.96	0.79
1:A:79:LEU:HD11	1:A:104:ILE:HD12	1.63	0.79
1:A:94:SER:O	4:A:1372:HOH:O	2.00	0.79
1:C:167:ILE:HG21	4:C:3345:HOH:O	1.80	0.79
1:D:118:ILE:CB	4:D:4408:HOH:O	2.27	0.79
1:B:142:GLN:HB2	4:B:2339:HOH:O	1.83	0.79
1:C:178:PRO:HG3	4:C:3346:HOH:O	1.83	0.79
1:C:199:ARG:HD3	4:C:3392:HOH:O	1.81	0.79
1:E:183:THR:CG2	4:E:5370:HOH:O	2.28	0.79
1:A:8:ALA:O	4:A:1333:HOH:O	2.01	0.79
1:B:95:CYS:CA	4:B:2349:HOH:O	2.27	0.79
1:B:228:LYS:C	4:B:2364:HOH:O	2.26	0.79
1:D:195:MET:CE	4:D:4366:HOH:O	2.22	0.79
1:A:45:LEU:HD11	4:A:1379:HOH:O	1.82	0.79
1:D:113:PRO:N	4:D:4329:HOH:O	2.15	0.79
1:C:266:ARG:HH11	1:C:266:ARG:HG2	1.47	0.79
1:A:37:MET:HA	1:A:42:VAL:HG21	1.64	0.79
1:A:178:PRO:O	4:A:1324:HOH:O	2.01	0.79
1:C:266:ARG:CA	4:C:3340:HOH:O	2.29	0.79
1:D:56:ASN:ND2	4:D:4446:HOH:O	2.16	0.79
1:B:60:VAL:HG12	1:B:89:ARG:HH22	1.49	0.79
1:C:129:ARG:NH1	3:C:3301:GLU:CG	2.45	0.79
1:D:112:ARG:HD2	4:D:4347:HOH:O	1.81	0.79
1:E:132:ALA:HA	4:E:5351:HOH:O	1.82	0.79
1:E:61:GLN:O	4:E:5324:HOH:O	2.00	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:179:ALA:HB1	4:E:5322:HOH:O	1.81	0.78
1:E:188:LEU:N	4:E:5343:HOH:O	2.15	0.78
1:C:98:GLY:HA2	4:C:3310:HOH:O	1.83	0.78
1:A:120:CYS:CA	4:A:1368:HOH:O	2.31	0.78
1:A:238:THR:N	4:A:1391:HOH:O	2.14	0.78
1:B:187:ALA:HA	4:B:2341:HOH:O	1.83	0.78
1:D:94:SER:OG	4:D:4344:HOH:O	2.01	0.78
1:D:162:VAL:HG13	1:D:166:LEU:HD12	1.63	0.78
1:C:48:MET:HG3	4:C:3363:HOH:O	1.83	0.78
2:D:4300:NAI:H3D	4:D:4410:HOH:O	1.82	0.78
1:B:258:VAL:C	4:B:2382:HOH:O	2.25	0.78
2:D:4300:NAI:O1N	3:D:4301:GLU:N	2.15	0.78
2:E:5300:NAI:C1D	3:E:5301:GLU:N	2.47	0.78
1:A:77:PHE:C	4:A:1356:HOH:O	2.25	0.78
1:B:228:LYS:O	4:B:2364:HOH:O	2.02	0.78
1:C:128:VAL:HG12	1:C:129:ARG:H	1.49	0.78
1:E:185:LEU:CA	4:E:5323:HOH:O	2.25	0.78
1:D:275:GLU:O	4:D:4456:HOH:O	2.00	0.78
1:E:-1:ARG:NE	4:E:5319:HOH:O	2.14	0.78
2:A:1300:NAI:H2N	3:A:1301:GLU:HB3	1.63	0.78
1:B:108:LEU:O	4:B:2328:HOH:O	2.02	0.78
1:B:129:ARG:HH21	2:B:2300:NAI:C7N	1.91	0.78
1:B:256:ASN:HB3	4:B:2369:HOH:O	1.82	0.78
1:D:158:PHE:CE2	2:D:4300:NAI:O3B	2.36	0.78
1:D:179:ALA:O	4:D:4335:HOH:O	2.01	0.78
1:E:207:ALA:N	4:E:5408:HOH:O	2.15	0.78
1:A:155:SER:O	4:A:1425:HOH:O	2.01	0.78
1:D:223:HIS:CD2	4:D:4321:HOH:O	2.37	0.78
1:B:161:GLU:OE2	4:B:2346:HOH:O	2.00	0.77
1:A:112:ARG:HD3	4:A:1392:HOH:O	1.77	0.77
1:C:53:THR:HG22	1:C:55:HIS:H	1.46	0.77
1:D:146:GLY:O	4:D:4443:HOH:O	2.01	0.77
2:D:4300:NAI:C2N	3:D:4301:GLU:C	2.57	0.77
1:E:53:THR:CG2	4:E:5332:HOH:O	2.29	0.77
1:B:141:ALA:O	1:B:145:ASP:HB3	1.85	0.77
1:B:155:SER:CA	2:B:2300:NAI:N7N	2.47	0.77
1:D:4:GLY:O	4:D:4327:HOH:O	2.02	0.77
1:D:43:SER:HB2	4:D:4405:HOH:O	1.83	0.77
1:E:105:GLU:OE1	4:E:5437:HOH:O	2.02	0.77
1:A:102:SER:CA	4:A:1358:HOH:O	2.33	0.77
1:B:135:TYR:CE1	1:B:161:GLU:HB3	2.20	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:LEU:HA	4:B:2392:HOH:O	1.80	0.77
1:C:160:THR:HG22	4:C:3323:HOH:O	1.82	0.77
2:D:4300:NAI:C5N	3:D:4301:GLU:C	2.57	0.77
1:D:204:ARG:NH2	4:D:4411:HOH:O	2.17	0.77
1:E:137:THR:HG23	4:E:5426:HOH:O	1.84	0.77
1:C:271:MET:HA	1:C:274:GLN:HB3	1.67	0.77
1:D:30:ILE:HA	4:D:4365:HOH:O	1.83	0.77
1:D:88:ASP:O	4:D:4432:HOH:O	2.02	0.77
1:E:172:GLY:HA2	1:E:261:SER:OG	1.85	0.77
1:E:80:ASP:CB	4:E:5336:HOH:O	2.18	0.77
2:E:5300:NAI:C5B	2:E:5300:NAI:O2A	2.32	0.77
1:E:59:THR:O	4:E:5372:HOH:O	2.03	0.77
1:B:11:LEU:N	4:B:2343:HOH:O	2.18	0.76
1:C:248:GLY:N	4:C:3402:HOH:O	2.16	0.76
1:C:255:ILE:HA	4:C:3332:HOH:O	1.85	0.76
1:D:115:PRO:HA	4:D:4374:HOH:O	1.85	0.76
1:B:74:ILE:HD12	4:B:2306:HOH:O	1.84	0.76
1:D:64:ASP:OD2	4:D:4353:HOH:O	2.03	0.76
1:D:115:PRO:O	4:D:4304:HOH:O	2.02	0.76
1:E:129:ARG:HB3	4:E:5401:HOH:O	1.85	0.76
1:A:75:ILE:HG22	1:A:76:PRO:HD3	1.67	0.76
1:A:168:ASP:OD1	4:A:1328:HOH:O	2.03	0.76
1:D:27:ALA:O	4:D:4425:HOH:O	2.02	0.76
3:A:1301:GLU:HB2	4:A:1408:HOH:O	1.86	0.76
1:B:1:MET:O	4:B:2332:HOH:O	2.04	0.76
1:D:194:LYS:NZ	4:D:4319:HOH:O	2.06	0.76
1:A:122:THR:HG22	1:A:123:ASN:N	1.99	0.76
1:B:251:ARG:CD	4:B:2330:HOH:O	2.34	0.76
1:D:57:LYS:HE2	4:D:4376:HOH:O	1.79	0.76
1:D:156:VAL:O	1:D:156:VAL:HG12	1.83	0.76
1:E:185:LEU:N	4:E:5323:HOH:O	2.19	0.76
1:A:218:LEU:HD22	2:A:1300:NAI:C5B	2.14	0.76
1:C:15:LEU:CD1	4:C:3348:HOH:O	2.34	0.76
1:C:71:LYS:H	1:C:71:LYS:HD3	1.48	0.76
1:E:236:GLY:O	4:E:5307:HOH:O	2.03	0.76
1:D:220:SER:HB2	4:D:4419:HOH:O	1.83	0.76
1:E:58:GLU:HB2	4:E:5332:HOH:O	1.85	0.76
1:E:199:ARG:O	4:E:5320:HOH:O	2.02	0.76
1:A:-1:ARG:HG3	4:A:1424:HOH:O	1.85	0.76
1:D:224:PRO:CG	4:D:4355:HOH:O	2.33	0.76
1:E:169:ALA:CA	4:E:5375:HOH:O	2.34	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ARG:NH1	4:A:1316:HOH:O	2.18	0.76
2:A:1300:NAI:C3N	3:A:1301:GLU:HB3	2.15	0.76
1:B:45:LEU:O	4:B:2385:HOH:O	2.03	0.76
1:C:163:GLU:HB2	4:C:3397:HOH:O	1.86	0.76
2:C:3300:NAI:O4D	2:C:3300:NAI:PN	2.44	0.76
1:E:231:VAL:O	4:E:5321:HOH:O	2.03	0.76
1:E:263:ILE:N	4:E:5342:HOH:O	2.18	0.76
2:E:5300:NAI:O1N	3:E:5301:GLU:O	2.03	0.76
1:A:130:GLU:OE1	2:A:1300:NAI:H2D	1.85	0.76
1:B:6:ILE:HA	1:B:33:SER:HB3	1.66	0.76
1:B:129:ARG:HH22	3:B:2301:GLU:HG3	1.51	0.76
1:B:152:LEU:O	4:B:2392:HOH:O	2.04	0.76
1:C:198:PRO:N	4:C:3361:HOH:O	2.19	0.76
1:D:9:GLY:H	1:D:41:THR:HG21	1.48	0.76
1:A:3:VAL:HG22	1:A:65:VAL:HB	1.66	0.75
1:B:10:GLN:HB3	4:B:2343:HOH:O	1.85	0.75
1:E:206:GLY:HA3	4:E:5408:HOH:O	1.85	0.75
1:C:217:LEU:CD1	4:C:3417:HOH:O	2.33	0.75
1:E:134:VAL:CG1	4:E:5413:HOH:O	2.11	0.75
1:B:259:GLU:HA	4:B:2382:HOH:O	1.83	0.75
1:C:252:SER:O	1:C:254:LEU:N	2.18	0.75
1:D:3:VAL:O	4:D:4365:HOH:O	2.03	0.75
1:A:-1:ARG:HG3	4:A:1332:HOH:O	1.87	0.75
1:B:232:SER:OG	4:B:2352:HOH:O	2.03	0.75
1:C:154:SER:O	2:C:3300:NAI:N7N	2.19	0.75
1:E:91:ILE:CA	4:E:5344:HOH:O	2.28	0.75
1:E:178:PRO:N	4:E:5315:HOH:O	2.19	0.75
1:D:257:ALA:O	4:D:4349:HOH:O	2.03	0.75
1:E:158:PHE:HB3	4:E:5351:HOH:O	1.86	0.75
1:A:149:MET:HA	1:A:149:MET:HE3	1.68	0.75
1:A:183:THR:CA	4:A:1354:HOH:O	2.21	0.75
1:D:218:LEU:CD2	2:D:4300:NAI:H52A	2.13	0.75
2:D:4300:NAI:C2N	3:D:4301:GLU:N	2.47	0.75
1:D:194:LYS:O	1:D:195:MET:HE2	1.87	0.75
1:E:121:MET:HB3	4:E:5407:HOH:O	1.85	0.75
1:A:33:SER:O	1:A:35:PRO:HD3	1.87	0.75
1:D:223:HIS:NE2	4:D:4321:HOH:O	2.18	0.75
1:E:253:LEU:HD23	4:E:5364:HOH:O	1.85	0.75
1:A:64:ASP:OD2	4:A:1403:HOH:O	2.03	0.74
1:B:9:GLY:N	4:B:2314:HOH:O	2.19	0.74
1:C:82:ILE:HG22	1:C:86:ILE:HD13	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:221:GLU:O	1:E:223:HIS:N	2.19	0.74
1:A:29:LYS:HA	4:A:1329:HOH:O	1.88	0.74
1:A:186:ASP:CA	4:A:1370:HOH:O	2.34	0.74
2:B:2300:NAI:O4D	2:B:2300:NAI:PN	2.44	0.74
1:B:195:MET:HE2	1:B:195:MET:CA	2.17	0.74
1:C:163:GLU:CB	4:C:3397:HOH:O	2.36	0.74
1:D:124:THR:OG1	4:D:4312:HOH:O	2.04	0.74
1:D:173:LEU:O	4:D:4315:HOH:O	2.05	0.74
1:C:137:THR:OG1	4:C:3384:HOH:O	2.04	0.74
1:E:162:VAL:HB	4:E:5413:HOH:O	1.87	0.74
1:E:183:THR:OG1	4:E:5390:HOH:O	2.04	0.74
1:E:216:MET:HE2	1:E:227:LEU:HD13	1.69	0.74
1:A:188:LEU:N	4:A:1303:HOH:O	2.21	0.74
1:A:199:ARG:HD3	4:A:1351:HOH:O	1.87	0.74
1:C:158:PHE:CE2	2:C:3300:NAI:O3B	2.39	0.74
1:E:162:VAL:N	4:E:5413:HOH:O	2.19	0.74
1:B:12:ALA:CB	4:B:2314:HOH:O	2.32	0.74
1:B:129:ARG:CZ	2:B:2300:NAI:C7N	2.63	0.74
1:E:111:PHE:CE1	4:E:5326:HOH:O	2.36	0.74
1:C:178:PRO:CB	4:C:3396:HOH:O	2.29	0.74
1:A:13:PHE:HB2	4:A:1379:HOH:O	1.87	0.74
1:B:239:ILE:HG21	4:E:5303:HOH:O	1.87	0.74
1:D:229:ASP:CB	4:D:4393:HOH:O	2.22	0.74
1:B:45:LEU:HA	1:B:48:MET:SD	2.28	0.73
1:A:163:GLU:HG3	4:A:1417:HOH:O	1.87	0.73
1:A:186:ASP:HB3	4:A:1354:HOH:O	1.89	0.73
1:B:222:GLN:O	1:B:223:HIS:HB2	1.88	0.73
2:D:4300:NAI:O4D	2:D:4300:NAI:PN	2.44	0.73
1:A:137:THR:O	4:A:1367:HOH:O	2.05	0.73
1:B:75:ILE:H	1:B:75:ILE:HD12	1.53	0.73
1:C:75:ILE:HD13	4:C:3377:HOH:O	1.87	0.73
1:A:171:THR:CA	4:A:1402:HOH:O	2.11	0.73
1:C:1:MET:O	4:C:3306:HOH:O	2.06	0.73
1:A:183:THR:C	4:A:1354:HOH:O	2.32	0.73
1:C:29:LYS:HE3	4:C:3404:HOH:O	1.88	0.73
1:A:35:PRO:O	1:A:36:ASP:HB2	1.88	0.73
1:A:122:THR:O	4:A:1428:HOH:O	2.05	0.73
1:D:112:ARG:HB3	4:D:4329:HOH:O	1.88	0.73
1:E:179:ALA:CA	4:E:5369:HOH:O	2.14	0.73
1:A:125:PRO:HG2	1:A:131:GLY:HA2	1.68	0.73
1:C:62:HIS:ND1	4:C:3362:HOH:O	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:ASN:HB2	1:C:125:PRO:HD2	1.69	0.73
1:A:2:SER:OG	4:A:1403:HOH:O	2.07	0.73
1:A:183:THR:O	4:A:1354:HOH:O	2.07	0.73
1:A:266:ARG:HG2	1:A:266:ARG:HH11	1.54	0.73
1:A:269:GLN:HG2	1:A:270:SER:N	2.02	0.73
1:B:65:VAL:HG22	1:B:91:ILE:HD13	1.70	0.73
1:B:85:ASP:HB2	4:B:2376:HOH:O	1.89	0.73
1:B:120:CYS:N	4:B:2349:HOH:O	2.10	0.73
1:D:246:GLU:OE2	4:D:4417:HOH:O	2.07	0.73
1:A:130:GLU:CD	2:A:1300:NAI:H2D	2.13	0.72
1:D:178:PRO:CB	4:D:4454:HOH:O	2.27	0.72
1:E:73:HIS:CB	4:E:5415:HOH:O	2.30	0.72
1:B:157:GLY:O	2:B:2300:NAI:H42N	1.89	0.72
1:C:135:TYR:CE1	1:C:161:GLU:HB3	2.23	0.72
1:A:240:HIS:NE2	4:A:1375:HOH:O	2.22	0.72
1:C:193:VAL:HG12	4:C:3309:HOH:O	1.88	0.72
1:D:180:TYR:N	4:D:4308:HOH:O	2.18	0.72
1:B:60:VAL:HG12	1:B:89:ARG:NH2	2.03	0.72
1:E:211:LEU:O	4:E:5314:HOH:O	2.08	0.72
1:A:126:VAL:HG22	1:A:156:VAL:HG12	1.71	0.72
1:B:4:GLY:HA3	1:B:66:LEU:HD23	1.72	0.72
1:B:160:THR:HG22	1:B:161:GLU:N	2.04	0.72
2:E:5300:NAI:PA	2:E:5300:NAI:C4B	2.78	0.72
1:D:100:THR:HA	4:D:4422:HOH:O	1.89	0.72
1:E:234:PRO:O	4:E:5309:HOH:O	2.08	0.72
1:B:186:ASP:OD2	4:B:2356:HOH:O	2.07	0.72
1:C:209:ALA:O	4:C:3386:HOH:O	2.08	0.72
1:D:231:VAL:HB	4:D:4402:HOH:O	1.89	0.72
1:E:126:VAL:HG21	4:E:5385:HOH:O	1.88	0.72
1:A:186:ASP:HA	4:A:1370:HOH:O	1.88	0.72
1:D:101:ILE:HB	1:D:164:GLU:OE1	1.90	0.72
1:D:161:GLU:CD	4:D:4398:HOH:O	2.33	0.72
1:C:171:THR:OG1	4:C:3351:HOH:O	2.08	0.72
1:E:153:LEU:CB	4:E:5432:HOH:O	2.38	0.72
1:A:201:LEU:O	1:A:205:LEU:HG	1.89	0.72
1:B:142:GLN:CG	1:B:143:VAL:H	1.91	0.72
1:D:100:THR:HG22	1:D:102:SER:H	1.55	0.72
1:D:246:GLU:OE1	4:D:4383:HOH:O	2.08	0.72
1:E:91:ILE:CB	4:E:5344:HOH:O	2.02	0.72
1:E:246:GLU:OE2	4:E:5312:HOH:O	2.07	0.72
1:C:163:GLU:HG3	4:C:3397:HOH:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:ILE:HD12	1:D:66:LEU:HD21	1.71	0.71
1:D:211:LEU:O	4:D:4406:HOH:O	2.07	0.71
1:E:141:ALA:HB2	4:E:5388:HOH:O	1.89	0.71
1:E:158:PHE:CD1	2:E:5300:NAI:H4B	2.25	0.71
1:E:251:ARG:NH1	4:E:5366:HOH:O	2.22	0.71
1:B:150:GLU:OE1	4:B:2312:HOH:O	2.08	0.71
1:D:11:LEU:N	4:D:4387:HOH:O	2.23	0.71
1:E:130:GLU:OE2	2:E:5300:NAI:H2D	1.90	0.71
1:D:97:ALA:HB1	1:D:265:THR:HG23	1.72	0.71
1:D:124:THR:O	1:D:127:VAL:HG23	1.89	0.71
1:E:57:LYS:H	1:E:57:LYS:HD3	1.56	0.71
1:E:58:GLU:OE1	4:E:5332:HOH:O	2.07	0.71
1:A:27:ALA:N	4:A:1382:HOH:O	2.21	0.71
1:A:89:ARG:NH2	4:A:1395:HOH:O	2.23	0.71
1:B:28:HIS:O	4:B:2344:HOH:O	2.08	0.71
1:B:129:ARG:C	4:B:2372:HOH:O	2.33	0.71
1:A:2:SER:HB3	4:A:1334:HOH:O	1.89	0.71
1:C:126:VAL:HG11	4:C:3317:HOH:O	1.89	0.71
1:D:83:GLY:O	1:D:86:ILE:HG22	1.89	0.71
1:E:206:GLY:CA	4:E:5408:HOH:O	2.36	0.71
1:D:37:MET:CG	4:D:4306:HOH:O	2.22	0.71
1:E:70:VAL:N	4:E:5305:HOH:O	2.15	0.71
1:A:3:VAL:N	4:A:1334:HOH:O	2.22	0.71
1:A:88:ASP:HB2	1:A:112:ARG:NH2	2.05	0.71
1:B:2:SER:HA	1:B:30:ILE:HG12	1.72	0.71
1:D:124:THR:CA	4:D:4375:HOH:O	2.39	0.71
1:A:86:ILE:CD1	1:A:108:LEU:HD11	2.15	0.71
1:E:199:ARG:HB3	4:E:5416:HOH:O	1.90	0.71
1:B:117:VAL:O	4:B:2370:HOH:O	2.09	0.71
1:C:222:GLN:HA	4:C:3304:HOH:O	1.89	0.71
1:D:161:GLU:OE2	4:D:4398:HOH:O	2.08	0.71
1:C:3:VAL:HB	1:C:30:ILE:CG1	2.21	0.71
1:C:273:ASP:C	4:C:3393:HOH:O	2.33	0.71
1:D:185:LEU:HD21	1:D:210:LEU:HD12	1.72	0.71
1:C:91:ILE:HG23	1:C:116:ARG:HB2	1.73	0.70
1:D:32:ALA:HB3	1:D:52:LEU:HD23	1.72	0.70
1:D:150:GLU:OE2	4:D:4390:HOH:O	2.09	0.70
1:E:153:LEU:CA	4:E:5432:HOH:O	2.39	0.70
1:E:215:LYS:HE3	4:E:5430:HOH:O	1.84	0.70
1:A:190:ASP:O	4:A:1420:HOH:O	2.09	0.70
1:A:269:GLN:HA	4:A:1407:HOH:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-1:ARG:HB3	4:A:1342:HOH:O	1.90	0.70
1:C:126:VAL:HG12	4:C:3307:HOH:O	1.89	0.70
1:C:218:LEU:HB3	2:C:3300:NAI:H52N	1.73	0.70
1:C:264:ARG:NE	4:C:3353:HOH:O	2.10	0.70
1:A:75:ILE:HG22	1:A:76:PRO:CD	2.21	0.70
1:B:19:PHE:HA	1:B:22:ALA:HB3	1.73	0.70
1:B:100:THR:HG22	1:B:101:ILE:N	2.06	0.70
1:B:187:ALA:O	1:B:190:ASP:HB2	1.91	0.70
1:C:6:ILE:HD12	1:C:56:ASN:HB3	1.73	0.70
1:C:122:THR:CB	1:C:133:THR:HG22	2.19	0.70
1:D:128:VAL:O	1:D:129:ARG:HB2	1.92	0.70
1:A:122:THR:CG2	1:A:123:ASN:H	2.04	0.70
1:A:124:THR:N	4:A:1325:HOH:O	2.15	0.70
1:A:158:PHE:HA	4:A:1412:HOH:O	1.91	0.70
1:A:266:ARG:HD2	4:A:1331:HOH:O	1.82	0.70
1:D:116:ARG:HA	4:D:4389:HOH:O	1.91	0.70
1:D:168:ASP:OD1	4:D:4337:HOH:O	2.09	0.70
1:E:100:THR:HG22	1:E:102:SER:H	1.56	0.70
1:A:182:PHE:N	4:A:1419:HOH:O	2.13	0.70
1:A:187:ALA:C	4:A:1303:HOH:O	2.34	0.70
1:B:218:LEU:CD2	2:B:2300:NAI:H52A	2.21	0.70
1:C:15:LEU:HD11	4:C:3348:HOH:O	1.88	0.70
1:C:274:GLN:NE2	4:C:3339:HOH:O	2.22	0.70
1:D:184:ALA:HB2	4:D:4340:HOH:O	1.92	0.70
1:E:57:LYS:HD3	1:E:57:LYS:N	2.07	0.70
1:E:165:ASP:O	4:E:5349:HOH:O	2.09	0.70
1:A:161:GLU:CB	4:A:1364:HOH:O	2.26	0.70
1:C:29:LYS:CB	4:C:3306:HOH:O	2.39	0.70
1:C:195:MET:HA	1:C:195:MET:CE	2.21	0.70
1:E:156:VAL:O	1:E:156:VAL:HG12	1.90	0.70
1:A:120:CYS:C	4:A:1327:HOH:O	2.35	0.70
1:A:130:GLU:O	4:A:1307:HOH:O	2.10	0.70
1:C:266:ARG:NE	4:C:3303:HOH:O	2.24	0.70
1:E:60:VAL:HG21	1:E:82:ILE:HG23	1.71	0.70
1:C:7:GLY:HA2	1:C:70:VAL:HG22	1.74	0.70
1:C:29:LYS:C	1:C:30:ILE:HD12	2.17	0.70
1:C:165:ASP:O	4:C:3311:HOH:O	2.10	0.70
1:E:194:LYS:CA	4:E:5303:HOH:O	2.19	0.70
1:B:208:GLN:OE1	4:B:2359:HOH:O	2.09	0.70
1:D:56:ASN:ND2	4:D:4369:HOH:O	2.25	0.70
1:E:174:SER:CB	4:E:5391:HOH:O	2.40	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:GLN:HB2	4:B:2359:HOH:O	1.91	0.69
1:C:27:ALA:HB1	4:C:3363:HOH:O	1.92	0.69
1:D:97:ALA:HA	4:D:4333:HOH:O	1.91	0.69
1:D:103:SER:HA	4:D:4449:HOH:O	1.91	0.69
1:E:136:ALA:O	4:E:5434:HOH:O	2.09	0.69
1:B:100:THR:HG22	1:B:101:ILE:H	1.55	0.69
1:C:56:ASN:O	4:C:3383:HOH:O	2.10	0.69
1:C:85:ASP:O	4:C:3382:HOH:O	2.10	0.69
1:D:64:ASP:CG	4:D:4353:HOH:O	2.34	0.69
1:A:106:LYS:O	4:A:1432:HOH:O	2.09	0.69
1:C:10:GLN:NE2	4:C:3390:HOH:O	2.25	0.69
1:C:198:PRO:HG2	1:C:201:LEU:HB3	1.75	0.69
1:D:231:VAL:O	4:D:4401:HOH:O	2.09	0.69
1:E:121:MET:HE3	1:E:121:MET:HA	1.75	0.69
1:B:8:ALA:HA	1:B:12:ALA:CB	2.22	0.69
1:D:124:THR:CG2	4:D:4375:HOH:O	2.20	0.69
1:E:91:ILE:N	4:E:5344:HOH:O	2.26	0.69
1:E:169:ALA:HA	4:E:5375:HOH:O	1.92	0.69
1:A:130:GLU:OE2	2:A:1300:NAI:H2D	1.92	0.69
1:A:168:ASP:HB2	4:A:1338:HOH:O	1.92	0.69
1:C:115:PRO:HB3	4:C:3358:HOH:O	1.93	0.69
2:D:4300:NAI:C6N	3:D:4301:GLU:C	2.65	0.69
1:A:162:VAL:HG13	1:A:166:LEU:HD12	1.75	0.69
1:A:193:VAL:CG2	4:A:1369:HOH:O	2.40	0.69
1:C:51:LYS:HB2	1:C:51:LYS:HZ3	1.58	0.69
1:C:128:VAL:HG12	1:C:129:ARG:N	2.06	0.69
1:D:125:PRO:O	1:D:128:VAL:HG12	1.92	0.69
1:E:102:SER:HB3	4:E:5347:HOH:O	1.91	0.69
1:E:121:MET:HE2	1:E:122:THR:O	1.92	0.69
2:E:5300:NAI:PN	2:E:5300:NAI:PA	2.89	0.69
2:E:5300:NAI:O2A	2:E:5300:NAI:O4B	2.11	0.69
1:A:122:THR:CG2	1:A:123:ASN:N	2.56	0.69
1:B:231:VAL:CG1	4:B:2363:HOH:O	2.40	0.69
1:C:100:THR:HG22	1:C:102:SER:H	1.57	0.69
1:C:118:ILE:H	1:C:118:ILE:HD13	1.57	0.69
1:C:140:HIS:HB2	4:C:3385:HOH:O	1.91	0.69
1:E:164:GLU:O	4:E:5395:HOH:O	2.11	0.69
1:A:29:LYS:CA	4:A:1329:HOH:O	2.41	0.69
1:D:61:GLN:O	4:D:4430:HOH:O	2.11	0.69
1:E:80:ASP:OD1	4:E:5326:HOH:O	2.10	0.69
1:E:253:LEU:N	4:E:5364:HOH:O	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:262:CYS:CB	4:E:5342:HOH:O	2.37	0.69
4:A:1315:HOH:O	1:E:228:LYS:HE2	1.92	0.68
1:C:203:VAL:CA	4:C:3355:HOH:O	2.34	0.68
1:D:67:PHE:N	4:D:4327:HOH:O	2.26	0.68
1:E:133:THR:CG2	4:E:5385:HOH:O	2.40	0.68
1:A:230:ASN:CB	4:A:1317:HOH:O	2.40	0.68
1:B:229:ASP:OD1	4:B:2386:HOH:O	2.09	0.68
1:C:101:ILE:CG1	4:C:3394:HOH:O	2.32	0.68
1:D:3:VAL:HB	1:D:30:ILE:CD1	2.22	0.68
1:E:11:LEU:O	1:E:15:LEU:HD12	1.93	0.68
1:E:175:GLY:O	4:E:5397:HOH:O	2.10	0.68
1:E:251:ARG:CD	4:E:5330:HOH:O	2.40	0.68
1:C:129:ARG:CD	2:C:3300:NAI:O7N	2.41	0.68
1:C:257:ALA:O	4:C:3378:HOH:O	2.11	0.68
1:C:266:ARG:HG2	4:C:3340:HOH:O	1.92	0.68
1:D:133:THR:HG21	1:D:153:LEU:HD12	1.75	0.68
1:E:2:SER:HB3	4:E:5387:HOH:O	1.93	0.68
1:A:-1:ARG:HG2	4:A:1332:HOH:O	1.87	0.68
1:A:269:GLN:C	1:A:271:MET:H	2.02	0.68
1:D:175:GLY:O	4:D:4309:HOH:O	2.10	0.68
1:E:251:ARG:N	4:E:5317:HOH:O	2.26	0.68
1:A:150:GLU:OE2	4:A:1383:HOH:O	2.11	0.68
1:B:6:ILE:CD1	1:B:59:THR:HB	2.24	0.68
1:A:194:LYS:HE2	1:E:240:HIS:CE1	2.29	0.68
1:C:124:THR:N	1:C:125:PRO:HD2	2.08	0.68
1:D:88:ASP:HA	4:D:4432:HOH:O	1.91	0.68
1:D:251:ARG:HD3	4:D:4427:HOH:O	1.94	0.68
1:B:155:SER:C	2:B:2300:NAI:H72N	2.02	0.68
1:C:48:MET:O	1:C:48:MET:HE3	1.94	0.68
1:E:169:ALA:C	1:E:171:THR:H	2.01	0.68
1:B:6:ILE:HD13	1:B:59:THR:HB	1.75	0.68
1:C:252:SER:OG	4:C:3308:HOH:O	2.07	0.68
1:D:16:ALA:HB1	1:D:48:MET:HE1	1.74	0.68
1:E:225:GLY:HA2	4:E:5353:HOH:O	1.86	0.68
1:E:251:ARG:HD2	4:E:5330:HOH:O	1.94	0.68
1:C:185:LEU:CD2	4:C:3324:HOH:O	2.42	0.68
1:B:124:THR:N	1:B:125:PRO:HD2	2.09	0.68
1:C:180:TYR:HD2	4:C:3302:HOH:O	1.76	0.68
1:C:203:VAL:HG13	4:C:3355:HOH:O	1.92	0.68
1:D:1:MET:HE1	1:D:152:LEU:HD21	1.76	0.68
1:D:150:GLU:HB2	4:D:4443:HOH:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:114:ALA:O	4:E:5436:HOH:O	2.11	0.68
1:A:22:ALA:CB	4:A:1425:HOH:O	2.41	0.67
1:B:94:SER:C	4:B:2349:HOH:O	2.36	0.67
1:D:181:ALA:O	4:D:4330:HOH:O	2.11	0.67
1:E:190:ASP:OD1	4:E:5381:HOH:O	2.12	0.67
1:A:266:ARG:NE	4:A:1331:HOH:O	2.21	0.67
1:B:50:VAL:HA	4:B:2378:HOH:O	1.95	0.67
1:B:124:THR:O	1:B:127:VAL:HG23	1.94	0.67
1:D:148:LEU:HB2	4:D:4348:HOH:O	1.93	0.67
1:E:147:ARG:O	1:E:151:GLN:HB2	1.94	0.67
1:E:190:ASP:CG	4:E:5381:HOH:O	2.35	0.67
1:B:101:ILE:O	1:B:105:GLU:HB2	1.93	0.67
1:C:29:LYS:HB3	4:C:3306:HOH:O	1.93	0.67
1:D:229:ASP:N	4:D:4310:HOH:O	2.25	0.67
1:C:150:GLU:O	4:C:3319:HOH:O	2.13	0.67
1:E:199:ARG:NH2	4:E:5316:HOH:O	2.28	0.67
1:A:76:PRO:O	4:A:1356:HOH:O	2.12	0.67
1:B:61:GLN:HA	4:B:2325:HOH:O	1.94	0.67
1:B:71:LYS:HB3	1:B:72:PRO:CD	2.22	0.67
1:E:153:LEU:C	4:E:5432:HOH:O	2.37	0.67
1:D:30:ILE:CB	4:D:4425:HOH:O	2.28	0.67
1:D:266:ARG:C	1:D:268:LEU:H	2.03	0.67
1:E:123:ASN:HB3	4:E:5397:HOH:O	1.94	0.67
1:C:66:LEU:HD23	1:C:67:PHE:N	2.10	0.67
1:C:223:HIS:N	4:C:3304:HOH:O	2.21	0.67
1:A:158:PHE:CZ	2:A:1300:NAI:O3B	2.48	0.67
1:A:165:ASP:O	4:A:1393:HOH:O	2.12	0.67
1:D:168:ASP:CG	4:D:4337:HOH:O	2.37	0.67
1:A:-1:ARG:N	4:A:1427:HOH:O	2.08	0.67
1:E:122:THR:CB	1:E:133:THR:HG22	2.23	0.67
1:A:124:THR:OG1	4:A:1325:HOH:O	2.13	0.66
1:B:178:PRO:O	4:B:2373:HOH:O	2.13	0.66
1:C:29:LYS:CE	4:C:3404:HOH:O	2.33	0.66
1:C:260:ALA:HB3	4:C:3378:HOH:O	1.94	0.66
1:C:275:GLU:N	4:C:3393:HOH:O	2.23	0.66
1:E:75:ILE:HG21	1:E:104:ILE:HD11	1.78	0.66
1:E:179:ALA:O	4:E:5322:HOH:O	2.14	0.66
1:C:75:ILE:HA	4:C:3407:HOH:O	1.94	0.66
1:D:62:HIS:ND1	1:D:62:HIS:O	2.27	0.66
1:A:120:CYS:CB	4:A:1368:HOH:O	2.42	0.66
1:B:255:ILE:HG12	4:B:2303:HOH:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:185:LEU:HD21	1:E:210:LEU:HD12	1.76	0.66
1:E:193:VAL:C	4:E:5303:HOH:O	2.37	0.66
1:A:79:LEU:HD11	1:A:104:ILE:CD1	2.24	0.66
1:A:193:VAL:C	1:A:195:MET:H	2.04	0.66
1:C:251:ARG:O	1:C:252:SER:O	2.13	0.66
1:D:32:ALA:HB3	1:D:52:LEU:CD2	2.25	0.66
1:D:266:ARG:NE	4:D:4378:HOH:O	2.27	0.66
1:E:48:MET:HG2	1:E:48:MET:O	1.94	0.66
1:C:198:PRO:CD	4:C:3361:HOH:O	2.42	0.66
1:C:265:THR:HG22	4:C:3340:HOH:O	1.94	0.66
1:D:61:GLN:O	4:D:4415:HOH:O	2.13	0.66
1:D:151:GLN:HB3	4:D:4444:HOH:O	1.94	0.66
1:A:26:ALA:HB1	4:A:1382:HOH:O	1.96	0.66
1:A:253:LEU:HD23	4:A:1405:HOH:O	1.95	0.66
1:B:129:ARG:CA	4:B:2372:HOH:O	2.42	0.66
1:B:153:LEU:O	4:B:2392:HOH:O	2.07	0.66
1:B:182:PHE:CD1	4:B:2373:HOH:O	2.47	0.66
1:B:219:HIS:HE1	2:B:2300:NAI:O5D	1.73	0.66
1:C:231:VAL:O	1:C:231:VAL:HG12	1.95	0.66
1:D:232:SER:HB3	1:D:239:ILE:HG12	1.78	0.66
1:E:209:ALA:C	4:E:5360:HOH:O	2.37	0.66
1:A:124:THR:N	1:A:125:PRO:HD2	2.10	0.66
1:C:101:ILE:HD11	1:C:117:VAL:O	1.95	0.66
1:A:193:VAL:HG23	4:A:1369:HOH:O	1.96	0.66
1:B:129:ARG:HH21	3:B:2301:GLU:HB2	1.59	0.66
1:D:251:ARG:CZ	4:D:4427:HOH:O	2.42	0.66
1:E:220:SER:O	1:E:221:GLU:HB2	1.95	0.66
1:B:168:ASP:CB	4:B:2357:HOH:O	2.43	0.66
1:D:93:VAL:HA	4:D:4408:HOH:O	1.95	0.66
1:E:193:VAL:O	4:E:5303:HOH:O	2.12	0.66
1:D:3:VAL:HB	1:D:30:ILE:HD12	1.78	0.66
1:D:256:ASN:O	4:D:4318:HOH:O	2.13	0.66
1:E:55:HIS:HB3	1:E:57:LYS:HE2	1.78	0.66
1:A:206:GLY:O	4:A:1421:HOH:O	2.14	0.65
1:B:256:ASN:C	4:B:2381:HOH:O	2.38	0.65
1:A:1:MET:CB	4:A:1427:HOH:O	2.25	0.65
1:B:189:ALA:CA	4:B:2302:HOH:O	2.35	0.65
1:C:118:ILE:HG22	1:C:137:THR:HA	1.76	0.65
1:E:114:ALA:HB1	1:E:140:HIS:CG	2.31	0.65
1:B:94:SER:HB2	4:B:2306:HOH:O	1.95	0.65
1:C:50:VAL:N	4:C:3363:HOH:O	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:GLY:HA3	4:C:3367:HOH:O	1.88	0.65
1:D:3:VAL:HG22	1:D:65:VAL:CG1	2.27	0.65
1:D:90:HIS:O	4:D:4455:HOH:O	2.14	0.65
1:D:264:ARG:NH2	4:D:4380:HOH:O	2.15	0.65
2:D:4300:NAI:N1N	3:D:4301:GLU:CA	2.55	0.65
1:E:118:ILE:O	4:E:5325:HOH:O	2.13	0.65
1:A:85:ASP:HB2	4:A:1437:HOH:O	1.95	0.65
1:A:240:HIS:HA	4:A:1352:HOH:O	1.97	0.65
1:B:160:THR:N	4:B:2311:HOH:O	2.23	0.65
1:B:172:GLY:HA2	1:B:261:SER:OG	1.96	0.65
1:C:29:LYS:CG	4:C:3404:HOH:O	2.39	0.65
1:C:29:LYS:N	4:C:3404:HOH:O	2.29	0.65
1:D:174:SER:CA	4:D:4315:HOH:O	2.39	0.65
1:A:182:PHE:O	4:A:1354:HOH:O	2.13	0.65
1:A:187:ALA:HB1	4:A:1303:HOH:O	1.97	0.65
1:A:198:PRO:HG2	1:A:201:LEU:HB3	1.77	0.65
1:B:3:VAL:H	1:B:30:ILE:HG23	1.61	0.65
1:E:178:PRO:CD	4:E:5315:HOH:O	2.44	0.65
1:A:123:ASN:C	1:A:125:PRO:HD2	2.22	0.65
1:B:188:LEU:C	1:B:190:ASP:H	2.05	0.65
1:B:218:LEU:CD1	2:B:2300:NAI:H52N	2.25	0.65
1:A:142:GLN:N	4:A:1390:HOH:O	2.05	0.65
1:C:251:ARG:CA	4:C:3359:HOH:O	2.40	0.65
1:A:198:PRO:HD2	1:A:201:LEU:HD23	1.77	0.65
1:D:53:THR:HG22	1:D:55:HIS:N	2.11	0.65
1:D:222:GLN:O	1:D:223:HIS:CB	2.44	0.65
1:E:83:GLY:HA2	1:E:86:ILE:HD12	1.79	0.65
1:E:163:GLU:OE2	4:E:5399:HOH:O	2.14	0.65
2:E:5300:NAI:O2A	2:E:5300:NAI:C4B	2.45	0.65
1:A:135:TYR:OH	1:A:150:GLU:HG3	1.97	0.64
1:B:9:GLY:H	1:B:12:ALA:CB	2.05	0.64
1:B:63:SER:HB2	1:B:89:ARG:NH1	2.13	0.64
1:B:73:HIS:ND1	4:B:2390:HOH:O	2.26	0.64
1:B:74:ILE:HG23	1:B:78:ILE:HG21	1.79	0.64
1:B:133:THR:O	4:B:2311:HOH:O	2.15	0.64
1:A:126:VAL:HG22	1:A:156:VAL:CG1	2.26	0.64
1:B:126:VAL:HA	4:B:2372:HOH:O	1.98	0.64
1:B:185:LEU:O	1:B:187:ALA:N	2.30	0.64
1:D:224:PRO:N	4:D:4372:HOH:O	2.29	0.64
1:E:220:SER:HB2	1:E:222:GLN:HG2	1.79	0.64
1:A:55:HIS:C	1:A:57:LYS:H	2.05	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:GLY:CA	4:A:1310:HOH:O	2.39	0.64
1:B:128:VAL:O	1:B:129:ARG:HB2	1.97	0.64
1:D:223:HIS:CE1	4:D:4355:HOH:O	2.51	0.64
1:A:181:ALA:O	4:A:1419:HOH:O	2.12	0.64
1:B:134:VAL:HA	4:B:2311:HOH:O	1.98	0.64
1:C:43:SER:O	1:C:46:ARG:HB2	1.97	0.64
1:C:131:GLY:CA	4:C:3307:HOH:O	2.41	0.64
1:D:125:PRO:HB2	1:D:131:GLY:HA2	1.80	0.64
1:D:275:GLU:C	4:D:4456:HOH:O	2.41	0.64
1:E:225:GLY:C	4:E:5353:HOH:O	2.40	0.64
1:A:128:VAL:O	1:A:129:ARG:HB2	1.97	0.64
1:B:95:CYS:HA	1:B:120:CYS:O	1.97	0.64
1:C:24:VAL:N	4:C:3369:HOH:O	2.09	0.64
1:C:124:THR:O	1:C:127:VAL:HG23	1.97	0.64
1:C:169:ALA:HB2	4:C:3320:HOH:O	1.97	0.64
1:E:178:PRO:HB2	4:E:5393:HOH:O	1.96	0.64
1:A:11:LEU:HD12	4:A:1399:HOH:O	1.97	0.64
1:A:26:ALA:C	4:A:1382:HOH:O	2.40	0.64
1:A:94:SER:CA	4:A:1321:HOH:O	2.45	0.64
1:E:0:GLY:O	4:E:5371:HOH:O	2.13	0.64
1:E:124:THR:O	1:E:127:VAL:HG23	1.96	0.64
1:E:151:GLN:HB3	4:E:5428:HOH:O	1.98	0.64
1:A:111:PHE:O	4:A:1365:HOH:O	2.14	0.64
1:A:194:LYS:O	1:A:195:MET:SD	2.55	0.64
1:B:269:GLN:C	1:B:271:MET:H	2.06	0.64
1:C:185:LEU:N	4:C:3352:HOH:O	2.31	0.64
1:C:198:PRO:HD3	4:C:3361:HOH:O	1.98	0.64
1:A:26:ALA:HB3	1:A:29:LYS:HB2	1.78	0.64
3:A:1301:GLU:HG2	4:A:1408:HOH:O	1.97	0.64
1:C:62:HIS:CE1	4:C:3362:HOH:O	2.50	0.64
1:C:178:PRO:CA	4:C:3396:HOH:O	2.46	0.64
1:D:99:VAL:O	4:D:4317:HOH:O	2.15	0.64
1:A:135:TYR:CE2	1:A:150:GLU:HG2	2.33	0.64
4:B:2308:HOH:O	1:D:239:ILE:HG21	1.92	0.64
1:E:13:PHE:CE1	4:E:5306:HOH:O	2.51	0.64
1:E:56:ASN:O	1:E:60:VAL:HG23	1.98	0.64
1:E:130:GLU:OE2	2:E:5300:NAI:C2D	2.46	0.64
1:E:232:SER:HB2	4:E:5345:HOH:O	1.97	0.64
1:A:156:VAL:HG12	1:A:156:VAL:O	1.98	0.64
1:B:240:HIS:C	4:B:2329:HOH:O	2.40	0.64
1:C:223:HIS:ND1	1:C:224:PRO:HD2	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:ALA:HB3	1:D:24:VAL:HG23	1.80	0.64
1:D:115:PRO:HA	4:D:4307:HOH:O	1.98	0.64
1:D:151:GLN:C	4:D:4444:HOH:O	2.41	0.64
1:E:63:SER:CA	4:E:5417:HOH:O	2.43	0.64
1:E:203:VAL:HG23	4:E:5320:HOH:O	1.98	0.64
1:E:218:LEU:HD22	2:E:5300:NAI:H52A	1.79	0.64
1:A:119:ARG:HG2	4:A:1372:HOH:O	1.90	0.63
1:C:112:ARG:HH11	1:C:112:ARG:HG3	1.63	0.63
1:A:33:SER:OG	1:A:56:ASN:HB3	1.98	0.63
1:A:36:ASP:O	1:A:37:MET:HB2	1.98	0.63
1:B:4:GLY:HA2	1:B:59:THR:HG22	1.79	0.63
1:B:73:HIS:O	1:B:78:ILE:HD13	1.98	0.63
1:C:117:VAL:HG23	4:C:3315:HOH:O	1.98	0.63
1:C:213:ALA:CB	4:C:3386:HOH:O	2.24	0.63
1:A:129:ARG:HD2	4:A:1371:HOH:O	1.98	0.63
1:B:182:PHE:CE1	4:B:2373:HOH:O	2.51	0.63
1:B:259:GLU:CA	4:B:2382:HOH:O	2.43	0.63
1:C:29:LYS:HG2	4:C:3404:HOH:O	1.98	0.63
1:C:155:SER:HA	2:C:3300:NAI:N7N	2.09	0.63
1:C:160:THR:HG22	1:C:161:GLU:N	2.13	0.63
1:D:217:LEU:HB3	4:D:4323:HOH:O	1.98	0.63
1:A:164:GLU:HA	1:A:167:ILE:HG12	1.80	0.63
1:A:271:MET:HG2	1:A:271:MET:O	1.98	0.63
1:C:123:ASN:N	4:C:3331:HOH:O	2.17	0.63
1:C:172:GLY:HA2	1:C:261:SER:OG	1.98	0.63
1:E:163:GLU:CD	4:E:5399:HOH:O	2.36	0.63
1:E:198:PRO:HG2	1:E:201:LEU:HB3	1.81	0.63
1:D:87:GLU:CB	4:D:4322:HOH:O	2.34	0.63
1:A:89:ARG:HG3	1:A:90:HIS:N	2.14	0.63
1:B:158:PHE:CZ	2:B:2300:NAI:C3B	2.82	0.63
1:E:158:PHE:CE2	2:E:5300:NAI:O3B	2.52	0.63
1:E:177:GLY:HA2	1:E:180:TYR:CD1	2.34	0.63
1:E:211:LEU:CD1	4:E:5314:HOH:O	2.46	0.63
1:E:229:ASP:CA	4:E:5337:HOH:O	2.20	0.63
1:A:55:HIS:HB3	1:A:57:LYS:HD2	1.80	0.63
1:B:256:ASN:CB	4:B:2369:HOH:O	2.42	0.63
1:A:100:THR:HG22	1:A:102:SER:H	1.64	0.63
1:C:114:ALA:HB1	1:C:140:HIS:ND1	2.14	0.63
1:E:30:ILE:HB	1:E:50:VAL:HG22	1.79	0.63
1:E:94:SER:N	4:E:5325:HOH:O	2.05	0.63
1:A:123:ASN:HB2	4:A:1325:HOH:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:GLY:C	4:A:1310:HOH:O	2.42	0.62
1:B:160:THR:HG22	1:B:161:GLU:H	1.62	0.62
1:C:172:GLY:O	1:C:258:VAL:HG22	1.99	0.62
1:C:266:ARG:HG2	1:C:266:ARG:NH1	2.14	0.62
1:E:225:GLY:O	4:E:5353:HOH:O	2.16	0.62
1:A:139:THR:N	4:A:1310:HOH:O	2.31	0.62
1:C:3:VAL:O	1:C:30:ILE:HA	1.98	0.62
1:D:88:ASP:C	4:D:4432:HOH:O	2.37	0.62
1:A:174:SER:CB	4:A:1339:HOH:O	2.46	0.62
1:C:218:LEU:CB	2:C:3300:NAI:H52N	2.28	0.62
1:D:31:MET:HE2	1:D:62:HIS:HB3	1.82	0.62
1:E:17:LYS:HB3	4:E:5306:HOH:O	1.90	0.62
1:B:109:SER:OG	1:B:115:PRO:HD2	1.98	0.62
1:B:129:ARG:N	4:B:2372:HOH:O	2.32	0.62
1:C:19:PHE:O	4:C:3369:HOH:O	2.15	0.62
1:C:155:SER:CA	2:C:3300:NAI:H72N	2.10	0.62
1:C:218:LEU:HB3	2:C:3300:NAI:C5D	2.30	0.62
1:A:101:ILE:HG12	1:A:119:ARG:HB2	1.81	0.62
1:B:259:GLU:N	4:B:2382:HOH:O	2.33	0.62
1:D:103:SER:CA	4:D:4449:HOH:O	2.45	0.62
1:A:121:MET:N	4:A:1327:HOH:O	2.33	0.62
1:D:169:ALA:C	1:D:171:THR:H	2.07	0.62
1:D:176:SER:O	1:D:179:ALA:HB3	1.99	0.62
1:A:78:ILE:N	4:A:1356:HOH:O	2.31	0.62
1:B:162:VAL:HG12	1:B:163:GLU:HG2	1.82	0.62
1:B:264:ARG:O	1:B:268:LEU:HG	2.00	0.62
1:C:25:LEU:HD11	1:C:30:ILE:HD11	1.81	0.62
1:D:71:LYS:O	1:D:75:ILE:HD12	1.99	0.62
1:E:179:ALA:C	4:E:5369:HOH:O	2.39	0.62
2:D:4300:NAI:H3D	4:D:4423:HOH:O	2.00	0.62
1:B:141:ALA:HB1	1:B:145:ASP:OD2	2.00	0.62
1:B:225:GLY:O	1:B:228:LYS:HB3	1.99	0.62
1:C:124:THR:C	1:C:126:VAL:H	2.07	0.62
1:C:258:VAL:O	1:C:258:VAL:CG1	2.47	0.62
1:A:118:ILE:HD12	1:A:149:MET:SD	2.39	0.61
1:A:172:GLY:HA2	1:A:261:SER:HB3	1.82	0.61
1:B:122:THR:HG22	1:B:133:THR:OG1	1.99	0.61
1:B:200:ARG:NH1	1:B:204:ARG:HH21	1.98	0.61
1:C:55:HIS:C	1:C:57:LYS:H	2.09	0.61
1:C:71:LYS:HB2	1:C:73:HIS:CE1	2.35	0.61
1:C:185:LEU:HD23	4:C:3324:HOH:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:ILE:CA	4:D:4365:HOH:O	2.41	0.61
1:A:13:PHE:CA	4:A:1379:HOH:O	2.47	0.61
1:A:123:ASN:HD21	1:A:132:ALA:N	1.97	0.61
1:A:255:ILE:C	4:A:1335:HOH:O	2.42	0.61
1:B:125:PRO:HG2	1:B:131:GLY:HA2	1.82	0.61
1:E:122:THR:HG22	1:E:133:THR:CB	2.28	0.61
1:A:258:VAL:HG23	4:A:1302:HOH:O	1.94	0.61
1:C:68:LEU:HD11	1:C:78:ILE:HG21	1.82	0.61
1:C:250:PHE:N	4:C:3312:HOH:O	2.33	0.61
1:D:31:MET:HE3	4:D:4404:HOH:O	1.99	0.61
1:D:53:THR:HG21	1:D:58:GLU:OE1	2.00	0.61
1:D:58:GLU:HB3	4:D:4358:HOH:O	1.99	0.61
1:A:2:SER:CB	4:A:1403:HOH:O	2.47	0.61
1:C:3:VAL:HB	1:C:30:ILE:HG12	1.82	0.61
1:A:93:VAL:HG13	1:A:118:ILE:HG13	1.82	0.61
1:B:119:ARG:HD2	1:B:164:GLU:OE2	2.00	0.61
1:C:37:MET:HA	1:C:42:VAL:HG11	1.82	0.61
1:C:208:GLN:OE1	4:C:3395:HOH:O	2.16	0.61
1:E:86:ILE:HD12	1:E:108:LEU:HD22	1.81	0.61
1:A:263:ILE:CD1	1:A:263:ILE:H	2.14	0.61
1:B:129:ARG:CZ	2:B:2300:NAI:C3N	2.78	0.61
1:B:231:VAL:HG13	4:B:2363:HOH:O	1.99	0.61
1:C:119:ARG:NH2	4:C:3310:HOH:O	2.31	0.61
1:D:229:ASP:HA	4:D:4316:HOH:O	2.01	0.61
1:A:241:ALA:O	1:A:244:VAL:HG22	2.01	0.61
1:B:14:ALA:CA	1:B:127:VAL:HG22	2.28	0.61
2:B:2300:NAI:N1N	3:B:2301:GLU:OXT	2.33	0.61
1:C:122:THR:CB	4:C:3331:HOH:O	2.15	0.61
2:C:3300:NAI:N1N	3:C:3301:GLU:OXT	2.33	0.61
1:A:68:LEU:HD12	1:A:94:SER:HB2	1.82	0.61
1:B:220:SER:C	4:B:2322:HOH:O	2.42	0.61
1:C:133:THR:HG22	4:C:3331:HOH:O	2.00	0.61
1:E:106:LYS:CB	4:E:5384:HOH:O	2.47	0.61
1:B:64:ASP:O	1:B:90:HIS:HA	1.99	0.61
1:B:70:VAL:HG23	4:B:2368:HOH:O	2.01	0.61
1:B:129:ARG:NH2	3:B:2301:GLU:HG3	2.14	0.61
1:C:171:THR:OG1	4:C:3380:HOH:O	2.15	0.61
1:C:269:GLN:C	1:C:271:MET:H	2.08	0.61
1:D:220:SER:HB2	1:D:222:GLN:HG2	1.82	0.61
1:E:113:PRO:HD2	4:E:5367:HOH:O	2.01	0.61
1:A:220:SER:HB2	4:A:1441:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:GLU:N	4:A:1366:HOH:O	2.29	0.61
1:B:133:THR:HG22	4:B:2387:HOH:O	2.01	0.61
1:A:115:PRO:HD2	1:A:140:HIS:CD2	2.36	0.60
1:B:153:LEU:C	1:B:155:SER:H	2.07	0.60
1:B:266:ARG:O	1:B:269:GLN:HG2	2.01	0.60
1:C:48:MET:HB3	4:C:3371:HOH:O	1.89	0.60
1:D:30:ILE:CG1	4:D:4425:HOH:O	2.48	0.60
1:D:38:ASP:OD2	1:D:40:ALA:HB3	2.01	0.60
1:E:135:TYR:CE1	1:E:161:GLU:HB3	2.36	0.60
1:E:228:LYS:C	4:E:5337:HOH:O	2.44	0.60
1:E:251:ARG:NE	4:E:5348:HOH:O	2.34	0.60
1:A:79:LEU:HD11	1:A:104:ILE:HG23	1.83	0.60
1:B:245:LEU:CA	4:B:2353:HOH:O	2.40	0.60
1:C:49:GLY:CA	4:C:3363:HOH:O	2.47	0.60
1:E:77:PHE:HD1	1:E:77:PHE:H	1.47	0.60
1:B:178:PRO:HG2	4:B:2345:HOH:O	2.02	0.60
1:C:264:ARG:NH2	4:C:3353:HOH:O	2.23	0.60
1:D:168:ASP:HA	4:D:4337:HOH:O	2.01	0.60
1:D:266:ARG:CZ	4:D:4378:HOH:O	2.46	0.60
1:D:269:GLN:C	1:D:271:MET:H	2.10	0.60
1:A:45:LEU:HD21	4:A:1379:HOH:O	2.01	0.60
1:B:154:SER:C	2:B:2300:NAI:H71N	2.02	0.60
1:B:218:LEU:HD22	2:B:2300:NAI:O5B	2.00	0.60
1:C:93:VAL:CG1	1:C:118:ILE:HD11	2.30	0.60
1:E:179:ALA:C	4:E:5322:HOH:O	2.44	0.60
1:C:45:LEU:O	1:C:48:MET:HB3	2.02	0.60
1:D:126:VAL:HG13	1:D:156:VAL:CG1	2.30	0.60
1:D:246:GLU:CG	4:D:4383:HOH:O	2.44	0.60
1:D:266:ARG:CD	4:D:4311:HOH:O	2.49	0.60
1:A:222:GLN:O	1:A:223:HIS:CB	2.49	0.60
1:B:70:VAL:HG12	1:B:71:LYS:H	1.66	0.60
2:B:2300:NAI:H2N	3:B:2301:GLU:HB3	1.78	0.60
1:D:78:ILE:HG23	1:D:82:ILE:HD13	1.83	0.60
1:D:80:ASP:CG	4:D:4370:HOH:O	2.43	0.60
1:D:185:LEU:CG	4:D:4330:HOH:O	2.28	0.60
1:D:203:VAL:HG12	1:D:204:ARG:N	2.17	0.60
1:A:186:ASP:CB	4:A:1354:HOH:O	2.45	0.60
1:D:265:THR:CB	4:D:4360:HOH:O	2.06	0.60
1:E:133:THR:HG21	4:E:5385:HOH:O	2.01	0.60
1:A:95:CYS:N	4:A:1321:HOH:O	2.33	0.60
1:A:106:LYS:HG3	4:A:1344:HOH:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:VAL:HG22	1:B:149:MET:HE1	1.82	0.60
1:B:102:SER:HA	1:B:105:GLU:HB2	1.82	0.60
1:B:223:HIS:ND1	1:B:224:PRO:HD2	2.16	0.60
1:B:251:ARG:C	4:B:2303:HOH:O	2.44	0.60
1:C:249:GLY:O	1:C:252:SER:HB3	2.02	0.60
1:E:86:ILE:CD1	1:E:108:LEU:HD22	2.32	0.60
1:B:258:VAL:HG22	4:B:2382:HOH:O	2.02	0.60
1:C:3:VAL:HB	1:C:30:ILE:HG13	1.84	0.60
1:C:105:GLU:CG	4:C:3315:HOH:O	2.41	0.60
1:E:22:ALA:HA	1:E:129:ARG:NH2	2.17	0.60
1:E:133:THR:HG22	4:E:5385:HOH:O	2.01	0.60
1:B:129:ARG:NH2	3:B:2301:GLU:CG	2.56	0.60
1:C:195:MET:HE3	1:C:195:MET:CA	2.27	0.60
1:C:275:GLU:C	4:C:3401:HOH:O	2.45	0.60
1:D:37:MET:HE3	1:D:42:VAL:HB	1.84	0.60
1:C:115:PRO:HG3	4:C:3358:HOH:O	2.01	0.59
1:C:169:ALA:CA	4:C:3320:HOH:O	2.49	0.59
1:D:1:MET:HE2	1:D:25:LEU:HD21	1.84	0.59
1:D:116:ARG:O	4:D:4455:HOH:O	2.16	0.59
1:D:121:MET:HE1	1:D:171:THR:HG23	1.84	0.59
1:D:174:SER:HA	4:D:4315:HOH:O	1.98	0.59
1:D:211:LEU:CD1	4:D:4406:HOH:O	2.42	0.59
1:A:123:ASN:ND2	1:A:132:ALA:H	2.00	0.59
1:A:182:PHE:CD1	4:A:1324:HOH:O	2.45	0.59
1:B:82:ILE:HG22	1:B:86:ILE:CD1	2.31	0.59
1:C:125:PRO:HB2	1:C:130:GLU:O	2.02	0.59
1:C:238:THR:O	1:C:241:ALA:N	2.35	0.59
1:D:222:GLN:N	4:D:4384:HOH:O	2.35	0.59
1:E:162:VAL:CB	4:E:5413:HOH:O	2.47	0.59
1:A:28:HIS:CD2	4:A:1329:HOH:O	2.56	0.59
1:A:239:ILE:N	4:A:1391:HOH:O	2.34	0.59
1:B:235:GLY:O	4:B:2318:HOH:O	2.17	0.59
1:C:258:VAL:C	4:C:3391:HOH:O	2.38	0.59
1:D:211:LEU:HD12	1:D:211:LEU:C	2.27	0.59
1:E:64:ASP:N	4:E:5417:HOH:O	2.31	0.59
1:E:70:VAL:O	1:E:71:LYS:HB2	2.02	0.59
1:A:51:LYS:NZ	4:A:1406:HOH:O	2.14	0.59
1:B:94:SER:O	1:B:96:ALA:N	2.35	0.59
1:C:266:ARG:NH2	4:C:3311:HOH:O	2.15	0.59
1:A:94:SER:OG	4:A:1321:HOH:O	2.15	0.59
1:B:41:THR:O	1:B:45:LEU:HG	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ARG:HH12	2:B:2300:NAI:C2N	2.06	0.59
1:B:195:MET:HA	1:B:195:MET:CE	2.26	0.59
1:B:235:GLY:C	4:B:2318:HOH:O	2.44	0.59
1:B:251:ARG:O	1:B:254:LEU:N	2.31	0.59
1:C:4:GLY:C	1:C:66:LEU:HG	2.27	0.59
1:C:35:PRO:O	1:C:36:ASP:HB2	2.02	0.59
1:E:136:ALA:HB3	4:E:5434:HOH:O	2.01	0.59
1:A:122:THR:HG22	1:A:123:ASN:H	1.64	0.59
1:B:11:LEU:CD2	4:B:2343:HOH:O	2.43	0.59
1:B:101:ILE:HG13	1:B:102:SER:N	2.17	0.59
1:B:231:VAL:O	4:B:2363:HOH:O	2.17	0.59
1:D:123:ASN:CB	4:D:4309:HOH:O	2.43	0.59
2:D:4300:NAI:N1N	3:D:4301:GLU:C	2.60	0.59
1:E:185:LEU:CG	4:E:5383:HOH:O	2.11	0.59
1:B:168:ASP:HB3	4:B:2357:HOH:O	2.00	0.59
1:D:116:ARG:HB2	4:D:4455:HOH:O	2.03	0.59
1:E:176:SER:CA	4:E:5333:HOH:O	2.20	0.59
1:A:223:HIS:ND1	1:A:224:PRO:HD2	2.16	0.59
2:A:1300:NAI:C5D	4:A:1431:HOH:O	2.44	0.59
1:B:189:ALA:HA	4:B:2302:HOH:O	1.99	0.59
1:C:51:LYS:HB2	1:C:51:LYS:NZ	2.17	0.59
1:E:168:ASP:OD2	1:E:266:ARG:HG3	2.03	0.59
1:E:223:HIS:ND1	1:E:224:PRO:HD2	2.18	0.59
1:A:112:ARG:HD3	4:A:1365:HOH:O	2.02	0.59
1:B:77:PHE:C	1:B:78:ILE:HD12	2.27	0.59
1:C:156:VAL:O	1:C:156:VAL:HG12	2.02	0.59
1:D:13:PHE:HA	1:D:16:ALA:HB3	1.85	0.59
1:D:197:LEU:HD22	1:D:201:LEU:HD23	1.85	0.59
1:A:68:LEU:HB2	4:A:1321:HOH:O	2.02	0.59
1:A:133:THR:HG21	1:A:153:LEU:CD1	2.25	0.59
1:C:177:GLY:HA2	1:C:180:TYR:CD1	2.37	0.59
1:D:6:ILE:CD1	1:D:66:LEU:HD21	2.32	0.59
1:A:60:VAL:HG21	1:A:82:ILE:HD12	1.85	0.58
1:A:268:LEU:HD21	4:A:1322:HOH:O	2.03	0.58
1:B:53:THR:HG23	1:B:58:GLU:OE2	2.03	0.58
1:A:22:ALA:HB2	4:A:1425:HOH:O	2.02	0.58
1:A:178:PRO:C	4:A:1324:HOH:O	2.42	0.58
1:B:176:SER:HB3	1:B:180:TYR:CE2	2.37	0.58
1:C:246:GLU:O	4:C:3402:HOH:O	2.17	0.58
1:D:16:ALA:CB	1:D:48:MET:HE1	2.32	0.58
1:A:190:ASP:N	1:A:199:ARG:HH12	2.00	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:ARG:CG	4:C:3340:HOH:O	2.50	0.58
1:D:117:VAL:O	1:D:138:GLY:HA3	2.02	0.58
1:D:264:ARG:O	1:D:268:LEU:HB2	2.03	0.58
1:D:266:ARG:O	1:D:268:LEU:N	2.36	0.58
1:E:37:MET:O	4:E:5392:HOH:O	2.16	0.58
1:E:89:ARG:NH2	4:E:5324:HOH:O	2.36	0.58
1:E:122:THR:CG2	1:E:133:THR:HB	2.30	0.58
1:B:123:ASN:HB2	1:B:125:PRO:HD2	1.84	0.58
1:E:222:GLN:O	1:E:223:HIS:CB	2.51	0.58
1:B:215:LYS:HG3	4:B:2377:HOH:O	2.03	0.58
1:C:250:PHE:O	4:C:3359:HOH:O	2.17	0.58
1:D:97:ALA:CA	4:D:4333:HOH:O	2.50	0.58
1:E:123:ASN:HB2	4:E:5310:HOH:O	2.04	0.58
1:E:274:GLN:HG3	1:E:275:GLU:N	2.17	0.58
1:B:13:PHE:HB2	1:B:41:THR:HG21	1.86	0.58
1:D:1:MET:CE	1:D:25:LEU:HD21	2.33	0.58
1:D:75:ILE:HG21	1:D:104:ILE:HD11	1.86	0.58
1:D:113:PRO:CD	4:D:4329:HOH:O	2.49	0.58
1:E:75:ILE:HG13	1:E:99:VAL:HG21	1.85	0.58
1:E:188:LEU:HB3	4:E:5396:HOH:O	2.02	0.58
1:A:267:GLU:O	1:A:271:MET:HB3	2.03	0.58
1:B:8:ALA:HB1	1:B:45:LEU:CD1	2.34	0.58
1:B:93:VAL:CG2	1:B:149:MET:HE1	2.33	0.58
1:C:194:LYS:N	4:C:3309:HOH:O	2.35	0.58
1:D:264:ARG:NE	4:D:4380:HOH:O	2.26	0.58
1:A:175:GLY:O	4:A:1436:HOH:O	2.16	0.58
1:B:221:GLU:O	1:B:223:HIS:N	2.37	0.58
1:C:79:LEU:HD22	1:C:108:LEU:HD11	1.85	0.58
1:C:131:GLY:N	4:C:3307:HOH:O	2.37	0.58
1:D:258:VAL:HG12	1:D:259:GLU:N	2.18	0.58
1:A:136:ALA:HA	4:A:1404:HOH:O	2.02	0.58
1:D:98:GLY:HA3	1:D:269:GLN:HB2	1.86	0.58
1:D:57:LYS:HD3	4:D:4438:HOH:O	2.04	0.57
1:E:100:THR:HG22	1:E:101:ILE:N	2.19	0.57
1:E:125:PRO:CG	4:E:5302:HOH:O	2.52	0.57
1:E:251:ARG:CZ	4:E:5366:HOH:O	2.52	0.57
1:B:71:LYS:HB2	1:B:73:HIS:CE1	2.39	0.57
1:E:117:VAL:O	1:E:138:GLY:HA3	2.03	0.57
1:A:258:VAL:C	4:A:1366:HOH:O	2.46	0.57
1:A:264:ARG:NE	4:A:1322:HOH:O	2.12	0.57
1:B:159:CYS:HA	4:B:2311:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:ILE:CD1	4:C:3394:HOH:O	2.52	0.57
1:A:68:LEU:HB2	1:A:94:SER:HA	1.87	0.57
1:B:185:LEU:O	1:B:186:ASP:C	2.47	0.57
1:B:192:GLY:N	4:B:2355:HOH:O	2.37	0.57
1:E:106:LYS:HA	4:E:5398:HOH:O	2.04	0.57
1:E:159:CYS:N	4:E:5425:HOH:O	2.35	0.57
1:A:231:VAL:O	1:A:231:VAL:HG12	2.04	0.57
1:B:160:THR:CG2	1:B:161:GLU:H	2.17	0.57
1:D:177:GLY:HA2	1:D:180:TYR:CD1	2.40	0.57
1:A:259:GLU:OE1	4:A:1330:HOH:O	2.18	0.57
1:C:185:LEU:CA	4:C:3352:HOH:O	2.53	0.57
1:C:221:GLU:HA	1:C:221:GLU:OE2	2.02	0.57
1:D:130:GLU:OE2	2:D:4300:NAI:H2D	2.05	0.57
1:E:169:ALA:C	1:E:171:THR:N	2.61	0.57
1:C:121:MET:HG3	4:C:3351:HOH:O	2.04	0.57
1:B:1:MET:HB2	1:B:64:ASP:HB2	1.85	0.57
1:B:70:VAL:HG12	1:B:71:LYS:N	2.18	0.57
1:B:176:SER:O	1:B:177:GLY:C	2.46	0.57
1:C:45:LEU:O	1:C:45:LEU:HD23	2.05	0.57
1:E:73:HIS:CD2	4:E:5429:HOH:O	2.56	0.57
1:E:169:ALA:O	1:E:171:THR:N	2.38	0.57
1:C:185:LEU:HA	4:C:3352:HOH:O	2.04	0.57
1:E:141:ALA:CB	4:E:5388:HOH:O	2.52	0.57
1:A:29:LYS:CG	4:A:1329:HOH:O	2.52	0.57
1:A:187:ALA:CB	4:A:1303:HOH:O	2.52	0.57
1:B:101:ILE:HG23	1:B:164:GLU:OE2	2.05	0.57
1:E:47:LYS:CE	4:E:5338:HOH:O	2.37	0.57
1:A:89:ARG:HG3	1:A:90:HIS:H	1.69	0.56
1:B:34:SER:C	1:B:36:ASP:H	2.12	0.56
1:B:160:THR:CG2	1:B:161:GLU:N	2.67	0.56
1:C:264:ARG:O	1:C:268:LEU:HG	2.05	0.56
1:E:229:ASP:HA	4:E:5340:HOH:O	2.05	0.56
1:A:163:GLU:N	4:A:1355:HOH:O	2.32	0.56
1:A:264:ARG:NH2	4:A:1322:HOH:O	2.36	0.56
1:B:74:ILE:O	1:B:79:LEU:HG	2.06	0.56
1:B:82:ILE:CA	4:B:2376:HOH:O	2.44	0.56
1:B:219:HIS:CE1	2:B:2300:NAI:PN	2.99	0.56
1:C:56:ASN:C	4:C:3383:HOH:O	2.48	0.56
1:C:203:VAL:CG1	4:C:3355:HOH:O	2.49	0.56
1:A:249:GLY:HA2	4:A:1318:HOH:O	2.04	0.56
2:A:1300:NAI:C1D	2:A:1300:NAI:C6N	2.78	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:LEU:C	4:B:2368:HOH:O	2.48	0.56
1:B:176:SER:HA	4:B:2327:HOH:O	2.05	0.56
2:B:2300:NAI:C5N	3:B:2301:GLU:OXT	2.53	0.56
1:C:169:ALA:HA	4:C:3320:HOH:O	2.05	0.56
1:C:197:LEU:HD12	4:C:3367:HOH:O	2.04	0.56
1:D:181:ALA:C	4:D:4330:HOH:O	2.48	0.56
1:E:22:ALA:HA	1:E:129:ARG:HH21	1.69	0.56
1:E:119:ARG:HA	4:E:5325:HOH:O	2.04	0.56
1:E:222:GLN:HG3	1:E:227:LEU:HD21	1.87	0.56
1:B:74:ILE:O	1:B:78:ILE:HB	2.05	0.56
1:D:62:HIS:HA	4:D:4415:HOH:O	2.05	0.56
1:D:229:ASP:CA	4:D:4310:HOH:O	2.54	0.56
1:A:70:VAL:HG22	1:A:75:ILE:HD12	1.86	0.56
1:B:115:PRO:HB3	4:B:2328:HOH:O	2.05	0.56
1:B:231:VAL:HG12	4:B:2363:HOH:O	2.02	0.56
1:B:259:GLU:OE1	4:B:2334:HOH:O	2.17	0.56
1:C:236:GLY:HA2	4:C:3398:HOH:O	1.98	0.56
1:D:194:LYS:C	1:D:195:MET:HE2	2.30	0.56
1:B:94:SER:OG	1:B:119:ARG:HA	2.06	0.56
1:B:222:GLN:O	1:B:223:HIS:CB	2.52	0.56
1:B:236:GLY:HA2	1:B:239:ILE:CG2	2.30	0.56
1:C:163:GLU:CG	4:C:3397:HOH:O	2.45	0.56
1:C:194:LYS:CA	4:C:3309:HOH:O	2.44	0.56
1:C:260:ALA:N	4:C:3381:HOH:O	2.39	0.56
1:D:103:SER:N	4:D:4449:HOH:O	2.38	0.56
1:B:184:ALA:O	1:B:188:LEU:HG	2.06	0.56
1:C:114:ALA:HB1	1:C:140:HIS:CE1	2.41	0.56
1:C:181:ALA:N	4:C:3336:HOH:O	2.39	0.56
1:D:82:ILE:HD12	1:D:82:ILE:N	2.20	0.56
1:D:169:ALA:O	1:D:171:THR:N	2.39	0.56
1:E:33:SER:O	1:E:35:PRO:HD3	2.06	0.56
1:E:63:SER:HB3	4:E:5372:HOH:O	2.06	0.56
1:C:75:ILE:HB	1:C:76:PRO:HD3	1.88	0.56
1:D:141:ALA:CA	4:D:4386:HOH:O	2.38	0.56
1:E:62:HIS:C	4:E:5372:HOH:O	2.43	0.56
1:E:162:VAL:CG1	1:E:166:LEU:HB2	2.35	0.56
1:A:215:LYS:O	1:A:216:MET:C	2.49	0.56
1:B:198:PRO:HD2	1:B:201:LEU:HD23	1.87	0.56
1:B:241:ALA:CA	4:B:2329:HOH:O	2.44	0.56
1:E:151:GLN:N	4:E:5327:HOH:O	2.30	0.56
1:E:183:THR:C	4:E:5370:HOH:O	2.48	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:ILE:HG13	1:C:99:VAL:HG21	1.87	0.56
1:C:141:ALA:HA	1:C:145:ASP:OD1	2.05	0.56
1:D:113:PRO:HD2	4:D:4329:HOH:O	2.06	0.56
1:D:164:GLU:HA	1:D:167:ILE:HG12	1.87	0.56
1:E:105:GLU:HB2	4:E:5437:HOH:O	2.06	0.56
1:A:2:SER:HB2	4:A:1403:HOH:O	2.04	0.55
1:A:135:TYR:HE2	1:A:150:GLU:HG2	1.70	0.55
1:B:200:ARG:O	1:B:204:ARG:HG2	2.06	0.55
1:C:118:ILE:HD13	1:C:118:ILE:N	2.19	0.55
1:C:249:GLY:O	1:C:253:LEU:HD13	2.06	0.55
1:D:136:ALA:HB3	4:D:4367:HOH:O	2.05	0.55
1:D:269:GLN:O	1:D:271:MET:N	2.39	0.55
1:A:38:ASP:O	1:A:39:LEU:C	2.49	0.55
1:A:172:GLY:HA2	1:A:261:SER:CB	2.35	0.55
1:A:249:GLY:C	4:A:1314:HOH:O	2.41	0.55
1:A:116:ARG:NH2	1:A:145:ASP:OD1	2.38	0.55
1:B:35:PRO:HG2	1:B:71:LYS:NZ	2.21	0.55
1:C:86:ILE:HG22	1:C:87:GLU:N	2.21	0.55
1:D:143:VAL:C	1:D:145:ASP:H	2.13	0.55
1:E:218:LEU:CD2	4:E:5424:HOH:O	2.54	0.55
1:A:194:LYS:C	4:E:5309:HOH:O	2.50	0.55
1:B:198:PRO:HG2	1:B:201:LEU:HB3	1.88	0.55
1:C:45:LEU:HD21	1:C:50:VAL:HB	1.87	0.55
1:C:124:THR:O	1:C:126:VAL:N	2.39	0.55
1:C:218:LEU:CB	2:C:3300:NAI:C5D	2.84	0.55
1:D:57:LYS:HE3	4:D:4376:HOH:O	1.97	0.55
1:D:81:GLU:HB3	1:D:82:ILE:HD12	1.89	0.55
1:D:97:ALA:C	4:D:4333:HOH:O	2.43	0.55
1:D:180:TYR:HD2	4:D:4308:HOH:O	1.88	0.55
1:E:74:ILE:C	1:E:76:PRO:HD2	2.31	0.55
1:E:91:ILE:O	4:E:5344:HOH:O	2.18	0.55
1:B:231:VAL:HB	4:B:2364:HOH:O	2.05	0.55
1:C:53:THR:CG2	1:C:58:GLU:HB2	2.35	0.55
1:D:252:SER:N	4:D:4342:HOH:O	2.39	0.55
1:A:76:PRO:C	1:A:78:ILE:H	2.14	0.55
1:A:230:ASN:ND2	4:A:1317:HOH:O	2.11	0.55
1:A:266:ARG:NH2	4:A:1440:HOH:O	2.36	0.55
1:B:68:LEU:HB3	4:B:2368:HOH:O	2.05	0.55
1:B:102:SER:HA	1:B:105:GLU:CB	2.37	0.55
1:B:220:SER:O	1:B:221:GLU:CB	2.55	0.55
1:E:75:ILE:O	1:E:79:LEU:HG	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125:PRO:O	1:E:129:ARG:O	2.25	0.55
1:A:120:CYS:N	4:A:1372:HOH:O	2.40	0.55
1:C:29:LYS:NZ	4:C:3344:HOH:O	2.25	0.55
1:C:185:LEU:HD21	1:C:210:LEU:HD12	1.88	0.55
1:C:236:GLY:O	1:C:237:ALA:HB3	2.06	0.55
1:C:253:LEU:H	1:C:253:LEU:HD12	1.71	0.55
2:C:3300:NAI:H2N	3:C:3301:GLU:HB3	1.79	0.55
1:D:101:ILE:HD11	1:D:117:VAL:O	2.07	0.55
1:D:128:VAL:O	1:D:129:ARG:CB	2.55	0.55
1:D:170:VAL:O	1:D:170:VAL:HG12	2.07	0.55
1:E:106:LYS:HB2	4:E:5384:HOH:O	2.06	0.55
1:E:170:VAL:O	1:E:170:VAL:HG12	2.06	0.55
1:E:177:GLY:C	4:E:5315:HOH:O	2.47	0.55
1:A:182:PHE:CZ	4:A:1324:HOH:O	2.48	0.55
1:A:219:HIS:O	1:A:220:SER:HB3	2.06	0.55
1:B:251:ARG:O	1:B:252:SER:C	2.50	0.55
1:C:26:ALA:C	1:C:28:HIS:H	2.15	0.55
2:C:3300:NAI:C5N	3:C:3301:GLU:OXT	2.53	0.55
1:D:31:MET:HE2	1:D:62:HIS:CB	2.37	0.55
1:D:62:HIS:CA	4:D:4448:HOH:O	2.53	0.55
1:A:238:THR:C	4:A:1391:HOH:O	2.50	0.55
1:D:183:THR:HG21	4:D:4428:HOH:O	2.07	0.55
1:D:231:VAL:CG1	4:D:4401:HOH:O	2.16	0.55
1:A:221:GLU:N	4:A:1441:HOH:O	2.11	0.55
1:E:101:ILE:O	1:E:105:GLU:HG3	2.06	0.55
1:A:238:THR:OG1	4:A:1320:HOH:O	2.14	0.54
1:D:167:ILE:HG23	4:D:4324:HOH:O	2.06	0.54
1:D:229:ASP:HA	4:D:4310:HOH:O	2.07	0.54
1:E:16:ALA:O	1:E:20:THR:HG23	2.07	0.54
1:E:60:VAL:CG2	1:E:82:ILE:HD12	2.34	0.54
1:B:186:ASP:HB3	4:B:2305:HOH:O	2.06	0.54
1:C:211:LEU:C	1:C:211:LEU:HD13	2.32	0.54
1:D:78:ILE:O	1:D:82:ILE:HD13	2.07	0.54
1:E:128:VAL:O	1:E:129:ARG:C	2.39	0.54
1:B:82:ILE:O	1:B:86:ILE:HG13	2.08	0.54
1:B:129:ARG:O	1:B:157:GLY:HA2	2.07	0.54
1:C:237:ALA:HB2	4:C:3411:HOH:O	1.93	0.54
1:E:126:VAL:HG13	1:E:156:VAL:HG11	1.89	0.54
1:A:94:SER:C	4:A:1321:HOH:O	2.50	0.54
1:A:129:ARG:HA	1:A:156:VAL:O	2.08	0.54
1:A:230:ASN:HB3	4:A:1317:HOH:O	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:VAL:O	1:B:89:ARG:NH2	2.39	0.54
1:B:178:PRO:CG	4:B:2345:HOH:O	2.56	0.54
1:C:87:GLU:N	1:C:90:HIS:HE1	2.06	0.54
1:C:266:ARG:NH2	4:C:3320:HOH:O	2.40	0.54
1:A:16:ALA:C	1:A:48:MET:HE1	2.32	0.54
1:A:133:THR:O	1:A:159:CYS:HA	2.07	0.54
1:B:27:ALA:O	4:B:2378:HOH:O	2.19	0.54
1:C:51:LYS:HD3	1:C:51:LYS:H	1.72	0.54
1:E:9:GLY:O	1:E:12:ALA:HB3	2.06	0.54
1:B:101:ILE:HD12	1:B:138:GLY:HA2	1.89	0.54
1:C:7:GLY:CA	1:C:70:VAL:HG22	2.38	0.54
1:E:68:LEU:HB2	1:E:94:SER:HA	1.90	0.54
1:E:181:ALA:O	1:E:184:ALA:N	2.39	0.54
1:A:99:VAL:HG11	1:A:104:ILE:HD11	1.90	0.54
1:A:266:ARG:NE	4:A:1440:HOH:O	2.35	0.54
1:B:158:PHE:O	4:B:2387:HOH:O	2.18	0.54
1:C:89:ARG:HE	1:C:90:HIS:CD2	2.26	0.54
1:C:93:VAL:HG13	1:C:118:ILE:HD11	1.89	0.54
1:D:39:LEU:HA	4:D:4405:HOH:O	2.06	0.54
1:E:1:MET:HE3	1:E:3:VAL:CG2	2.37	0.54
1:A:91:ILE:H	1:A:91:ILE:HD12	1.72	0.54
1:B:99:VAL:CG2	4:B:2309:HOH:O	2.15	0.54
1:B:238:THR:O	1:B:240:HIS:N	2.41	0.54
1:B:259:GLU:CA	4:B:2307:HOH:O	2.34	0.54
1:C:87:GLU:H	1:C:90:HIS:HE1	1.55	0.54
1:C:91:ILE:N	1:C:91:ILE:HD12	2.23	0.54
1:C:122:THR:CG2	1:C:133:THR:HG22	2.37	0.54
2:C:3300:NAI:C3N	3:C:3301:GLU:CB	2.81	0.54
1:E:105:GLU:CB	4:E:5437:HOH:O	2.56	0.54
1:E:185:LEU:CD1	4:E:5383:HOH:O	2.51	0.54
1:A:178:PRO:CD	4:A:1436:HOH:O	2.32	0.54
1:B:152:LEU:C	4:B:2392:HOH:O	2.47	0.54
1:B:258:VAL:HG13	1:B:259:GLU:H	1.72	0.54
1:D:93:VAL:HG13	4:D:4408:HOH:O	2.07	0.54
1:E:14:ALA:HA	1:E:127:VAL:HG22	1.89	0.54
1:E:82:ILE:O	1:E:85:ASP:N	2.37	0.54
1:E:125:PRO:HG3	4:E:5302:HOH:O	2.07	0.54
1:E:211:LEU:HD12	4:E:5314:HOH:O	2.05	0.54
1:E:218:LEU:HA	4:E:5424:HOH:O	2.08	0.54
1:B:78:ILE:HD12	1:B:78:ILE:N	2.23	0.54
1:B:137:THR:HG21	4:B:2339:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:VAL:HB	1:B:166:LEU:HD12	1.90	0.54
1:B:218:LEU:CD1	2:B:2300:NAI:C5D	2.81	0.54
1:C:49:GLY:N	4:C:3363:HOH:O	2.40	0.54
1:C:164:GLU:HG2	4:C:3372:HOH:O	2.07	0.54
1:D:3:VAL:HG22	1:D:65:VAL:HG13	1.90	0.54
1:E:130:GLU:OE2	2:E:5300:NAI:C1D	2.55	0.54
1:E:169:ALA:N	4:E:5375:HOH:O	2.37	0.54
1:A:100:THR:HG22	1:A:102:SER:N	2.22	0.53
1:B:82:ILE:CG2	1:B:86:ILE:HD11	2.36	0.53
1:B:93:VAL:HG12	1:B:95:CYS:SG	2.48	0.53
1:B:153:LEU:O	1:B:155:SER:N	2.41	0.53
1:C:129:ARG:NH2	2:C:3300:NAI:H2N	2.23	0.53
1:D:31:MET:HE1	4:D:4358:HOH:O	2.07	0.53
1:D:77:PHE:HD1	1:D:77:PHE:H	1.56	0.53
1:D:183:THR:CG2	4:D:4428:HOH:O	2.55	0.53
1:A:101:ILE:HG13	1:A:164:GLU:OE1	2.09	0.53
1:B:91:ILE:HD12	1:B:91:ILE:N	2.24	0.53
1:B:155:SER:C	2:B:2300:NAI:N7N	2.66	0.53
1:C:112:ARG:HH11	1:C:113:PRO:CD	2.09	0.53
1:C:116:ARG:HA	1:C:140:HIS:HB2	1.90	0.53
1:C:122:THR:HG22	1:C:133:THR:HB	1.90	0.53
1:C:134:VAL:CG1	1:C:162:VAL:HG22	2.38	0.53
1:D:242:LEU:O	1:D:243:HIS:C	2.51	0.53
1:A:26:ALA:CB	1:A:29:LYS:HE3	2.38	0.53
1:B:45:LEU:HB3	4:B:2385:HOH:O	2.08	0.53
1:B:158:PHE:CE1	2:B:2300:NAI:C4B	2.82	0.53
1:B:169:ALA:O	1:B:171:THR:N	2.42	0.53
1:C:50:VAL:CG2	4:C:3363:HOH:O	2.55	0.53
1:C:82:ILE:HG22	1:C:86:ILE:CD1	2.36	0.53
1:C:123:ASN:ND2	1:C:132:ALA:HB3	2.20	0.53
1:D:72:PRO:HA	1:D:75:ILE:HD13	1.90	0.53
1:D:134:VAL:CG2	1:D:162:VAL:HB	2.37	0.53
1:A:50:VAL:HG12	1:A:51:LYS:N	2.23	0.53
1:A:255:ILE:CG2	4:A:1335:HOH:O	2.47	0.53
1:C:19:PHE:O	1:C:22:ALA:HB3	2.09	0.53
1:D:57:LYS:CD	4:D:4438:HOH:O	2.55	0.53
1:E:60:VAL:HG21	1:E:82:ILE:CG2	2.37	0.53
1:A:93:VAL:HG22	1:A:118:ILE:HD11	1.91	0.53
1:A:115:PRO:O	1:A:140:HIS:HB2	2.08	0.53
1:B:139:THR:O	1:B:139:THR:HG22	2.09	0.53
1:B:190:ASP:OD2	1:D:228:LYS:NZ	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:GLY:O	1:D:234:PRO:HB3	2.09	0.53
1:B:238:THR:C	1:B:240:HIS:N	2.66	0.53
1:C:180:TYR:CA	4:C:3302:HOH:O	2.20	0.53
1:E:98:GLY:O	4:E:5400:HOH:O	2.19	0.53
1:E:178:PRO:HD3	4:E:5315:HOH:O	2.06	0.53
1:E:269:GLN:OE1	4:E:5400:HOH:O	2.19	0.53
1:C:6:ILE:H	1:C:66:LEU:HD21	1.74	0.53
1:C:108:LEU:C	4:C:3358:HOH:O	2.51	0.53
1:C:257:ALA:C	1:C:259:GLU:H	2.17	0.53
1:D:79:LEU:HD22	1:D:104:ILE:HD13	1.89	0.53
1:E:121:MET:CE	1:E:122:THR:H	2.21	0.53
1:E:231:VAL:HG12	1:E:231:VAL:O	2.08	0.53
1:C:3:VAL:HA	1:C:65:VAL:O	2.08	0.53
1:C:104:ILE:HG22	1:C:117:VAL:HG21	1.90	0.53
1:C:236:GLY:HA2	1:C:239:ILE:HG22	1.91	0.53
1:C:261:SER:CA	4:C:3354:HOH:O	2.21	0.53
1:D:119:ARG:CD	4:D:4422:HOH:O	2.24	0.53
2:D:4300:NAI:C3D	4:D:4410:HOH:O	2.47	0.53
1:E:3:VAL:O	1:E:30:ILE:HA	2.09	0.53
1:A:29:LYS:N	4:A:1329:HOH:O	2.41	0.53
1:A:106:LYS:HB3	4:A:1432:HOH:O	2.09	0.53
1:B:188:LEU:O	1:B:190:ASP:N	2.42	0.53
1:D:31:MET:N	4:D:4365:HOH:O	2.42	0.53
1:A:178:PRO:CG	4:A:1436:HOH:O	2.55	0.53
1:B:45:LEU:HD23	1:B:48:MET:SD	2.48	0.53
1:B:75:ILE:HD12	1:B:75:ILE:N	2.22	0.53
1:B:199:ARG:HD3	4:B:2340:HOH:O	2.08	0.53
1:C:39:LEU:HA	1:C:43:SER:CB	2.39	0.53
1:C:115:PRO:CB	4:C:3358:HOH:O	2.51	0.53
1:C:257:ALA:CA	4:C:3378:HOH:O	2.17	0.53
1:D:229:ASP:CG	4:D:4393:HOH:O	2.49	0.53
1:E:7:GLY:H	1:E:33:SER:HB2	1.73	0.53
1:E:75:ILE:CG2	1:E:104:ILE:HD11	2.39	0.53
1:E:91:ILE:C	4:E:5344:HOH:O	2.50	0.53
1:E:124:THR:N	1:E:125:PRO:HD2	2.24	0.53
1:A:135:TYR:OH	1:A:161:GLU:HG3	2.09	0.53
1:C:261:SER:N	4:C:3391:HOH:O	2.41	0.53
1:D:31:MET:CE	4:D:4358:HOH:O	2.55	0.53
1:E:150:GLU:O	1:E:152:LEU:N	2.41	0.53
1:E:228:LYS:HE3	1:E:242:LEU:HD13	1.91	0.53
1:A:6:ILE:HD11	1:A:66:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:GLY:O	1:A:195:MET:HB2	2.09	0.52
1:B:157:GLY:O	2:B:2300:NAI:C4N	2.56	0.52
2:B:2300:NAI:C3N	3:B:2301:GLU:CB	2.81	0.52
1:C:25:LEU:HD11	1:C:30:ILE:CD1	2.38	0.52
1:E:55:HIS:CB	1:E:57:LYS:HE2	2.38	0.52
1:A:236:GLY:HA2	1:A:239:ILE:HG22	1.91	0.52
1:B:8:ALA:HA	1:B:12:ALA:HB2	1.90	0.52
1:B:94:SER:OG	4:B:2333:HOH:O	2.03	0.52
1:B:130:GLU:OE2	2:B:2300:NAI:H2D	2.09	0.52
1:E:45:LEU:HA	1:E:48:MET:CE	2.39	0.52
1:E:177:GLY:O	1:E:180:TYR:N	2.42	0.52
1:A:-1:ARG:CB	4:A:1342:HOH:O	2.52	0.52
1:A:198:PRO:HG2	1:A:201:LEU:CB	2.40	0.52
1:C:24:VAL:O	1:C:24:VAL:HG12	2.09	0.52
2:C:3300:NAI:O2B	4:C:3408:HOH:O	2.18	0.52
1:D:193:VAL:C	1:D:195:MET:H	2.17	0.52
1:E:112:ARG:NE	4:E:5328:HOH:O	2.41	0.52
1:A:218:LEU:CD2	2:A:1300:NAI:H52A	2.22	0.52
1:B:5:PHE:HZ	1:B:15:LEU:CB	2.15	0.52
1:B:12:ALA:O	1:B:16:ALA:HB2	2.08	0.52
1:B:73:HIS:HB2	4:B:2320:HOH:O	2.09	0.52
1:C:199:ARG:O	1:C:203:VAL:HG23	2.09	0.52
1:D:169:ALA:C	1:D:171:THR:N	2.63	0.52
1:D:266:ARG:C	1:D:268:LEU:N	2.62	0.52
1:E:109:SER:C	1:E:111:PHE:H	2.18	0.52
1:E:185:LEU:HD22	4:E:5408:HOH:O	2.09	0.52
1:A:62:HIS:ND1	1:A:62:HIS:O	2.43	0.52
1:A:242:LEU:O	1:A:243:HIS:C	2.51	0.52
1:A:251:ARG:HG3	4:A:1314:HOH:O	2.08	0.52
1:C:147:ARG:O	1:C:151:GLN:HG3	2.10	0.52
1:D:123:ASN:HB2	1:D:125:PRO:HD2	1.91	0.52
1:D:232:SER:HA	4:D:4343:HOH:O	2.08	0.52
1:E:97:ALA:CB	4:E:5358:HOH:O	2.58	0.52
1:E:206:GLY:C	4:E:5408:HOH:O	2.48	0.52
1:E:221:GLU:HG3	4:E:5350:HOH:O	2.09	0.52
1:A:70:VAL:CG2	1:A:75:ILE:HD12	2.40	0.52
1:A:91:ILE:HD12	1:A:91:ILE:N	2.24	0.52
1:A:143:VAL:O	1:A:143:VAL:HG12	2.09	0.52
1:B:18:GLY:O	1:B:20:THR:N	2.43	0.52
1:C:33:SER:OG	1:C:56:ASN:HA	2.09	0.52
1:D:252:SER:OG	1:D:253:LEU:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3:VAL:HG12	1:E:4:GLY:N	2.23	0.52
1:B:245:LEU:C	1:B:247:SER:H	2.16	0.52
1:B:245:LEU:O	1:B:247:SER:N	2.43	0.52
1:C:158:PHE:CD1	2:C:3300:NAI:H4B	2.44	0.52
1:A:36:ASP:O	1:A:37:MET:CB	2.56	0.52
1:A:256:ASN:HA	4:A:1335:HOH:O	2.10	0.52
2:A:1300:NAI:C4D	4:A:1435:HOH:O	2.58	0.52
1:D:224:PRO:HB2	4:D:4355:HOH:O	2.10	0.52
1:A:32:ALA:O	1:A:52:LEU:HA	2.10	0.52
1:B:13:PHE:HB2	1:B:41:THR:CG2	2.40	0.52
1:E:195:MET:HA	1:E:195:MET:CE	2.35	0.52
1:E:242:LEU:HD11	4:E:5345:HOH:O	2.09	0.52
1:A:6:ILE:CD1	1:A:66:LEU:HD11	2.39	0.52
1:C:169:ALA:CB	4:C:3320:HOH:O	2.55	0.52
1:E:124:THR:C	1:E:126:VAL:H	2.16	0.52
1:E:124:THR:C	1:E:126:VAL:N	2.68	0.52
2:E:5300:NAI:O1N	3:E:5301:GLU:C	2.53	0.52
1:B:75:ILE:CB	1:B:76:PRO:HD3	2.26	0.51
1:B:245:LEU:C	1:B:247:SER:N	2.67	0.51
1:C:218:LEU:HD13	2:C:3300:NAI:C4D	2.39	0.51
1:C:242:LEU:O	1:C:245:LEU:N	2.40	0.51
1:C:251:ARG:C	1:C:252:SER:O	2.53	0.51
1:D:60:VAL:O	1:D:90:HIS:NE2	2.39	0.51
1:D:73:HIS:O	1:D:76:PRO:HD2	2.10	0.51
1:E:206:GLY:O	1:E:209:ALA:HB3	2.10	0.51
1:A:94:SER:CB	4:A:1321:HOH:O	2.58	0.51
1:A:121:MET:HG3	4:A:1402:HOH:O	2.09	0.51
1:A:191:GLY:CA	4:A:1420:HOH:O	2.24	0.51
1:B:118:ILE:HG21	1:B:149:MET:SD	2.50	0.51
1:B:156:VAL:O	1:B:156:VAL:HG12	2.11	0.51
1:C:61:GLN:C	1:C:63:SER:N	2.66	0.51
1:C:122:THR:CG2	4:C:3317:HOH:O	2.50	0.51
1:C:266:ARG:N	4:C:3340:HOH:O	2.42	0.51
1:D:141:ALA:CB	4:D:4386:HOH:O	2.57	0.51
1:E:46:ARG:C	1:E:48:MET:H	2.17	0.51
1:A:79:LEU:CD1	1:A:104:ILE:HG23	2.40	0.51
1:A:239:ILE:C	4:A:1352:HOH:O	2.52	0.51
1:B:158:PHE:CE1	2:B:2300:NAI:O1A	2.64	0.51
1:B:159:CYS:CA	4:B:2311:HOH:O	2.56	0.51
1:C:15:LEU:HD12	4:C:3348:HOH:O	2.01	0.51
1:C:29:LYS:HG3	4:C:3306:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:THR:HG22	1:C:101:ILE:N	2.25	0.51
1:C:251:ARG:HD2	4:C:3376:HOH:O	2.09	0.51
1:D:166:LEU:O	1:D:168:ASP:N	2.44	0.51
1:E:218:LEU:CA	4:E:5424:HOH:O	2.57	0.51
1:A:11:LEU:O	1:A:11:LEU:HD23	2.10	0.51
1:B:2:SER:OG	1:B:30:ILE:HA	2.10	0.51
1:B:29:LYS:C	1:B:30:ILE:HG13	2.35	0.51
1:B:153:LEU:C	1:B:155:SER:N	2.69	0.51
1:C:7:GLY:HA3	1:C:69:ALA:C	2.35	0.51
1:C:61:GLN:C	1:C:63:SER:H	2.19	0.51
1:D:179:ALA:C	4:D:4308:HOH:O	2.49	0.51
1:D:191:GLY:O	1:D:192:GLY:C	2.53	0.51
1:E:34:SER:HB3	1:E:54:PRO:HA	1.91	0.51
1:E:136:ALA:CB	4:E:5434:HOH:O	2.58	0.51
1:B:73:HIS:C	1:B:75:ILE:H	2.19	0.51
1:B:168:ASP:HB2	4:B:2357:HOH:O	2.06	0.51
1:C:52:LEU:C	1:C:52:LEU:HD23	2.35	0.51
1:C:223:HIS:C	4:C:3417:HOH:O	2.54	0.51
1:D:143:VAL:C	1:D:145:ASP:N	2.67	0.51
1:D:228:LYS:HB2	4:D:4397:HOH:O	2.11	0.51
1:E:39:LEU:HA	1:E:43:SER:HB2	1.93	0.51
1:E:94:SER:HB3	4:E:5325:HOH:O	2.09	0.51
1:E:136:ALA:HB2	1:E:167:ILE:HD11	1.93	0.51
1:E:262:CYS:HB3	4:E:5342:HOH:O	2.06	0.51
2:B:2300:NAI:H2A	4:B:2380:HOH:O	2.09	0.51
1:E:89:ARG:HG2	1:E:89:ARG:HH11	1.76	0.51
1:E:225:GLY:HA3	4:E:5353:HOH:O	1.98	0.51
1:A:141:ALA:CA	4:A:1390:HOH:O	2.04	0.51
1:B:9:GLY:O	1:B:41:THR:HG21	2.11	0.51
1:B:140:HIS:O	1:B:141:ALA:HB2	2.11	0.51
1:E:118:ILE:N	1:E:118:ILE:HD12	2.26	0.51
1:E:168:ASP:HB2	4:E:5349:HOH:O	2.10	0.51
1:A:30:ILE:HG22	1:A:31:MET:N	2.26	0.51
1:A:163:GLU:O	1:A:165:ASP:N	2.43	0.51
1:B:7:GLY:HA3	1:B:69:ALA:C	2.35	0.51
1:B:188:LEU:O	4:B:2302:HOH:O	2.19	0.51
1:C:51:LYS:H	1:C:51:LYS:HZ2	1.58	0.51
1:C:86:ILE:HB	1:C:112:ARG:HB2	1.93	0.51
1:C:122:THR:CA	4:C:3331:HOH:O	2.51	0.51
1:E:114:ALA:N	4:E:5367:HOH:O	2.39	0.51
1:A:236:GLY:O	1:A:237:ALA:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:LEU:HD12	1:C:14:ALA:HB3	1.92	0.51
1:C:218:LEU:CD1	2:C:3300:NAI:H51N	2.40	0.51
1:C:237:ALA:HB3	4:C:3406:HOH:O	2.11	0.51
1:D:75:ILE:HB	1:D:76:PRO:HD3	1.92	0.51
1:D:224:PRO:CB	4:D:4355:HOH:O	2.58	0.51
1:D:266:ARG:NH1	4:D:4442:HOH:O	2.01	0.51
1:A:193:VAL:C	1:A:195:MET:N	2.68	0.51
1:A:219:HIS:NE2	2:A:1300:NAI:H51N	2.25	0.51
1:C:45:LEU:HD23	1:C:45:LEU:C	2.36	0.51
1:C:269:GLN:HG3	1:C:270:SER:H	1.76	0.51
1:A:121:MET:CG	1:A:171:THR:HG23	2.41	0.50
1:A:156:VAL:CG1	1:A:156:VAL:O	2.59	0.50
1:C:193:VAL:C	4:C:3309:HOH:O	2.54	0.50
1:C:255:ILE:CA	4:C:3332:HOH:O	2.53	0.50
1:C:270:SER:O	1:C:274:GLN:HB2	2.10	0.50
1:D:215:LYS:HG3	1:D:219:HIS:CE1	2.46	0.50
1:E:175:GLY:C	4:E:5333:HOH:O	2.54	0.50
1:A:60:VAL:HG21	1:A:82:ILE:HG23	1.92	0.50
1:C:185:LEU:HD22	4:C:3324:HOH:O	2.07	0.50
1:E:102:SER:CB	4:E:5347:HOH:O	2.52	0.50
1:E:158:PHE:CD2	2:E:5300:NAI:O3B	2.64	0.50
1:B:215:LYS:HE3	4:B:2377:HOH:O	2.12	0.50
1:C:149:MET:C	1:C:151:GLN:H	2.18	0.50
1:A:6:ILE:HD11	1:A:60:VAL:HG22	1.93	0.50
1:C:218:LEU:CG	2:C:3300:NAI:H52N	2.40	0.50
1:D:123:ASN:HB2	4:D:4312:HOH:O	2.11	0.50
1:E:112:ARG:CG	4:E:5328:HOH:O	2.36	0.50
1:E:132:ALA:CB	4:E:5391:HOH:O	2.41	0.50
1:A:11:LEU:CB	4:A:1389:HOH:O	2.15	0.50
1:D:73:HIS:CE1	1:D:74:ILE:HG12	2.46	0.50
1:D:251:ARG:HG2	1:D:251:ARG:HH11	1.77	0.50
1:E:36:ASP:O	1:E:37:MET:HE2	2.12	0.50
1:A:112:ARG:CD	4:A:1365:HOH:O	2.57	0.50
1:A:238:THR:C	1:A:240:HIS:N	2.65	0.50
1:B:180:TYR:O	1:B:183:THR:HB	2.11	0.50
1:C:9:GLY:O	1:C:10:GLN:C	2.55	0.50
1:D:101:ILE:HG22	1:D:102:SER:N	2.26	0.50
1:A:174:SER:HB2	4:A:1339:HOH:O	2.08	0.50
1:A:269:GLN:C	1:A:271:MET:N	2.70	0.50
1:B:123:ASN:O	1:B:126:VAL:HG23	2.12	0.50
1:C:126:VAL:C	1:C:128:VAL:N	2.67	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:THR:CG2	1:C:161:GLU:N	2.74	0.50
1:D:135:TYR:CE1	4:D:4398:HOH:O	2.27	0.50
1:A:115:PRO:HD2	1:A:140:HIS:HD2	1.75	0.50
1:A:134:VAL:HG13	1:A:162:VAL:CG2	2.42	0.50
1:A:189:ALA:O	1:A:190:ASP:C	2.54	0.50
1:B:79:LEU:HD12	1:B:107:LYS:HD3	1.94	0.50
1:B:124:THR:C	1:B:126:VAL:H	2.20	0.50
1:B:233:SER:O	1:B:234:PRO:C	2.54	0.50
1:C:176:SER:O	1:C:177:GLY:C	2.53	0.50
1:D:30:ILE:HG12	4:D:4425:HOH:O	2.11	0.50
1:E:25:LEU:N	1:E:25:LEU:HD23	2.26	0.50
1:E:28:HIS:C	1:E:28:HIS:CD2	2.88	0.50
1:A:130:GLU:OE2	2:A:1300:NAI:C2D	2.60	0.50
1:C:187:ALA:O	1:C:188:LEU:C	2.55	0.50
1:C:187:ALA:O	1:C:190:ASP:HB2	2.12	0.50
1:C:274:GLN:O	1:C:274:GLN:HG2	2.12	0.50
1:D:257:ALA:O	1:D:258:VAL:C	2.55	0.50
1:E:45:LEU:HD23	1:E:48:MET:CE	2.42	0.50
1:E:198:PRO:HD2	1:E:201:LEU:HD23	1.93	0.50
1:A:45:LEU:HD21	4:A:1387:HOH:O	2.10	0.49
1:A:123:ASN:HB2	4:A:1436:HOH:O	2.12	0.49
1:A:253:LEU:CD2	4:A:1405:HOH:O	2.54	0.49
1:B:25:LEU:HD22	1:B:30:ILE:HD11	1.93	0.49
1:B:264:ARG:O	1:B:264:ARG:HD2	2.11	0.49
1:C:82:ILE:HA	1:C:85:ASP:HB2	1.93	0.49
1:D:124:THR:O	1:D:126:VAL:N	2.45	0.49
1:E:19:PHE:CE2	1:E:152:LEU:HG	2.47	0.49
1:A:13:PHE:N	4:A:1379:HOH:O	2.45	0.49
1:A:16:ALA:O	1:A:48:MET:HE1	2.12	0.49
1:A:29:LYS:HG3	4:A:1329:HOH:O	2.11	0.49
1:B:18:GLY:O	1:B:19:PHE:C	2.55	0.49
1:B:91:ILE:HD12	1:B:91:ILE:H	1.77	0.49
1:B:100:THR:CG2	1:B:101:ILE:N	2.76	0.49
1:D:97:ALA:HA	4:D:4435:HOH:O	2.11	0.49
1:E:70:VAL:CA	4:E:5305:HOH:O	2.56	0.49
1:B:58:GLU:O	1:B:61:GLN:HG3	2.12	0.49
1:B:135:TYR:O	1:B:161:GLU:HB2	2.13	0.49
1:C:79:LEU:O	4:C:3329:HOH:O	2.20	0.49
1:E:98:GLY:HA2	4:E:5400:HOH:O	2.10	0.49
1:E:129:ARG:C	4:E:5401:HOH:O	2.49	0.49
1:E:232:SER:OG	1:E:239:ILE:HB	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:262:CYS:O	1:E:263:ILE:C	2.54	0.49
2:A:1300:NAI:H52N	4:A:1435:HOH:O	2.12	0.49
1:B:147:ARG:HG3	1:B:147:ARG:O	2.11	0.49
1:B:236:GLY:C	1:B:238:THR:H	2.20	0.49
1:C:74:ILE:O	1:C:74:ILE:HG22	2.12	0.49
1:C:115:PRO:CG	4:C:3358:HOH:O	2.57	0.49
1:C:197:LEU:CG	4:C:3367:HOH:O	2.60	0.49
1:E:13:PHE:CZ	4:E:5306:HOH:O	2.66	0.49
1:E:46:ARG:C	1:E:48:MET:N	2.70	0.49
1:E:95:CYS:N	4:E:5423:HOH:O	2.42	0.49
1:E:134:VAL:CG1	1:E:162:VAL:HB	2.42	0.49
1:E:228:LYS:O	4:E:5337:HOH:O	2.19	0.49
1:A:236:GLY:C	4:A:1391:HOH:O	2.54	0.49
1:B:74:ILE:HD11	1:B:96:ALA:HB3	1.94	0.49
1:B:100:THR:CG2	1:B:101:ILE:H	2.24	0.49
1:A:6:ILE:HD13	1:A:59:THR:CG2	2.43	0.49
1:A:31:MET:HA	1:A:51:LYS:O	2.12	0.49
1:C:9:GLY:O	1:C:12:ALA:HB3	2.13	0.49
1:C:45:LEU:CD2	1:C:50:VAL:HB	2.42	0.49
1:C:104:ILE:HG21	1:C:117:VAL:HG11	1.94	0.49
1:D:222:GLN:O	1:D:223:HIS:HB3	2.12	0.49
1:A:117:VAL:HG12	4:A:1343:HOH:O	2.11	0.49
1:A:178:PRO:CB	4:A:1324:HOH:O	2.61	0.49
1:D:58:GLU:CB	4:D:4358:HOH:O	2.57	0.49
1:D:70:VAL:HG12	1:D:74:ILE:HB	1.95	0.49
1:E:70:VAL:O	1:E:70:VAL:HG12	2.13	0.49
1:E:150:GLU:O	1:E:151:GLN:C	2.56	0.49
1:E:190:ASP:HB2	4:E:5381:HOH:O	2.12	0.49
1:A:172:GLY:C	4:A:1302:HOH:O	2.55	0.49
1:B:83:GLY:C	1:B:85:ASP:H	2.19	0.49
1:B:160:THR:HA	4:B:2312:HOH:O	2.12	0.49
1:B:194:LYS:HG2	1:B:195:MET:HE3	1.94	0.49
1:D:30:ILE:C	4:D:4365:HOH:O	2.56	0.49
1:E:36:ASP:OD1	1:E:37:MET:N	2.46	0.49
1:E:121:MET:HE3	1:E:122:THR:H	1.78	0.49
1:E:222:GLN:O	1:E:223:HIS:HB2	2.12	0.49
1:E:236:GLY:HA2	1:E:239:ILE:HG22	1.93	0.49
1:B:71:LYS:H	1:B:71:LYS:HD2	1.76	0.49
1:C:72:PRO:HG2	1:C:97:ALA:O	2.13	0.49
1:C:75:ILE:N	1:C:76:PRO:CD	2.75	0.49
1:D:112:ARG:C	4:D:4329:HOH:O	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:124:THR:O	1:E:126:VAL:N	2.45	0.49
1:A:41:THR:O	1:A:44:ALA:HB3	2.12	0.49
1:B:105:GLU:OE1	1:B:105:GLU:HA	2.13	0.49
1:B:195:MET:CA	1:B:195:MET:CE	2.88	0.49
1:C:119:ARG:NE	4:C:3345:HOH:O	2.46	0.49
1:C:240:HIS:N	4:C:3398:HOH:O	2.34	0.49
1:D:68:LEU:HD12	1:D:94:SER:HB2	1.94	0.49
1:D:121:MET:CE	1:D:171:THR:HG23	2.42	0.49
1:A:101:ILE:CG1	1:A:119:ARG:HB2	2.43	0.48
1:A:211:LEU:CD1	1:A:211:LEU:C	2.86	0.48
1:B:79:LEU:HD22	1:B:104:ILE:HG23	1.95	0.48
1:B:137:THR:CG2	4:B:2339:HOH:O	2.59	0.48
1:C:26:ALA:O	1:C:28:HIS:N	2.46	0.48
1:D:93:VAL:CG1	1:D:149:MET:HE1	2.43	0.48
2:D:4300:NAI:C3N	4:D:4413:HOH:O	2.61	0.48
2:D:4300:NAI:H2N	4:D:4436:HOH:O	2.11	0.48
1:E:113:PRO:HD2	4:E:5328:HOH:O	2.12	0.48
1:E:251:ARG:NH2	4:E:5366:HOH:O	2.45	0.48
1:E:264:ARG:O	1:E:265:THR:C	2.55	0.48
1:A:28:HIS:C	4:A:1329:HOH:O	2.56	0.48
1:A:31:MET:HE3	1:A:51:LYS:HB3	1.96	0.48
1:A:45:LEU:CD2	4:A:1387:HOH:O	2.60	0.48
1:A:171:THR:N	4:A:1402:HOH:O	2.34	0.48
1:B:75:ILE:HB	1:B:76:PRO:CD	2.27	0.48
1:B:134:VAL:HG13	1:B:160:THR:O	2.12	0.48
1:D:231:VAL:HG12	1:D:231:VAL:O	2.13	0.48
1:D:249:GLY:O	1:D:250:PHE:C	2.56	0.48
2:E:5300:NAI:N1N	3:E:5301:GLU:N	2.61	0.48
1:A:121:MET:HE2	1:A:121:MET:HA	1.95	0.48
1:A:178:PRO:HG2	4:A:1436:HOH:O	2.13	0.48
1:B:74:ILE:HD11	1:B:96:ALA:CB	2.43	0.48
1:D:31:MET:HE3	1:D:58:GLU:HB3	1.96	0.48
1:A:169:ALA:O	1:A:170:VAL:C	2.57	0.48
1:B:122:THR:CG2	1:B:133:THR:HB	2.40	0.48
1:C:3:VAL:O	1:C:30:ILE:HG13	2.12	0.48
1:C:140:HIS:CB	4:C:3385:HOH:O	2.56	0.48
1:C:147:ARG:HG2	1:C:151:GLN:OE1	2.13	0.48
1:D:22:ALA:HA	1:D:129:ARG:CZ	2.44	0.48
1:D:80:ASP:OD2	1:D:107:LYS:NZ	2.45	0.48
1:E:211:LEU:C	4:E:5314:HOH:O	2.55	0.48
1:E:221:GLU:N	4:E:5350:HOH:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:ALA:HA	1:A:127:VAL:HG22	1.94	0.48
1:C:122:THR:HG22	1:C:133:THR:CB	2.43	0.48
1:C:233:SER:O	1:C:234:PRO:C	2.56	0.48
1:D:118:ILE:CG1	4:D:4408:HOH:O	2.57	0.48
1:D:231:VAL:CG2	4:D:4402:HOH:O	2.61	0.48
1:E:45:LEU:HA	1:E:48:MET:HE3	1.94	0.48
1:A:42:VAL:CG2	4:A:1349:HOH:O	2.05	0.48
1:A:211:LEU:C	1:A:211:LEU:HD12	2.39	0.48
1:C:150:GLU:C	1:C:154:SER:HB2	2.38	0.48
1:C:222:GLN:CA	4:C:3304:HOH:O	2.56	0.48
1:D:193:VAL:C	1:D:195:MET:N	2.71	0.48
1:E:41:THR:O	1:E:42:VAL:C	2.57	0.48
1:E:68:LEU:HD12	1:E:94:SER:HB2	1.96	0.48
1:A:6:ILE:HG22	1:A:6:ILE:O	2.13	0.48
1:B:180:TYR:CD2	1:B:180:TYR:N	2.77	0.48
1:B:221:GLU:HB2	4:B:2322:HOH:O	2.13	0.48
1:B:231:VAL:O	1:B:231:VAL:HG12	2.12	0.48
1:C:3:VAL:C	4:C:3356:HOH:O	2.49	0.48
1:C:7:GLY:HA3	1:C:69:ALA:O	2.12	0.48
1:C:72:PRO:HA	1:C:75:ILE:HG13	1.95	0.48
1:C:112:ARG:CG	1:C:113:PRO:HD2	2.34	0.48
1:D:60:VAL:HG21	1:D:82:ILE:CG2	2.39	0.48
1:D:223:HIS:ND1	1:D:224:PRO:HD2	2.29	0.48
1:E:46:ARG:HG3	1:E:46:ARG:NH1	2.28	0.48
1:E:187:ALA:CB	4:E:5363:HOH:O	2.34	0.48
1:A:194:LYS:HA	4:E:5309:HOH:O	2.13	0.48
1:A:222:GLN:O	1:A:223:HIS:HB3	2.13	0.48
1:B:178:PRO:HD2	4:B:2345:HOH:O	2.13	0.48
1:C:27:ALA:CB	4:C:3363:HOH:O	2.58	0.48
1:C:33:SER:HA	1:C:53:THR:O	2.14	0.48
1:D:15:LEU:HA	1:D:126:VAL:HG11	1.96	0.48
1:E:106:LYS:CG	4:E:5398:HOH:O	2.62	0.48
1:E:112:ARG:CD	4:E:5328:HOH:O	2.62	0.48
1:E:123:ASN:CB	4:E:5310:HOH:O	2.59	0.48
1:E:134:VAL:HG21	1:E:170:VAL:HG11	1.96	0.48
1:E:199:ARG:NE	4:E:5346:HOH:O	2.26	0.48
1:E:212:GLY:O	1:E:213:ALA:C	2.56	0.48
1:A:28:HIS:N	4:A:1382:HOH:O	2.47	0.48
1:A:112:ARG:HG2	4:A:1392:HOH:O	2.13	0.48
1:C:83:GLY:CA	4:C:3329:HOH:O	2.60	0.48
1:D:161:GLU:HG3	4:D:4394:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:HIS:HB3	1:E:57:LYS:HG2	1.95	0.48
1:E:179:ALA:CB	4:E:5322:HOH:O	2.51	0.48
1:E:191:GLY:O	1:E:192:GLY:C	2.56	0.48
1:A:240:HIS:HD2	4:A:1352:HOH:O	1.95	0.48
1:B:112:ARG:HG3	1:B:113:PRO:HD2	1.95	0.48
1:B:124:THR:O	1:B:126:VAL:N	2.47	0.48
1:B:188:LEU:C	1:B:190:ASP:N	2.71	0.48
1:C:29:LYS:HB2	1:C:30:ILE:HD12	1.96	0.48
1:C:39:LEU:HA	1:C:43:SER:HB3	1.96	0.48
1:C:275:GLU:C	4:C:3393:HOH:O	2.56	0.48
1:E:91:ILE:CG2	1:E:118:ILE:HD13	2.44	0.48
1:E:193:VAL:HG21	1:E:199:ARG:HD2	1.96	0.48
1:E:223:HIS:O	1:E:224:PRO:C	2.57	0.48
1:B:84:ALA:H	1:B:111:PHE:HD2	1.62	0.47
1:B:101:ILE:HG12	1:B:164:GLU:OE1	2.14	0.47
1:B:147:ARG:HG3	1:B:151:GLN:HE21	1.79	0.47
1:C:25:LEU:HD21	1:C:30:ILE:CD1	2.44	0.47
1:C:134:VAL:HG11	1:C:162:VAL:HG22	1.95	0.47
1:C:240:HIS:CE1	1:D:194:LYS:HE2	2.49	0.47
1:D:119:ARG:NH1	4:D:4422:HOH:O	2.46	0.47
1:D:228:LYS:HG2	4:D:4310:HOH:O	2.13	0.47
1:D:262:CYS:O	4:D:4360:HOH:O	2.20	0.47
1:E:123:ASN:HB2	1:E:125:PRO:HD2	1.96	0.47
1:E:136:ALA:C	4:E:5434:HOH:O	2.55	0.47
1:A:64:ASP:O	1:A:90:HIS:CB	2.62	0.47
1:C:82:ILE:O	1:C:86:ILE:HG12	2.14	0.47
1:E:118:ILE:HG21	1:E:149:MET:HG2	1.96	0.47
1:A:123:ASN:H	1:A:123:ASN:HD22	1.62	0.47
1:B:115:PRO:CG	4:B:2328:HOH:O	2.61	0.47
1:B:194:LYS:HZ2	1:D:240:HIS:CE1	2.32	0.47
1:B:216:MET:HE1	4:B:2315:HOH:O	2.13	0.47
1:D:79:LEU:HD21	1:D:104:ILE:HA	1.95	0.47
1:D:184:ALA:CA	4:D:4340:HOH:O	2.63	0.47
1:E:46:ARG:HG3	1:E:46:ARG:HH11	1.79	0.47
1:E:226:GLN:HA	1:E:226:GLN:NE2	2.29	0.47
1:C:8:ALA:HB3	1:C:34:SER:HB2	1.96	0.47
1:C:199:ARG:HD2	4:C:3392:HOH:O	2.05	0.47
1:D:70:VAL:O	1:D:75:ILE:HD11	2.15	0.47
1:D:146:GLY:O	1:D:149:MET:HB3	2.14	0.47
1:E:15:LEU:HB3	1:E:19:PHE:CE1	2.50	0.47
1:A:82:ILE:CA	4:A:1437:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:VAL:HG12	1:A:167:ILE:CD1	2.44	0.47
1:B:154:SER:C	2:B:2300:NAI:N7N	2.66	0.47
1:C:89:ARG:NE	1:C:90:HIS:CD2	2.82	0.47
1:C:124:THR:C	1:C:126:VAL:N	2.71	0.47
1:D:172:GLY:HA2	1:D:261:SER:OG	2.14	0.47
1:E:67:PHE:HA	1:E:93:VAL:O	2.14	0.47
1:E:112:ARG:N	4:E:5422:HOH:O	2.47	0.47
1:E:184:ALA:N	4:E:5370:HOH:O	2.47	0.47
1:A:13:PHE:CB	4:A:1379:HOH:O	2.53	0.47
1:A:82:ILE:O	1:A:85:ASP:N	2.48	0.47
1:D:88:ASP:CB	4:D:4432:HOH:O	2.60	0.47
1:E:123:ASN:O	1:E:126:VAL:HB	2.15	0.47
1:A:4:GLY:HA2	1:A:31:MET:O	2.15	0.47
1:A:75:ILE:HG22	1:A:76:PRO:N	2.29	0.47
1:B:2:SER:O	1:B:3:VAL:HG23	2.15	0.47
1:B:172:GLY:O	1:B:258:VAL:HA	2.13	0.47
1:B:236:GLY:CA	4:B:2318:HOH:O	2.48	0.47
1:C:3:VAL:HG12	1:C:4:GLY:N	2.30	0.47
1:C:101:ILE:HD11	4:C:3394:HOH:O	2.14	0.47
1:C:218:LEU:CD2	2:C:3300:NAI:H52A	2.45	0.47
1:D:34:SER:HB2	1:D:36:ASP:O	2.14	0.47
1:D:109:SER:C	1:D:111:PHE:H	2.22	0.47
1:D:111:PHE:O	1:D:112:ARG:C	2.57	0.47
1:D:115:PRO:CA	4:D:4374:HOH:O	2.52	0.47
1:D:142:GLN:C	1:D:145:ASP:HB2	2.40	0.47
1:D:217:LEU:CD1	4:D:4372:HOH:O	2.26	0.47
1:D:251:ARG:CB	4:D:4342:HOH:O	2.28	0.47
1:E:82:ILE:HG22	1:E:86:ILE:HG13	1.97	0.47
1:E:259:GLU:O	1:E:260:ALA:C	2.57	0.47
1:A:11:LEU:N	4:A:1389:HOH:O	2.35	0.47
1:B:241:ALA:N	4:B:2329:HOH:O	2.47	0.47
1:C:50:VAL:HG23	4:C:3363:HOH:O	2.14	0.47
1:C:168:ASP:HB2	1:C:266:ARG:NH1	2.30	0.47
1:D:88:ASP:HB3	4:D:4432:HOH:O	2.14	0.47
1:D:238:THR:HG22	1:D:239:ILE:N	2.30	0.47
1:D:269:GLN:C	1:D:271:MET:N	2.70	0.47
1:E:111:PHE:O	1:E:112:ARG:C	2.56	0.47
1:E:158:PHE:CA	4:E:5425:HOH:O	2.23	0.47
1:A:55:HIS:O	1:A:57:LYS:N	2.40	0.47
1:B:158:PHE:CE2	2:B:2300:NAI:H4B	2.43	0.47
1:C:168:ASP:HB2	1:C:266:ARG:HH12	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:VAL:O	1:C:231:VAL:CG1	2.62	0.47
1:D:28:HIS:C	1:D:28:HIS:CD2	2.93	0.47
1:D:156:VAL:HG12	4:D:4331:HOH:O	2.15	0.47
1:E:95:CYS:CA	4:E:5423:HOH:O	2.63	0.47
1:E:123:ASN:CA	4:E:5310:HOH:O	2.63	0.47
1:A:45:LEU:HB2	1:A:52:LEU:HD11	1.96	0.47
1:A:109:SER:C	1:A:111:PHE:H	2.23	0.47
1:A:264:ARG:CZ	4:A:1322:HOH:O	2.59	0.47
1:B:37:MET:HE2	4:B:2393:HOH:O	2.13	0.47
1:C:128:VAL:CG1	1:C:129:ARG:N	2.78	0.47
1:C:203:VAL:C	4:C:3355:HOH:O	2.54	0.47
1:D:37:MET:HE3	1:D:42:VAL:CG1	2.45	0.47
1:D:185:LEU:HD21	1:D:210:LEU:CD1	2.42	0.47
1:E:162:VAL:HG11	1:E:166:LEU:HB2	1.95	0.47
1:E:243:HIS:ND1	4:E:5357:HOH:O	2.35	0.47
1:A:55:HIS:C	1:A:57:LYS:N	2.69	0.46
1:A:128:VAL:HG12	1:A:129:ARG:N	2.30	0.46
1:B:115:PRO:HD3	4:B:2328:HOH:O	2.13	0.46
1:B:129:ARG:NH1	2:B:2300:NAI:C2D	2.77	0.46
1:B:169:ALA:C	1:B:171:THR:N	2.70	0.46
1:C:53:THR:HG23	1:C:58:GLU:OE2	2.15	0.46
1:C:57:LYS:C	4:C:3383:HOH:O	2.58	0.46
1:C:143:VAL:O	1:C:143:VAL:HG12	2.15	0.46
1:D:266:ARG:HD2	4:D:4311:HOH:O	2.13	0.46
1:E:79:LEU:HD21	1:E:104:ILE:HG12	1.96	0.46
1:E:87:GLU:O	1:E:89:ARG:N	2.49	0.46
1:A:111:PHE:N	1:A:111:PHE:CD1	2.84	0.46
1:B:112:ARG:CD	1:B:113:PRO:HD2	2.45	0.46
1:B:143:VAL:HG12	1:B:144:GLU:N	2.30	0.46
1:C:28:HIS:HB2	4:C:3404:HOH:O	2.15	0.46
1:C:169:ALA:O	1:C:172:GLY:N	2.38	0.46
1:C:233:SER:N	4:C:3374:HOH:O	2.47	0.46
1:C:269:GLN:HG3	1:C:270:SER:N	2.30	0.46
1:D:39:LEU:O	1:D:40:ALA:O	2.34	0.46
1:E:113:PRO:CD	4:E:5367:HOH:O	2.60	0.46
1:B:105:GLU:OE2	1:B:139:THR:HB	2.15	0.46
1:B:119:ARG:HD3	1:B:167:ILE:HD13	1.98	0.46
2:B:2300:NAI:O4D	2:B:2300:NAI:O3	2.34	0.46
1:D:98:GLY:O	1:D:99:VAL:C	2.58	0.46
1:E:73:HIS:HB3	4:E:5415:HOH:O	2.08	0.46
1:E:75:ILE:N	1:E:76:PRO:CD	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ALA:HB3	1:A:29:LYS:HE3	1.97	0.46
1:B:101:ILE:HG23	1:B:164:GLU:CD	2.41	0.46
1:B:105:GLU:HG2	1:B:139:THR:OG1	2.15	0.46
1:C:6:ILE:HG21	1:C:78:ILE:HG21	1.96	0.46
1:D:246:GLU:CD	4:D:4383:HOH:O	2.56	0.46
1:D:265:THR:CG2	4:D:4360:HOH:O	2.51	0.46
1:B:70:VAL:CB	4:B:2368:HOH:O	2.63	0.46
1:C:240:HIS:CB	4:C:3398:HOH:O	2.52	0.46
1:D:17:LYS:HD2	1:D:127:VAL:CG1	2.45	0.46
1:D:70:VAL:HG12	1:D:71:LYS:N	2.31	0.46
1:D:112:ARG:HB3	4:D:4347:HOH:O	2.14	0.46
1:E:97:ALA:N	4:E:5358:HOH:O	2.23	0.46
1:E:218:LEU:HD23	4:E:5424:HOH:O	2.15	0.46
1:A:62:HIS:HE1	4:A:1334:HOH:O	1.98	0.46
1:A:160:THR:HG22	1:A:161:GLU:O	2.15	0.46
1:B:42:VAL:C	1:B:44:ALA:H	2.23	0.46
1:C:109:SER:OG	1:C:115:PRO:HD2	2.16	0.46
1:C:112:ARG:HG3	1:C:112:ARG:NH1	2.30	0.46
1:D:114:ALA:HB1	1:D:140:HIS:CG	2.51	0.46
1:D:166:LEU:O	1:D:167:ILE:C	2.59	0.46
1:E:229:ASP:N	4:E:5337:HOH:O	2.43	0.46
2:E:5300:NAI:C6N	4:E:5402:HOH:O	2.64	0.46
1:A:62:HIS:CE1	4:A:1334:HOH:O	2.69	0.46
1:B:52:LEU:O	1:B:54:PRO:HD3	2.16	0.46
1:B:218:LEU:CD2	2:B:2300:NAI:C5B	2.93	0.46
1:C:121:MET:CB	4:C:3327:HOH:O	2.64	0.46
1:D:220:SER:C	1:D:222:GLN:H	2.24	0.46
1:E:106:LYS:HG2	4:E:5398:HOH:O	2.15	0.46
1:E:115:PRO:O	1:E:140:HIS:HB2	2.16	0.46
1:A:263:ILE:CD1	1:A:263:ILE:N	2.78	0.46
1:B:36:ASP:O	1:B:37:MET:HB2	2.15	0.46
1:B:229:ASP:C	1:B:231:VAL:H	2.23	0.46
1:C:253:LEU:HD12	1:C:253:LEU:N	2.30	0.46
1:D:210:LEU:O	1:D:211:LEU:C	2.58	0.46
1:E:33:SER:O	1:E:35:PRO:CD	2.64	0.46
1:E:62:HIS:CE1	4:E:5387:HOH:O	2.69	0.46
1:A:79:LEU:HD22	1:A:108:LEU:HD13	1.96	0.46
1:B:6:ILE:CD1	1:B:56:ASN:O	2.60	0.46
1:C:163:GLU:HB2	1:C:165:ASP:OD2	2.16	0.46
1:C:252:SER:O	1:C:253:LEU:C	2.58	0.46
1:E:121:MET:CE	1:E:122:THR:N	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:135:TYR:CZ	1:E:161:GLU:HB3	2.51	0.46
1:E:215:LYS:O	1:E:219:HIS:HD2	1.99	0.46
1:A:132:ALA:HB3	4:A:1339:HOH:O	2.16	0.45
1:A:178:PRO:HB3	4:A:1324:HOH:O	2.14	0.45
1:C:178:PRO:N	4:C:3396:HOH:O	2.49	0.45
1:C:218:LEU:HD22	2:C:3300:NAI:O5B	2.16	0.45
1:D:29:LYS:O	1:D:30:ILE:HD13	2.16	0.45
2:D:4300:NAI:O4D	2:D:4300:NAI:O3	2.34	0.45
1:E:126:VAL:O	1:E:156:VAL:CG1	2.65	0.45
1:E:143:VAL:HG12	1:E:143:VAL:O	2.16	0.45
1:A:33:SER:HA	1:A:53:THR:O	2.16	0.45
1:B:241:ALA:O	1:B:242:LEU:C	2.57	0.45
2:C:3300:NAI:O4D	2:C:3300:NAI:O3	2.34	0.45
1:E:89:ARG:HG3	1:E:90:HIS:N	2.30	0.45
1:A:27:ALA:HB1	1:A:49:GLY:HA3	1.99	0.45
1:A:136:ALA:CA	4:A:1404:HOH:O	2.63	0.45
1:B:15:LEU:O	1:B:19:PHE:CE1	2.69	0.45
1:B:16:ALA:C	1:B:18:GLY:N	2.72	0.45
1:B:238:THR:HG22	1:B:239:ILE:N	2.30	0.45
1:C:14:ALA:HB1	1:C:126:VAL:HG23	1.98	0.45
1:C:237:ALA:CB	4:C:3406:HOH:O	2.64	0.45
1:D:232:SER:HB3	1:D:239:ILE:CG1	2.44	0.45
1:E:255:ILE:O	1:E:256:ASN:C	2.59	0.45
1:B:101:ILE:CD1	1:B:138:GLY:HA2	2.46	0.45
1:B:239:ILE:N	4:B:2352:HOH:O	2.49	0.45
2:B:2300:NAI:H1D	2:B:2300:NAI:O1N	2.17	0.45
1:C:73:HIS:CE1	1:C:74:ILE:HG12	2.51	0.45
1:C:118:ILE:O	1:C:118:ILE:HG12	2.17	0.45
2:C:3300:NAI:O1N	2:C:3300:NAI:H1D	2.17	0.45
1:A:149:MET:CE	1:A:153:LEU:HG	2.39	0.45
2:D:4300:NAI:H1D	2:D:4300:NAI:O1N	2.16	0.45
1:E:39:LEU:HD23	1:E:39:LEU:H	1.81	0.45
1:A:9:GLY:CA	1:A:41:THR:HG21	2.46	0.45
1:D:100:THR:HG22	1:D:101:ILE:N	2.31	0.45
1:D:237:ALA:O	1:D:240:HIS:HB2	2.17	0.45
1:E:74:ILE:C	1:E:76:PRO:CD	2.90	0.45
1:E:154:SER:O	2:E:5300:NAI:H42N	2.17	0.45
1:A:26:ALA:O	1:A:27:ALA:C	2.60	0.45
1:A:124:THR:C	1:A:126:VAL:H	2.24	0.45
1:B:35:PRO:HG2	1:B:71:LYS:HZ2	1.82	0.45
1:B:84:ALA:N	1:B:111:PHE:HD2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:LEU:CA	4:C:3371:HOH:O	2.44	0.45
1:C:171:THR:HA	4:C:3351:HOH:O	2.00	0.45
1:C:255:ILE:HG23	4:C:3332:HOH:O	2.16	0.45
1:D:242:LEU:O	1:D:244:VAL:N	2.50	0.45
1:E:1:MET:HG2	1:E:2:SER:N	2.31	0.45
1:E:74:ILE:CG2	1:E:78:ILE:HD11	2.46	0.45
1:E:106:LYS:HB3	4:E:5384:HOH:O	2.14	0.45
1:E:254:LEU:O	1:E:257:ALA:HB3	2.17	0.45
1:A:95:CYS:SG	4:A:1337:HOH:O	2.61	0.45
2:A:1300:NAI:C3N	3:A:1301:GLU:CB	2.91	0.45
1:B:222:GLN:OE1	1:B:226:GLN:HG2	2.15	0.45
1:C:189:ALA:HB2	1:C:203:VAL:HA	1.97	0.45
1:D:77:PHE:N	1:D:77:PHE:CD1	2.83	0.45
2:D:4300:NAI:C5N	3:D:4301:GLU:OXT	2.64	0.45
1:E:70:VAL:O	1:E:71:LYS:CB	2.65	0.45
1:E:137:THR:HG23	1:E:137:THR:O	2.17	0.45
1:E:181:ALA:C	4:E:5383:HOH:O	2.58	0.45
1:A:124:THR:O	1:A:126:VAL:N	2.50	0.45
1:B:89:ARG:HD2	1:B:89:ARG:C	2.41	0.45
1:B:190:ASP:O	4:B:2308:HOH:O	2.21	0.45
1:B:245:LEU:O	4:B:2353:HOH:O	2.21	0.45
1:B:258:VAL:HG13	1:B:259:GLU:N	2.31	0.45
1:D:133:THR:HG21	1:D:153:LEU:CD1	2.45	0.45
1:D:184:ALA:N	4:D:4340:HOH:O	2.50	0.45
2:D:4300:NAI:C3N	3:D:4301:GLU:CA	2.91	0.45
2:D:4300:NAI:H2N	3:D:4301:GLU:HA	1.89	0.45
1:E:13:PHE:HD1	1:E:48:MET:HE1	1.81	0.45
1:A:121:MET:CE	4:A:1346:HOH:O	2.64	0.45
1:A:225:GLY:O	1:A:228:LYS:HB3	2.17	0.45
1:B:37:MET:CE	4:B:2393:HOH:O	2.65	0.45
1:B:66:LEU:N	1:B:91:ILE:O	2.50	0.45
1:B:135:TYR:HE1	1:B:161:GLU:OE1	1.99	0.45
1:B:269:GLN:C	1:B:271:MET:N	2.74	0.45
1:C:60:VAL:N	4:C:3383:HOH:O	2.47	0.45
1:C:206:GLY:O	1:C:209:ALA:HB3	2.17	0.45
1:D:14:ALA:HA	1:D:127:VAL:HG22	1.98	0.45
1:E:47:LYS:NZ	4:E:5338:HOH:O	2.47	0.45
1:E:53:THR:HG21	1:E:58:GLU:CB	2.47	0.45
1:E:150:GLU:C	1:E:152:LEU:N	2.74	0.45
1:E:177:GLY:HA2	1:E:180:TYR:HD1	1.81	0.45
1:E:211:LEU:HD13	4:E:5314:HOH:O	2.13	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:251:ARG:CG	4:E:5304:HOH:O	2.64	0.45
1:A:233:SER:O	1:A:235:GLY:N	2.50	0.44
1:A:258:VAL:HG13	4:A:1366:HOH:O	2.16	0.44
1:B:199:ARG:NH1	4:B:2340:HOH:O	2.22	0.44
1:C:19:PHE:HE2	1:C:153:LEU:HD23	1.82	0.44
1:C:126:VAL:CG1	4:C:3307:HOH:O	2.57	0.44
1:C:160:THR:CG2	1:C:161:GLU:H	2.30	0.44
1:D:227:LEU:HD12	4:D:4363:HOH:O	2.16	0.44
1:E:43:SER:O	1:E:46:ARG:HB2	2.17	0.44
1:E:140:HIS:O	1:E:141:ALA:C	2.59	0.44
1:E:177:GLY:O	1:E:180:TYR:HB2	2.17	0.44
1:A:6:ILE:HD13	1:A:59:THR:HG21	2.00	0.44
1:A:120:CYS:HB2	4:A:1368:HOH:O	2.12	0.44
1:A:190:ASP:C	4:A:1420:HOH:O	2.58	0.44
1:A:219:HIS:CE1	4:A:1431:HOH:O	2.69	0.44
1:B:129:ARG:HH12	2:B:2300:NAI:C2D	2.29	0.44
1:C:61:GLN:O	1:C:89:ARG:NH2	2.49	0.44
1:D:195:MET:HG2	4:D:4366:HOH:O	2.16	0.44
1:A:123:ASN:N	1:A:123:ASN:HD22	2.16	0.44
1:A:124:THR:C	1:A:126:VAL:N	2.76	0.44
1:A:135:TYR:OH	1:A:150:GLU:CG	2.64	0.44
1:A:188:LEU:O	1:A:189:ALA:C	2.60	0.44
1:A:195:MET:N	4:E:5309:HOH:O	2.50	0.44
1:A:252:SER:HA	1:A:255:ILE:HD12	1.99	0.44
1:B:47:LYS:NZ	1:B:47:LYS:HB3	2.33	0.44
1:B:73:HIS:C	1:B:75:ILE:N	2.74	0.44
1:B:234:PRO:O	1:B:235:GLY:C	2.60	0.44
1:C:9:GLY:H	1:C:12:ALA:HB3	1.81	0.44
1:C:93:VAL:HG12	1:C:118:ILE:HD11	1.99	0.44
1:C:101:ILE:HB	1:C:164:GLU:OE1	2.17	0.44
1:D:10:GLN:N	4:D:4387:HOH:O	2.50	0.44
1:D:124:THR:C	1:D:126:VAL:N	2.75	0.44
2:D:4300:NAI:C3N	3:D:4301:GLU:HA	2.47	0.44
1:E:38:ASP:H	1:E:42:VAL:CG2	2.29	0.44
1:E:62:HIS:HE1	4:E:5387:HOH:O	2.00	0.44
1:E:104:ILE:HG22	1:E:117:VAL:HG21	1.99	0.44
1:E:172:GLY:HA2	1:E:261:SER:CB	2.47	0.44
1:E:229:ASP:C	1:E:231:VAL:H	2.25	0.44
1:A:191:GLY:O	1:A:192:GLY:C	2.59	0.44
1:A:200:ARG:O	1:A:204:ARG:HG2	2.17	0.44
1:A:256:ASN:CA	4:A:1335:HOH:O	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:ARG:HD2	4:B:2330:HOH:O	2.11	0.44
1:D:92:VAL:HB	1:D:117:VAL:HG22	1.99	0.44
1:E:62:HIS:ND1	4:E:5372:HOH:O	2.31	0.44
1:A:251:ARG:O	1:A:252:SER:C	2.60	0.44
1:A:255:ILE:O	1:A:258:VAL:N	2.48	0.44
1:B:10:GLN:C	4:B:2343:HOH:O	2.59	0.44
1:B:211:LEU:C	1:B:211:LEU:CD1	2.90	0.44
1:B:221:GLU:N	4:B:2322:HOH:O	2.50	0.44
1:C:8:ALA:HB3	1:C:34:SER:CB	2.48	0.44
1:C:61:GLN:O	1:C:63:SER:N	2.51	0.44
1:C:124:THR:N	1:C:125:PRO:CD	2.79	0.44
1:C:167:ILE:HG22	4:C:3345:HOH:O	2.03	0.44
1:D:80:ASP:O	1:D:81:GLU:C	2.60	0.44
1:E:184:ALA:O	1:E:187:ALA:HB3	2.17	0.44
1:E:242:LEU:O	1:E:243:HIS:C	2.60	0.44
1:A:11:LEU:CD1	4:A:1399:HOH:O	2.59	0.44
1:A:266:ARG:NH1	1:A:266:ARG:HG2	2.24	0.44
1:B:76:PRO:C	1:B:78:ILE:H	2.24	0.44
1:B:185:LEU:C	1:B:187:ALA:N	2.74	0.44
1:C:199:ARG:NH1	4:C:3392:HOH:O	2.48	0.44
1:A:1:MET:HG2	1:A:2:SER:N	2.33	0.44
1:E:211:LEU:CD1	1:E:211:LEU:C	2.91	0.44
1:E:220:SER:O	4:E:5362:HOH:O	2.21	0.44
1:E:251:ARG:HG2	4:E:5304:HOH:O	2.17	0.44
1:B:195:MET:HE2	1:B:195:MET:N	2.32	0.44
1:C:71:LYS:HB2	1:C:73:HIS:HE1	1.80	0.44
1:C:261:SER:HB3	4:C:3391:HOH:O	2.18	0.44
1:D:100:THR:HG22	1:D:102:SER:N	2.30	0.44
1:D:219:HIS:CE1	2:D:4300:NAI:H51N	2.37	0.44
1:A:101:ILE:HG21	1:A:138:GLY:HA2	2.00	0.44
1:A:121:MET:N	4:A:1368:HOH:O	2.49	0.44
1:A:149:MET:C	1:A:151:GLN:H	2.26	0.44
1:A:190:ASP:N	1:A:199:ARG:NH1	2.65	0.44
1:B:60:VAL:O	1:B:89:ARG:NH1	2.51	0.44
1:B:218:LEU:HB3	2:B:2300:NAI:H52N	2.00	0.44
1:C:13:PHE:O	1:C:16:ALA:HB3	2.18	0.44
1:C:26:ALA:HB3	1:C:29:LYS:HE3	1.99	0.44
1:C:30:ILE:HD12	1:C:30:ILE:N	2.32	0.44
1:C:75:ILE:CA	4:C:3407:HOH:O	2.60	0.44
1:C:266:ARG:O	1:C:269:GLN:HG2	2.18	0.44
1:D:115:PRO:CB	4:D:4374:HOH:O	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:GLN:O	1:D:223:HIS:HB2	2.18	0.44
1:D:266:ARG:HD3	4:D:4311:HOH:O	2.13	0.44
1:E:228:LYS:CE	1:E:242:LEU:HD13	2.48	0.44
1:E:264:ARG:C	1:E:266:ARG:N	2.74	0.44
1:A:3:VAL:HG11	1:A:67:PHE:HE1	1.82	0.43
1:A:176:SER:HB3	1:A:180:TYR:CE2	2.54	0.43
1:A:194:LYS:CB	4:A:1420:HOH:O	2.65	0.43
1:A:238:THR:CG2	4:A:1320:HOH:O	2.66	0.43
1:A:258:VAL:HG22	4:A:1302:HOH:O	2.09	0.43
1:A:267:GLU:O	1:A:268:LEU:C	2.57	0.43
1:B:142:GLN:CG	1:B:143:VAL:N	2.64	0.43
1:B:236:GLY:O	1:B:237:ALA:HB3	2.17	0.43
1:C:39:LEU:HA	1:C:43:SER:HB2	2.00	0.43
1:C:91:ILE:HG23	1:C:116:ARG:CB	2.43	0.43
1:C:140:HIS:N	4:C:3385:HOH:O	2.51	0.43
1:C:169:ALA:O	1:C:170:VAL:C	2.60	0.43
1:C:262:CYS:O	1:C:265:THR:HB	2.18	0.43
1:C:269:GLN:O	1:C:271:MET:N	2.45	0.43
1:D:92:VAL:N	4:D:4455:HOH:O	2.51	0.43
1:D:124:THR:N	4:D:4375:HOH:O	2.50	0.43
1:D:125:PRO:O	1:D:126:VAL:C	2.61	0.43
1:E:39:LEU:C	1:E:41:THR:H	2.24	0.43
1:E:242:LEU:O	1:E:244:VAL:N	2.50	0.43
1:E:259:GLU:O	1:E:262:CYS:N	2.50	0.43
1:A:76:PRO:C	1:A:78:ILE:N	2.76	0.43
1:A:218:LEU:CD1	4:A:1435:HOH:O	2.65	0.43
1:A:231:VAL:O	1:A:231:VAL:CG1	2.65	0.43
1:B:74:ILE:O	1:B:74:ILE:HG22	2.18	0.43
1:B:163:GLU:HG3	1:B:165:ASP:OD1	2.18	0.43
1:B:210:LEU:O	1:B:211:LEU:C	2.60	0.43
1:B:214:ALA:O	1:B:217:LEU:N	2.50	0.43
1:C:29:LYS:CG	4:C:3306:HOH:O	2.65	0.43
1:C:123:ASN:O	1:C:126:VAL:HG22	2.17	0.43
1:C:138:GLY:HA3	4:C:3394:HOH:O	2.18	0.43
1:D:121:MET:O	1:D:133:THR:HA	2.19	0.43
1:D:124:THR:N	1:D:125:PRO:CD	2.80	0.43
1:D:135:TYR:HE2	1:D:150:GLU:HG3	1.83	0.43
1:D:224:PRO:HG2	4:D:4355:HOH:O	2.12	0.43
1:E:109:SER:C	1:E:111:PHE:N	2.75	0.43
1:E:211:LEU:C	1:E:211:LEU:HD13	2.44	0.43
1:E:238:THR:CG2	4:E:5321:HOH:O	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ASP:O	1:A:90:HIS:HB3	2.18	0.43
1:A:123:ASN:N	1:A:123:ASN:ND2	2.64	0.43
1:A:123:ASN:CB	4:A:1436:HOH:O	2.67	0.43
1:B:211:LEU:C	1:B:211:LEU:HD12	2.43	0.43
1:B:238:THR:O	1:B:239:ILE:C	2.60	0.43
1:E:53:THR:HG22	1:E:55:HIS:N	2.19	0.43
1:E:94:SER:O	4:E:5423:HOH:O	2.19	0.43
1:E:126:VAL:HG22	1:E:156:VAL:HG12	2.01	0.43
1:A:139:THR:HG23	4:A:1430:HOH:O	2.18	0.43
1:A:193:VAL:O	1:A:195:MET:N	2.48	0.43
1:B:164:GLU:O	1:B:167:ILE:HB	2.18	0.43
1:C:15:LEU:O	1:C:19:PHE:CD1	2.71	0.43
1:C:93:VAL:HG12	1:C:118:ILE:CG1	2.48	0.43
1:C:240:HIS:CE1	4:C:3365:HOH:O	2.71	0.43
1:D:245:LEU:HD23	1:D:245:LEU:HA	1.87	0.43
1:E:233:SER:O	1:E:235:GLY:N	2.52	0.43
1:A:60:VAL:HG21	1:A:82:ILE:CG2	2.49	0.43
1:A:86:ILE:O	1:A:86:ILE:HG22	2.19	0.43
1:A:119:ARG:HA	4:A:1372:HOH:O	2.18	0.43
1:A:221:GLU:O	1:A:222:GLN:HB2	2.18	0.43
1:B:83:GLY:C	1:B:85:ASP:N	2.75	0.43
1:B:185:LEU:CD2	1:B:210:LEU:HD12	2.40	0.43
1:C:60:VAL:O	1:C:60:VAL:HG12	2.18	0.43
1:C:83:GLY:O	1:C:86:ILE:HG12	2.18	0.43
1:D:185:LEU:O	4:D:4361:HOH:O	2.21	0.43
1:E:107:LYS:HG3	4:E:5384:HOH:O	2.18	0.43
2:E:5300:NAI:O2D	3:E:5301:GLU:N	2.51	0.43
1:B:79:LEU:CD2	1:B:104:ILE:HG23	2.48	0.43
1:B:83:GLY:HA3	1:B:111:PHE:CD2	2.54	0.43
1:C:51:LYS:HD3	1:C:51:LYS:N	2.32	0.43
1:C:89:ARG:CD	1:C:90:HIS:N	2.68	0.43
1:C:112:ARG:NH1	1:C:113:PRO:HD2	2.11	0.43
1:D:42:VAL:HA	1:D:45:LEU:HD12	2.00	0.43
1:A:34:SER:HB2	1:A:37:MET:HG2	2.01	0.43
1:A:262:CYS:O	1:A:265:THR:N	2.52	0.43
1:B:32:ALA:O	1:B:53:THR:HB	2.18	0.43
1:C:38:ASP:H	1:C:42:VAL:HB	1.84	0.43
1:D:128:VAL:HG13	1:D:129:ARG:N	2.33	0.43
1:D:162:VAL:CG1	1:D:166:LEU:HB2	2.48	0.43
1:A:20:THR:OG1	1:A:48:MET:HE3	2.19	0.43
1:A:194:LYS:HE2	1:E:240:HIS:ND1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:VAL:O	1:B:129:ARG:CB	2.66	0.43
1:B:256:ASN:O	4:B:2381:HOH:O	2.21	0.43
1:D:27:ALA:C	1:D:29:LYS:H	2.26	0.43
1:D:73:HIS:ND1	1:D:74:ILE:HG12	2.34	0.43
1:E:106:LYS:CA	4:E:5398:HOH:O	2.66	0.43
1:E:129:ARG:HA	1:E:156:VAL:HG13	2.01	0.43
1:A:5:PHE:C	1:A:7:GLY:N	2.74	0.43
1:A:56:ASN:O	1:A:82:ILE:HD11	2.19	0.43
1:B:26:ALA:HB3	1:B:29:LYS:HB2	2.00	0.43
1:B:260:ALA:N	4:B:2381:HOH:O	2.50	0.43
1:C:35:PRO:O	1:C:36:ASP:CB	2.66	0.43
1:C:75:ILE:HG21	1:C:99:VAL:HG11	2.01	0.43
1:A:73:HIS:O	1:A:76:PRO:HD2	2.19	0.43
1:B:133:THR:N	4:B:2387:HOH:O	2.51	0.43
1:B:147:ARG:NH1	1:B:150:GLU:OE2	2.52	0.43
1:C:112:ARG:HG3	1:C:113:PRO:CD	2.39	0.43
1:D:258:VAL:O	1:D:259:GLU:C	2.62	0.43
1:E:77:PHE:O	1:E:78:ILE:C	2.61	0.43
1:E:125:PRO:HB2	1:E:130:GLU:O	2.19	0.43
1:E:131:GLY:O	1:E:157:GLY:HA3	2.19	0.43
1:A:6:ILE:HG23	1:A:56:ASN:HB2	2.00	0.42
1:B:111:PHE:N	1:B:111:PHE:CD1	2.87	0.42
1:B:171:THR:C	1:B:173:LEU:N	2.75	0.42
1:B:238:THR:O	1:B:241:ALA:N	2.51	0.42
1:B:245:LEU:C	4:B:2353:HOH:O	2.56	0.42
1:B:269:GLN:O	1:B:271:MET:N	2.47	0.42
1:C:24:VAL:O	1:C:25:LEU:HB2	2.16	0.42
1:C:46:ARG:C	1:C:48:MET:N	2.76	0.42
1:C:46:ARG:O	1:C:48:MET:N	2.52	0.42
1:C:79:LEU:HD11	1:C:104:ILE:CG1	2.48	0.42
1:C:250:PHE:C	4:C:3359:HOH:O	2.60	0.42
1:C:252:SER:HA	4:C:3364:HOH:O	2.19	0.42
1:D:89:ARG:CZ	1:D:90:HIS:CE1	3.02	0.42
1:A:149:MET:C	1:A:151:GLN:N	2.75	0.42
1:B:105:GLU:O	1:B:109:SER:HB2	2.18	0.42
1:C:123:ASN:HD21	1:C:132:ALA:CB	2.22	0.42
1:D:134:VAL:HG23	1:D:160:THR:O	2.19	0.42
1:E:115:PRO:CA	4:E:5436:HOH:O	2.52	0.42
1:E:136:ALA:HB2	1:E:167:ILE:CD1	2.49	0.42
1:E:243:HIS:O	1:E:247:SER:OG	2.35	0.42
1:A:39:LEU:O	1:A:40:ALA:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:THR:N	1:B:125:PRO:CD	2.80	0.42
1:B:204:ARG:HD3	1:B:204:ARG:N	2.35	0.42
1:C:125:PRO:HG3	4:C:3346:HOH:O	2.19	0.42
1:C:185:LEU:HG	4:C:3352:HOH:O	2.19	0.42
1:D:39:LEU:O	1:D:43:SER:HB3	2.19	0.42
1:D:57:LYS:O	1:D:61:GLN:HG3	2.19	0.42
1:E:117:VAL:C	1:E:118:ILE:HD12	2.44	0.42
1:E:188:LEU:C	4:E:5396:HOH:O	2.61	0.42
1:E:238:THR:CB	4:E:5321:HOH:O	2.60	0.42
1:A:92:VAL:O	1:A:117:VAL:HG23	2.20	0.42
1:A:119:ARG:O	1:A:135:TYR:HA	2.19	0.42
1:B:39:LEU:HA	1:B:43:SER:HB2	2.01	0.42
1:B:165:ASP:OD1	1:B:166:LEU:N	2.53	0.42
1:B:218:LEU:CB	2:B:2300:NAI:H52N	2.50	0.42
1:C:129:ARG:NH1	3:C:3301:GLU:HG2	2.32	0.42
1:A:169:ALA:O	1:A:172:GLY:N	2.51	0.42
1:A:258:VAL:HG12	1:A:259:GLU:N	2.34	0.42
1:A:269:GLN:O	1:A:271:MET:N	2.52	0.42
1:B:172:GLY:HA2	1:B:261:SER:CB	2.49	0.42
1:C:16:ALA:C	1:C:18:GLY:N	2.78	0.42
1:E:121:MET:HE2	1:E:122:THR:N	2.34	0.42
1:E:132:ALA:CA	4:E:5351:HOH:O	2.52	0.42
1:E:246:GLU:CA	4:E:5312:HOH:O	2.66	0.42
1:A:105:GLU:O	1:A:107:LYS:N	2.45	0.42
1:A:109:SER:C	1:A:111:PHE:N	2.78	0.42
1:A:119:ARG:CA	4:A:1372:HOH:O	2.68	0.42
1:A:149:MET:O	1:A:151:GLN:N	2.52	0.42
1:A:219:HIS:NE2	2:A:1300:NAI:C5D	2.82	0.42
1:A:249:GLY:O	1:A:252:SER:HB3	2.20	0.42
1:B:75:ILE:H	1:B:75:ILE:CD1	2.27	0.42
1:C:11:LEU:O	1:C:15:LEU:HG	2.20	0.42
1:C:22:ALA:CB	4:C:3369:HOH:O	2.40	0.42
1:C:46:ARG:C	1:C:48:MET:H	2.28	0.42
1:C:167:ILE:C	4:C:3380:HOH:O	2.62	0.42
1:E:17:LYS:O	1:E:18:GLY:C	2.61	0.42
1:E:89:ARG:NH2	1:E:90:HIS:HE1	2.17	0.42
1:E:199:ARG:NH2	4:E:5346:HOH:O	2.49	0.42
1:E:211:LEU:O	1:E:211:LEU:HD13	2.19	0.42
1:A:50:VAL:CG1	1:A:51:LYS:N	2.83	0.42
1:A:153:LEU:C	1:A:155:SER:N	2.76	0.42
1:A:173:LEU:HB3	1:A:174:SER:H	1.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:GLN:HG2	1:B:275:GLU:HG3	2.01	0.42
1:C:234:PRO:HB3	1:D:196:GLY:C	2.45	0.42
1:C:249:GLY:C	4:C:3312:HOH:O	2.63	0.42
1:D:133:THR:HG22	1:D:158:PHE:O	2.19	0.42
1:E:62:HIS:O	4:E:5417:HOH:O	2.22	0.42
1:E:214:ALA:C	1:E:216:MET:N	2.76	0.42
1:E:260:ALA:HA	4:E:5329:HOH:O	2.20	0.42
1:A:102:SER:O	1:A:104:ILE:N	2.53	0.42
1:A:166:LEU:O	1:A:168:ASP:N	2.52	0.42
1:A:194:LYS:CA	4:E:5309:HOH:O	2.66	0.42
1:A:249:GLY:CA	4:A:1318:HOH:O	2.66	0.42
1:B:158:PHE:HE2	2:B:2300:NAI:O3B	1.85	0.42
1:C:177:GLY:O	1:C:180:TYR:N	2.45	0.42
1:C:185:LEU:HD23	1:C:185:LEU:HA	1.90	0.42
1:C:234:PRO:O	1:C:235:GLY:C	2.61	0.42
1:C:256:ASN:C	4:C:3381:HOH:O	2.63	0.42
1:D:30:ILE:CB	1:D:50:VAL:HG22	2.40	0.42
1:D:38:ASP:O	1:D:39:LEU:C	2.63	0.42
1:D:70:VAL:CG1	1:D:74:ILE:HB	2.50	0.42
1:D:252:SER:O	1:D:253:LEU:C	2.61	0.42
1:A:80:ASP:OD2	1:A:107:LYS:NZ	2.42	0.42
1:A:162:VAL:CG1	1:A:166:LEU:HD12	2.45	0.42
1:B:176:SER:HB2	1:B:180:TYR:OH	2.20	0.42
1:B:191:GLY:O	1:B:194:LYS:HB3	2.20	0.42
1:C:86:ILE:HG22	1:C:87:GLU:H	1.84	0.42
1:C:223:HIS:O	1:C:224:PRO:C	2.62	0.42
1:D:62:HIS:HA	4:D:4448:HOH:O	2.16	0.42
1:D:251:ARG:NH1	1:D:251:ARG:HG2	2.35	0.42
1:E:39:LEU:HA	1:E:43:SER:CB	2.50	0.42
1:A:82:ILE:O	1:A:83:GLY:C	2.63	0.42
1:A:106:LYS:CB	4:A:1432:HOH:O	2.67	0.42
1:A:163:GLU:O	1:A:164:GLU:C	2.63	0.42
1:A:238:THR:O	1:A:239:ILE:C	2.63	0.42
1:B:16:ALA:C	1:B:18:GLY:H	2.28	0.42
1:B:89:ARG:HD2	1:B:89:ARG:O	2.20	0.42
1:B:164:GLU:HA	1:B:167:ILE:CD1	2.49	0.42
1:D:119:ARG:CZ	4:D:4422:HOH:O	2.68	0.42
1:E:78:ILE:O	1:E:81:GLU:HB2	2.19	0.42
1:A:33:SER:C	1:A:35:PRO:HD3	2.44	0.41
1:A:119:ARG:HH11	1:A:164:GLU:HG2	1.85	0.41
1:B:57:LYS:HG3	1:B:58:GLU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:PHE:N	4:B:2361:HOH:O	2.53	0.41
1:C:133:THR:O	1:C:159:CYS:HA	2.19	0.41
1:C:197:LEU:CD1	4:C:3367:HOH:O	2.66	0.41
1:D:219:HIS:NE2	2:D:4300:NAI:O5D	2.52	0.41
1:E:45:LEU:HD23	1:E:48:MET:HE1	2.02	0.41
1:E:53:THR:C	1:E:55:HIS:H	2.26	0.41
1:E:116:ARG:HA	4:E:5388:HOH:O	2.20	0.41
1:E:218:LEU:CB	4:E:5424:HOH:O	2.68	0.41
1:A:146:GLY:O	1:A:150:GLU:HB2	2.20	0.41
1:A:187:ALA:O	1:A:190:ASP:HB2	2.20	0.41
1:B:5:PHE:CE1	1:B:12:ALA:HA	2.55	0.41
1:B:28:HIS:C	1:B:30:ILE:H	2.28	0.41
1:B:45:LEU:CA	4:B:2385:HOH:O	2.69	0.41
1:C:240:HIS:HE1	4:C:3365:HOH:O	2.03	0.41
1:D:17:LYS:HD2	1:D:127:VAL:HG12	2.01	0.41
1:D:172:GLY:HA2	1:D:261:SER:CB	2.50	0.41
1:E:180:TYR:CE2	1:E:257:ALA:HB1	2.55	0.41
1:E:229:ASP:O	1:E:231:VAL:N	2.52	0.41
1:A:223:HIS:ND1	1:A:224:PRO:CD	2.83	0.41
1:B:229:ASP:CG	4:B:2386:HOH:O	2.56	0.41
1:C:68:LEU:C	4:C:3322:HOH:O	2.57	0.41
1:C:87:GLU:HB2	1:C:90:HIS:CE1	2.55	0.41
1:D:43:SER:CB	4:D:4405:HOH:O	2.56	0.41
1:D:173:LEU:C	1:D:173:LEU:HD23	2.45	0.41
1:D:212:GLY:O	1:D:213:ALA:C	2.63	0.41
1:D:227:LEU:HA	1:D:230:ASN:HB2	2.02	0.41
1:D:233:SER:O	1:D:234:PRO:C	2.64	0.41
1:E:6:ILE:HG12	1:E:66:LEU:HD11	2.02	0.41
1:A:73:HIS:HE1	4:E:5334:HOH:O	2.03	0.41
1:A:123:ASN:HD21	1:A:131:GLY:CA	2.34	0.41
1:B:86:ILE:HD12	1:B:108:LEU:HD22	2.03	0.41
1:B:162:VAL:O	1:B:163:GLU:C	2.64	0.41
1:C:12:ALA:HA	1:C:15:LEU:HD12	2.02	0.41
1:C:133:THR:HG21	4:C:3317:HOH:O	2.04	0.41
1:C:173:LEU:HD12	1:C:173:LEU:HA	1.85	0.41
1:C:213:ALA:O	1:C:216:MET:HB2	2.19	0.41
1:E:94:SER:CA	4:E:5325:HOH:O	2.60	0.41
1:A:171:THR:O	1:A:175:GLY:HA3	2.21	0.41
1:A:263:ILE:HD13	1:A:263:ILE:H	1.81	0.41
1:B:70:VAL:HB	4:B:2368:HOH:O	2.19	0.41
1:B:236:GLY:C	1:B:238:THR:N	2.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:LEU:HB3	1:C:19:PHE:CE1	2.55	0.41
1:C:16:ALA:O	1:C:18:GLY:N	2.53	0.41
1:C:55:HIS:C	1:C:57:LYS:N	2.74	0.41
1:D:229:ASP:O	4:D:4316:HOH:O	2.22	0.41
1:E:53:THR:C	1:E:55:HIS:N	2.77	0.41
1:E:69:ALA:CB	4:E:5379:HOH:O	2.48	0.41
1:E:187:ALA:C	4:E:5343:HOH:O	2.55	0.41
1:E:190:ASP:CB	4:E:5381:HOH:O	2.65	0.41
1:B:218:LEU:HD21	2:B:2300:NAI:H52A	2.02	0.41
1:B:233:SER:O	1:B:235:GLY:N	2.53	0.41
1:C:4:GLY:CA	1:C:66:LEU:HG	2.51	0.41
1:C:13:PHE:C	1:C:13:PHE:CD2	2.97	0.41
1:C:74:ILE:HG22	1:C:78:ILE:HG12	2.03	0.41
1:C:123:ASN:OD1	1:C:132:ALA:N	2.53	0.41
1:C:134:VAL:O	4:C:3327:HOH:O	2.22	0.41
1:D:21:ALA:C	1:D:23:GLY:N	2.75	0.41
1:D:89:ARG:CZ	1:D:90:HIS:HE1	2.34	0.41
1:E:57:LYS:N	1:E:57:LYS:CD	2.74	0.41
1:A:22:ALA:HB1	4:A:1425:HOH:O	2.15	0.41
1:A:38:ASP:O	1:A:40:ALA:N	2.54	0.41
1:A:41:THR:HG22	1:A:42:VAL:N	2.36	0.41
1:A:167:ILE:O	1:A:167:ILE:HG22	2.21	0.41
1:B:53:THR:HG21	1:B:58:GLU:HB2	2.03	0.41
1:B:89:ARG:NH1	1:B:90:HIS:HD1	2.18	0.41
1:B:140:HIS:O	1:B:141:ALA:CB	2.68	0.41
1:C:19:PHE:CE2	1:C:153:LEU:HD23	2.55	0.41
1:D:164:GLU:OE2	4:D:4422:HOH:O	2.21	0.41
1:D:236:GLY:O	1:D:237:ALA:HB3	2.21	0.41
1:E:129:ARG:CB	4:E:5401:HOH:O	2.56	0.41
1:A:116:ARG:HG3	4:A:1416:HOH:O	2.19	0.41
1:B:238:THR:C	1:B:240:HIS:H	2.29	0.41
1:C:6:ILE:HD12	1:C:56:ASN:CB	2.46	0.41
1:C:119:ARG:NH1	4:C:3372:HOH:O	2.53	0.41
1:C:238:THR:C	1:C:240:HIS:N	2.78	0.41
1:D:45:LEU:O	1:D:46:ARG:C	2.63	0.41
1:D:67:PHE:O	4:D:4327:HOH:O	2.21	0.41
1:D:80:ASP:O	1:D:82:ILE:N	2.54	0.41
1:D:161:GLU:O	1:D:162:VAL:HG23	2.21	0.41
1:D:242:LEU:C	1:D:244:VAL:N	2.76	0.41
1:E:21:ALA:C	1:E:23:GLY:H	2.29	0.41
1:E:117:VAL:O	1:E:138:GLY:CA	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:134:VAL:CG2	1:E:170:VAL:HG11	2.51	0.41
1:E:191:GLY:C	1:E:193:VAL:N	2.79	0.41
1:A:7:GLY:CA	4:A:1305:HOH:O	2.59	0.41
1:A:11:LEU:HD11	4:A:1346:HOH:O	2.20	0.41
1:A:13:PHE:HA	1:A:45:LEU:HD21	2.03	0.41
1:A:238:THR:C	1:A:240:HIS:H	2.29	0.41
1:A:240:HIS:CD2	1:C:194:LYS:HE3	2.56	0.41
1:B:8:ALA:HB1	1:B:45:LEU:HD12	2.03	0.41
1:B:28:HIS:CD2	1:B:49:GLY:O	2.73	0.41
1:B:164:GLU:CG	1:B:167:ILE:HD12	2.42	0.41
1:B:169:ALA:O	1:B:170:VAL:C	2.64	0.41
1:C:21:ALA:C	1:C:23:GLY:N	2.78	0.41
1:C:137:THR:O	4:C:3414:HOH:O	2.22	0.41
1:C:222:GLN:HG3	1:C:227:LEU:HD21	2.02	0.41
1:C:257:ALA:C	1:C:259:GLU:N	2.79	0.41
1:D:24:VAL:HG11	1:D:152:LEU:CD2	2.51	0.41
1:D:46:ARG:HG3	1:D:52:LEU:HD12	2.02	0.41
1:D:165:ASP:O	4:D:4368:HOH:O	2.22	0.41
1:D:187:ALA:O	1:D:190:ASP:HB2	2.20	0.41
1:D:269:GLN:NE2	4:D:4445:HOH:O	2.52	0.41
1:E:1:MET:HE3	1:E:3:VAL:HG23	2.02	0.41
1:E:75:ILE:HG21	1:E:99:VAL:HG11	2.02	0.41
1:E:100:THR:HG22	1:E:101:ILE:H	1.86	0.41
1:E:185:LEU:O	1:E:186:ASP:C	2.62	0.41
1:E:242:LEU:O	1:E:245:LEU:N	2.54	0.41
1:A:98:GLY:CA	4:A:1328:HOH:O	2.39	0.41
1:A:185:LEU:HG	4:A:1419:HOH:O	2.21	0.41
1:B:91:ILE:HG23	1:B:116:ARG:HB3	2.03	0.41
1:B:107:LYS:HE2	1:B:107:LYS:HB3	1.91	0.41
1:B:134:VAL:HG12	1:B:135:TYR:N	2.36	0.41
1:C:104:ILE:CG2	1:C:117:VAL:HG11	2.51	0.41
1:C:119:ARG:NH2	4:C:3345:HOH:O	2.53	0.41
1:C:252:SER:C	4:C:3364:HOH:O	2.63	0.41
1:D:89:ARG:NH1	1:D:90:HIS:CE1	2.89	0.41
1:D:135:TYR:CD1	1:D:135:TYR:C	2.99	0.41
1:D:193:VAL:HA	1:D:197:LEU:O	2.21	0.41
1:E:3:VAL:HG22	1:E:65:VAL:HB	2.03	0.41
1:A:77:PHE:N	1:A:77:PHE:CD1	2.89	0.40
1:A:199:ARG:O	1:A:200:ARG:C	2.63	0.40
1:A:242:LEU:O	1:A:244:VAL:N	2.53	0.40
1:B:228:LYS:HE2	1:B:229:ASP:OD1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:ILE:HD11	1:C:117:VAL:C	2.45	0.40
1:C:129:ARG:O	1:C:157:GLY:HA2	2.21	0.40
1:C:142:GLN:H	1:C:145:ASP:CG	2.29	0.40
1:C:160:THR:HG22	1:C:161:GLU:H	1.81	0.40
1:C:233:SER:N	4:C:3313:HOH:O	2.45	0.40
1:D:233:SER:C	1:D:235:GLY:N	2.79	0.40
1:E:215:LYS:O	1:E:219:HIS:CD2	2.74	0.40
1:A:26:ALA:HB2	1:A:29:LYS:HE3	2.03	0.40
1:B:12:ALA:O	1:B:16:ALA:CB	2.69	0.40
1:B:12:ALA:HB1	4:B:2314:HOH:O	2.13	0.40
1:B:76:PRO:HB2	1:B:77:PHE:CD1	2.56	0.40
1:C:82:ILE:HG22	1:C:82:ILE:O	2.21	0.40
1:D:156:VAL:O	1:D:156:VAL:CG1	2.56	0.40
1:D:206:GLY:O	1:D:209:ALA:HB3	2.22	0.40
1:D:251:ARG:CD	4:D:4427:HOH:O	2.59	0.40
1:E:31:MET:HE3	1:E:51:LYS:HD3	2.02	0.40
1:E:74:ILE:O	1:E:75:ILE:C	2.65	0.40
1:E:133:THR:O	1:E:159:CYS:HA	2.21	0.40
2:E:5300:NAI:C2D	3:E:5301:GLU:N	2.85	0.40
1:A:62:HIS:O	1:A:62:HIS:CG	2.74	0.40
1:A:149:MET:HE2	1:A:153:LEU:CG	2.42	0.40
1:A:240:HIS:HD2	1:C:194:LYS:HG3	1.86	0.40
1:A:241:ALA:O	1:A:242:LEU:C	2.64	0.40
1:B:160:THR:HG22	4:B:2360:HOH:O	2.07	0.40
1:B:169:ALA:C	1:B:171:THR:H	2.30	0.40
1:C:26:ALA:C	1:C:28:HIS:N	2.80	0.40
1:C:50:VAL:HG22	4:C:3363:HOH:O	2.18	0.40
1:C:128:VAL:CG1	1:C:129:ARG:H	2.26	0.40
1:D:90:HIS:C	4:D:4455:HOH:O	2.62	0.40
1:D:129:ARG:HD3	1:D:155:SER:O	2.21	0.40
1:E:63:SER:CB	4:E:5372:HOH:O	2.67	0.40
1:E:77:PHE:CD1	1:E:77:PHE:N	2.86	0.40
1:E:113:PRO:N	4:E:5367:HOH:O	2.55	0.40
1:A:40:ALA:O	1:A:44:ALA:HB2	2.22	0.40
1:A:100:THR:HG22	1:A:101:ILE:N	2.37	0.40
1:A:153:LEU:C	1:A:155:SER:H	2.28	0.40
1:A:236:GLY:C	1:A:238:THR:H	2.30	0.40
1:B:57:LYS:O	1:B:58:GLU:C	2.64	0.40
1:B:77:PHE:CD1	1:B:77:PHE:N	2.85	0.40
1:B:216:MET:CE	4:B:2315:HOH:O	2.69	0.40
1:C:79:LEU:HD11	1:C:104:ILE:HG12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:SER:HB2	1:C:180:TYR:CZ	2.56	0.40
1:C:228:LYS:NZ	1:C:229:ASP:OD1	2.55	0.40
1:D:251:ARG:NH1	4:D:4447:HOH:O	2.28	0.40
1:E:72:PRO:C	1:E:74:ILE:H	2.30	0.40
1:A:102:SER:O	1:A:103:SER:C	2.64	0.40
1:C:53:THR:HG23	1:C:58:GLU:CD	2.47	0.40
1:E:82:ILE:O	1:E:83:GLY:C	2.65	0.40
1:E:135:TYR:N	4:E:5413:HOH:O	2.54	0.40

All (22) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:ARG:NH1	2:B:2300:NAI:N7A[2_555]	1.66	0.54
1:A:204:ARG:CB	2:C:3300:NAI:C3B[2_555]	1.75	0.45
1:B:204:ARG:CB	2:B:2300:NAI:C3B[2_555]	1.76	0.44
2:B:2300:NAI:O5B	4:B:2359:HOH:O[2_555]	1.88	0.32
1:D:204:ARG:CB	2:E:5300:NAI:C2B[2_555]	1.94	0.26
1:B:204:ARG:CG	2:B:2300:NAI:C2B[2_555]	2.01	0.19
1:B:204:ARG:NE	2:B:2300:NAI:C8A[2_555]	2.03	0.17
1:E:250:PHE:CE2	4:D:4340:HOH:O[2_555]	2.03	0.17
4:A:1320:HOH:O	4:C:3330:HOH:O[2_555]	2.04	0.16
1:A:243:HIS:NE2	4:A:1335:HOH:O[2_555]	2.07	0.13
1:A:251:ARG:NH1	1:A:251:ARG:NH1[2_555]	2.09	0.11
4:A:1398:HOH:O	4:C:3376:HOH:O[2_555]	2.09	0.11
4:B:2337:HOH:O	4:B:2363:HOH:O[2_555]	2.09	0.11
1:C:231:VAL:CG1	4:A:1347:HOH:O[2_555]	2.10	0.10
4:A:1380:HOH:O	4:C:3336:HOH:O[2_555]	2.11	0.09
1:C:255:ILE:CG2	4:E:5357:HOH:O[2_555]	2.11	0.09
1:A:204:ARG:CG	2:C:3300:NAI:C2B[2_555]	2.15	0.05
1:A:204:ARG:CG	2:C:3300:NAI:O4B[2_555]	2.16	0.04
1:D:29:LYS:CE	4:D:4430:HOH:O[2_556]	2.16	0.04
4:A:1442:HOH:O	4:C:3379:HOH:O[2_555]	2.17	0.03
1:B:258:VAL:CG2	4:B:2355:HOH:O[2_555]	2.17	0.03
1:A:204:ARG:CB	2:C:3300:NAI:O4B[2_555]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	275/277 (99%)	189 (69%)	54 (20%)	32 (12%)	0	1
1	B	272/277 (98%)	168 (62%)	62 (23%)	42 (15%)	0	0
1	C	275/277 (99%)	198 (72%)	49 (18%)	28 (10%)	0	3
1	D	275/277 (99%)	190 (69%)	64 (23%)	21 (8%)	1	4
1	E	275/277 (99%)	178 (65%)	64 (23%)	33 (12%)	0	1
All	All	1372/1385 (99%)	923 (67%)	293 (21%)	156 (11%)	0	1

All (156) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ALA
1	A	36	ASP
1	A	39	LEU
1	A	107	LYS
1	A	129	ARG
1	A	164	GLU
1	A	173	LEU
1	B	10	GLN
1	B	19	PHE
1	B	36	ASP
1	B	37	MET
1	B	76	PRO
1	B	95	CYS
1	B	97	ALA
1	B	129	ARG
1	B	137	THR
1	B	140	HIS
1	B	141	ALA
1	B	142	GLN
1	B	221	GLU
1	B	222	GLN

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Mol	Chain	Res	Type
1	B	223	HIS
1	C	10	GLN
1	C	27	ALA
1	C	63	SER
1	C	65	VAL
1	C	113	PRO
1	C	252	SER
1	C	253	LEU
1	D	40	ALA
1	D	99	VAL
1	D	129	ARG
1	D	164	GLU
1	D	223	HIS
1	E	88	ASP
1	E	164	GLU
1	E	222	GLN
1	E	223	HIS
1	E	274	GLN
1	A	41	THR
1	A	42	VAL
1	A	235	GLY
1	B	61	GLN
1	B	77	PHE
1	B	113	PRO
1	B	154	SER
1	B	160	THR
1	B	170	VAL
1	B	177	GLY
1	B	186	ASP
1	B	189	ALA
1	C	16	ALA
1	C	36	ASP
1	C	64	ASP
1	C	107	LYS
1	D	8	ALA
1	D	167	ILE
1	D	267	GLU
1	D	270	SER
1	E	41	THR
1	E	42	VAL
1	E	50	VAL
1	E	78	ILE

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Mol	Chain	Res	Type
1	E	90	HIS
1	E	151	GLN
1	E	170	VAL
1	E	230	ASN
1	E	235	GLY
1	E	260	ALA
1	A	37	MET
1	A	77	PHE
1	A	103	SER
1	A	106	LYS
1	A	167	ILE
1	A	223	HIS
1	A	243	HIS
1	A	256	ASN
1	A	270	SER
1	B	38	ASP
1	B	94	SER
1	B	143	VAL
1	B	163	GLU
1	B	199	ARG
1	B	220	SER
1	B	230	ASN
1	B	270	SER
1	C	17	LYS
1	C	20	THR
1	C	47	LYS
1	C	56	ASN
1	C	125	PRO
1	C	139	THR
1	C	197	LEU
1	C	258	VAL
1	D	10	GLN
1	D	41	THR
1	D	81	GLU
1	D	170	VAL
1	D	258	VAL
1	E	243	HIS
1	E	250	PHE
1	A	40	ALA
1	A	87	GLU
1	A	102	SER
1	A	150	GLU

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Mol	Chain	Res	Type
1	A	163	GLU
1	A	187	ALA
1	A	220	SER
1	B	16	ALA
1	B	20	THR
1	B	125	PRO
1	B	246	GLU
1	C	46	ARG
1	C	72	PRO
1	C	173	LEU
1	D	235	GLY
1	D	257	ALA
1	E	36	ASP
1	E	77	PHE
1	E	130	GLU
1	E	163	GLU
1	E	221	GLU
1	E	237	ALA
1	E	259	GLU
1	A	177	GLY
1	A	234	PRO
1	B	71	LYS
1	C	11	LEU
1	C	40	ALA
1	C	62	HIS
1	C	150	GLU
1	C	270	SER
1	D	77	PHE
1	D	125	PRO
1	D	238	THR
1	E	113	PRO
1	E	143	VAL
1	A	56	ASN
1	A	263	ILE
1	C	177	GLY
1	D	42	VAL
1	D	111	PHE
1	E	81	GLU
1	A	125	PRO
1	B	239	ILE
1	E	74	ILE
1	E	125	PRO

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Mol	Chain	Res	Type
1	A	34	SER
1	B	24	VAL
1	B	235	GLY
1	E	234	PRO
1	B	234	PRO
1	B	127	VAL
1	E	34	SER
1	E	71	LYS
1	E	167	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	215/215 (100%)	185 (86%)	30 (14%)	3	15
1	B	213/215 (99%)	197 (92%)	16 (8%)	12	39
1	C	214/215 (100%)	197 (92%)	17 (8%)	11	37
1	D	215/215 (100%)	192 (89%)	23 (11%)	6	25
1	E	215/215 (100%)	199 (93%)	16 (7%)	13	40
All	All	1072/1075 (100%)	970 (90%)	102 (10%)	8	30

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	20	THR
1	A	25	LEU
1	A	36	ASP
1	A	38	ASP
1	A	75	ILE
1	A	91	ILE
1	A	111	PHE
1	A	120	CYS
1	A	121	MET

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Mol	Chain	Res	Type
1	A	123	ASN
1	A	124	THR
1	A	126	VAL
1	A	139	THR
1	A	148	LEU
1	A	149	MET
1	A	150	GLU
1	A	171	THR
1	A	180	TYR
1	A	183	THR
1	A	210	LEU
1	A	211	LEU
1	A	228	LYS
1	A	234	PRO
1	A	244	VAL
1	A	247	SER
1	A	258	VAL
1	A	263	ILE
1	A	265	THR
1	A	269	GLN
1	B	5	PHE
1	B	10	GLN
1	B	47	LYS
1	B	90	HIS
1	B	105	GLU
1	B	120	CYS
1	B	124	THR
1	B	140	HIS
1	B	161	GLU
1	B	178	PRO
1	B	211	LEU
1	B	234	PRO
1	B	238	THR
1	B	244	VAL
1	B	247	SER
1	B	265	THR
1	C	45	LEU
1	C	51	LYS
1	C	72	PRO
1	C	90	HIS
1	C	91	ILE
1	C	104	ILE

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Mol	Chain	Res	Type
1	C	118	ILE
1	C	120	CYS
1	C	121	MET
1	C	123	ASN
1	C	124	THR
1	C	190	ASP
1	C	195	MET
1	C	216	MET
1	C	228	LYS
1	C	244	VAL
1	C	265	THR
1	D	10	GLN
1	D	31	MET
1	D	37	MET
1	D	50	VAL
1	D	65	VAL
1	D	75	ILE
1	D	101	ILE
1	D	118	ILE
1	D	120	CYS
1	D	122	THR
1	D	124	THR
1	D	127	VAL
1	D	137	THR
1	D	144	GLU
1	D	145	ASP
1	D	153	LEU
1	D	168	ASP
1	D	203	VAL
1	D	211	LEU
1	D	215	LYS
1	D	244	VAL
1	D	258	VAL
1	D	259	GLU
1	E	31	MET
1	E	57	LYS
1	E	77	PHE
1	E	101	ILE
1	E	104	ILE
1	E	120	CYS
1	E	124	THR
1	E	126	VAL

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Mol	Chain	Res	Type
1	E	160	THR
1	E	168	ASP
1	E	176	SER
1	E	178	PRO
1	E	195	MET
1	E	211	LEU
1	E	228	LYS
1	E	233	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	HIS
1	A	73	HIS
1	A	90	HIS
1	A	123	ASN
1	A	140	HIS
1	A	208	GLN
1	A	226	GLN
1	A	240	HIS
1	A	269	GLN
1	B	56	ASN
1	B	151	GLN
1	C	90	HIS
1	C	240	HIS
1	C	243	HIS
1	D	28	HIS
1	D	55	HIS
1	D	61	GLN
1	D	140	HIS
1	D	219	HIS
1	D	222	GLN
1	E	28	HIS
1	E	219	HIS
1	E	226	GLN
1	E	243	HIS
1	E	269	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	GLU	C	3301	-	8,9,9	1.92	2 (25%)	8,11,11	5.91	1 (12%)
3	GLU	A	1301	-	8,9,9	1.62	1 (12%)	8,11,11	5.89	1 (12%)
3	GLU	B	2301	-	8,9,9	1.92	2 (25%)	8,11,11	5.91	1 (12%)
3	GLU	D	4301	-	8,9,9	1.43	1 (12%)	8,11,11	1.76	1 (12%)
2	NAI	D	4300	-	46,47,48	5.81	26 (56%)	61,71,73	4.17	27 (44%)
2	NAI	B	2300	-	46,47,48	5.80	26 (56%)	61,71,73	4.15	27 (44%)
2	NAI	A	1300	-	46,47,48	5.79	30 (65%)	61,71,73	5.74	37 (60%)
2	NAI	E	5300	-	46,47,48	8.97	30 (65%)	61,71,73	6.44	40 (65%)
2	NAI	C	3300	-	46,47,48	5.81	25 (54%)	61,71,73	4.16	27 (44%)
3	GLU	E	5301	-	8,9,9	1.44	1 (12%)	8,11,11	0.85	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLU	C	3301	-	-	5/9/9/9	-
3	GLU	A	1301	-	-	5/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLU	B	2301	-	-	5/9/9/9	-
3	GLU	D	4301	-	-	2/9/9/9	-
2	NAI	D	4300	-	1/1/13/16	13/29/72/72	0/5/5/5
2	NAI	B	2300	-	1/1/13/16	13/29/72/72	0/5/5/5
2	NAI	A	1300	-	2/2/13/16	15/29/72/72	0/5/5/5
2	NAI	E	5300	-	3/3/13/16	16/29/72/72	0/5/5/5
2	NAI	C	3300	-	1/1/13/16	13/29/72/72	0/5/5/5
3	GLU	E	5301	-	-	2/9/9/9	-

All (144) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	5300	NAI	PN-O3	-43.08	1.13	1.59
2	E	5300	NAI	PA-O3	19.02	1.80	1.59
2	C	3300	NAI	C8A-N7A	16.99	1.64	1.31
2	B	2300	NAI	C8A-N7A	16.98	1.64	1.31
2	D	4300	NAI	C8A-N7A	16.95	1.64	1.31
2	E	5300	NAI	C8A-N7A	16.92	1.64	1.31
2	D	4300	NAI	PA-O3	16.48	1.77	1.59
2	C	3300	NAI	PA-O3	16.45	1.77	1.59
2	B	2300	NAI	PA-O3	16.41	1.77	1.59
2	A	1300	NAI	O7N-C7N	15.91	1.61	1.24
2	A	1300	NAI	O4D-C4D	-14.49	1.12	1.45
2	D	4300	NAI	O4D-C4D	-14.47	1.12	1.45
2	C	3300	NAI	O4D-C4D	-14.47	1.12	1.45
2	B	2300	NAI	O4D-C4D	-14.46	1.12	1.45
2	E	5300	NAI	C1D-N1N	12.59	1.81	1.46
2	E	5300	NAI	C3D-C4D	-12.58	1.21	1.53
2	E	5300	NAI	C1B-N9A	-11.90	1.13	1.46
2	A	1300	NAI	PN-O3	11.13	1.71	1.59
2	E	5300	NAI	O7N-C7N	11.03	1.50	1.24
2	B	2300	NAI	PN-O3	10.07	1.70	1.59
2	D	4300	NAI	PN-O3	10.04	1.70	1.59
2	C	3300	NAI	PN-O3	9.99	1.70	1.59
2	A	1300	NAI	C7N-C3N	-9.74	1.27	1.48
2	A	1300	NAI	O4D-C1D	-9.30	1.20	1.42
2	D	4300	NAI	O4D-C1D	-9.30	1.20	1.42
2	C	3300	NAI	O4D-C1D	-9.29	1.20	1.42
2	B	2300	NAI	O4D-C1D	-9.26	1.20	1.42
2	C	3300	NAI	PA-O1A	9.22	1.82	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4300	NAI	PA-O1A	9.22	1.82	1.50
2	A	1300	NAI	PA-O1A	9.20	1.82	1.50
2	B	2300	NAI	PA-O1A	9.19	1.82	1.50
2	D	4300	NAI	C3D-C4D	-9.16	1.29	1.53
2	C	3300	NAI	C3D-C4D	-9.12	1.29	1.53
2	A	1300	NAI	C3D-C4D	-9.12	1.29	1.53
2	B	2300	NAI	C3D-C4D	-9.11	1.29	1.53
2	A	1300	NAI	C1D-N1N	8.09	1.68	1.46
2	A	1300	NAI	O4B-C1B	8.09	1.60	1.42
2	E	5300	NAI	C4A-N9A	8.04	1.54	1.37
2	C	3300	NAI	C4A-N9A	8.01	1.54	1.37
2	D	4300	NAI	C4A-N9A	8.00	1.54	1.37
2	B	2300	NAI	C4A-N9A	7.97	1.54	1.37
2	A	1300	NAI	C1B-N9A	-7.48	1.25	1.46
2	E	5300	NAI	O3D-C3D	-7.42	1.24	1.43
2	A	1300	NAI	C4A-N3A	7.40	1.48	1.34
2	E	5300	NAI	O5B-C5B	7.10	1.71	1.44
2	E	5300	NAI	C2A-N3A	7.08	1.46	1.33
2	A	1300	NAI	PN-O2N	6.99	1.75	1.50
2	C	3300	NAI	C7N-N7N	6.96	1.53	1.33
2	B	2300	NAI	C7N-N7N	6.96	1.53	1.33
2	E	5300	NAI	C7N-N7N	6.95	1.53	1.33
2	D	4300	NAI	O4B-C1B	6.93	1.58	1.42
2	D	4300	NAI	C7N-N7N	6.92	1.53	1.33
2	C	3300	NAI	O4B-C1B	6.92	1.58	1.42
2	E	5300	NAI	O4B-C1B	6.90	1.57	1.42
2	B	2300	NAI	O4B-C1B	6.89	1.57	1.42
2	C	3300	NAI	C1D-N1N	6.50	1.64	1.46
2	D	4300	NAI	C1D-N1N	6.47	1.64	1.46
2	B	2300	NAI	C1D-N1N	6.46	1.64	1.46
2	E	5300	NAI	PA-O1A	-6.45	1.28	1.50
2	A	1300	NAI	C2B-C1B	-6.35	1.33	1.53
2	E	5300	NAI	C2D-C1D	-6.34	1.33	1.53
2	A	1300	NAI	C8A-N7A	6.21	1.43	1.31
2	A	1300	NAI	C5A-C4A	-5.83	1.30	1.40
2	B	2300	NAI	PA-O2A	5.79	1.82	1.55
2	D	4300	NAI	PA-O2A	5.78	1.82	1.55
2	A	1300	NAI	PA-O2A	5.78	1.82	1.55
2	C	3300	NAI	PA-O2A	5.77	1.82	1.55
2	E	5300	NAI	PN-O5D	-5.72	1.37	1.59
2	A	1300	NAI	PA-O3	5.67	1.65	1.59
2	E	5300	NAI	C8A-N9A	5.34	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3300	NAI	C8A-N9A	5.31	1.46	1.37
2	D	4300	NAI	C8A-N9A	5.28	1.46	1.37
2	B	2300	NAI	C8A-N9A	5.27	1.46	1.37
2	E	5300	NAI	PN-O2N	5.17	1.68	1.50
2	C	3300	NAI	PN-O5D	-5.04	1.39	1.59
2	D	4300	NAI	PN-O5D	-5.03	1.39	1.59
2	B	2300	NAI	PN-O5D	-5.02	1.39	1.59
2	A	1300	NAI	PN-O1N	4.80	1.77	1.55
2	D	4300	NAI	O5B-C5B	4.47	1.61	1.44
2	B	2300	NAI	O5B-C5B	4.46	1.61	1.44
2	C	3300	NAI	O5B-C5B	4.44	1.61	1.44
2	C	3300	NAI	O7N-C7N	-4.20	1.14	1.24
2	B	2300	NAI	O7N-C7N	-4.19	1.14	1.24
2	D	4300	NAI	O7N-C7N	-4.19	1.14	1.24
2	E	5300	NAI	C5D-C4D	-4.17	1.39	1.51
2	E	5300	NAI	C5A-N7A	4.13	1.47	1.39
2	A	1300	NAI	C4N-C5N	-4.13	1.38	1.49
2	C	3300	NAI	C5A-N7A	4.12	1.47	1.39
2	D	4300	NAI	C5A-N7A	4.10	1.47	1.39
2	E	5300	NAI	O2D-C2D	-4.08	1.32	1.43
2	B	2300	NAI	C5A-N7A	4.06	1.47	1.39
2	B	2300	NAI	C6N-N1N	3.89	1.46	1.37
2	C	3300	NAI	C6N-N1N	3.89	1.46	1.37
2	D	4300	NAI	C6N-N1N	3.88	1.46	1.37
2	E	5300	NAI	C6N-N1N	3.84	1.46	1.37
2	D	4300	NAI	PA-O5B	-3.73	1.44	1.59
2	B	2300	NAI	PA-O5B	-3.72	1.44	1.59
2	C	3300	NAI	PA-O5B	-3.71	1.44	1.59
2	A	1300	NAI	PA-O5B	-3.61	1.45	1.59
3	C	3301	GLU	CB-CG	3.59	1.63	1.52
3	B	2301	GLU	CB-CG	3.59	1.63	1.52
3	A	1301	GLU	CB-CG	3.58	1.63	1.52
2	A	1300	NAI	C6N-N1N	3.52	1.45	1.37
3	E	5301	GLU	OXT-C	-3.40	1.19	1.30
3	D	4301	GLU	OXT-C	-3.37	1.19	1.30
3	C	3301	GLU	OXT-C	-3.34	1.20	1.30
3	B	2301	GLU	OXT-C	-3.32	1.20	1.30
2	A	1300	NAI	C4N-C3N	-3.01	1.44	1.50
2	A	1300	NAI	C7N-N7N	2.95	1.41	1.33
2	E	5300	NAI	PA-O5B	2.77	1.70	1.59
2	E	5300	NAI	O4D-C4D	-2.74	1.38	1.45
2	A	1300	NAI	C6N-C5N	2.70	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4300	NAI	C2N-C3N	2.69	1.42	1.35
2	C	3300	NAI	C2N-C3N	2.69	1.42	1.35
2	B	2300	NAI	C2N-C3N	2.68	1.42	1.35
2	E	5300	NAI	C2N-C3N	2.67	1.42	1.35
2	C	3300	NAI	C4A-N3A	-2.65	1.29	1.34
2	E	5300	NAI	C4A-N3A	-2.64	1.29	1.34
2	B	2300	NAI	C4A-N3A	-2.62	1.29	1.34
2	D	4300	NAI	C4A-N3A	-2.61	1.29	1.34
2	B	2300	NAI	O4B-C4B	2.46	1.50	1.45
2	C	3300	NAI	C2D-C3D	-2.45	1.46	1.53
2	A	1300	NAI	O4B-C4B	2.45	1.50	1.45
2	B	2300	NAI	C2D-C3D	-2.43	1.46	1.53
2	D	4300	NAI	O4B-C4B	2.42	1.50	1.45
2	A	1300	NAI	C2D-C3D	-2.41	1.46	1.53
2	E	5300	NAI	O4B-C4B	2.40	1.50	1.45
2	C	3300	NAI	O4B-C4B	2.40	1.50	1.45
2	C	3300	NAI	C2B-C3B	-2.40	1.46	1.53
2	D	4300	NAI	C2D-C3D	-2.39	1.46	1.53
2	A	1300	NAI	C2B-C3B	-2.39	1.46	1.53
2	D	4300	NAI	C5D-C4D	2.38	1.58	1.51
2	B	2300	NAI	C2B-C3B	-2.37	1.47	1.53
2	D	4300	NAI	C2B-C3B	-2.34	1.47	1.53
2	E	5300	NAI	C2B-C3B	-2.34	1.47	1.53
2	E	5300	NAI	PN-O1N	2.22	1.65	1.55
2	A	1300	NAI	C6A-C5A	2.20	1.42	1.39
2	C	3300	NAI	C6A-C5A	2.20	1.42	1.39
2	E	5300	NAI	C6A-C5A	2.20	1.42	1.39
2	B	2300	NAI	C6A-C5A	2.19	1.42	1.39
2	D	4300	NAI	C6A-C5A	2.18	1.42	1.39
2	A	1300	NAI	C8A-N9A	2.17	1.41	1.37
2	B	2300	NAI	O5D-C5D	2.12	1.52	1.44
2	A	1300	NAI	O5B-C5B	-2.00	1.37	1.44

All (162) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	5300	NAI	C1D-N1N-C6N	-19.57	79.40	120.77
2	E	5300	NAI	C1D-N1N-C2N	18.73	151.99	121.14
2	A	1300	NAI	C1B-N9A-C8A	-17.24	88.84	127.09
3	C	3301	GLU	CB-CG-CD	16.46	156.40	112.49
3	B	2301	GLU	CB-CG-CD	16.46	156.38	112.49
3	A	1301	GLU	CB-CG-CD	16.45	156.37	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1300	NAI	C4A-N9A-C1B	15.52	162.94	126.63
2	E	5300	NAI	O4D-C1D-N1N	15.50	137.63	108.08
2	E	5300	NAI	C1B-N9A-C8A	-15.34	93.04	127.09
2	A	1300	NAI	O4D-C1D-N1N	14.90	136.50	108.08
2	E	5300	NAI	O2A-PA-O3	-14.29	68.65	107.27
2	A	1300	NAI	O7N-C7N-N7N	-13.08	93.56	122.89
2	E	5300	NAI	O4B-C1B-N9A	13.03	133.11	108.09
2	A	1300	NAI	C3N-C7N-N7N	11.70	138.46	117.67
2	B	2300	NAI	O4D-C1D-N1N	11.30	129.64	108.08
2	D	4300	NAI	O4D-C1D-N1N	11.30	129.63	108.08
2	C	3300	NAI	O4D-C1D-N1N	11.29	129.61	108.08
2	E	5300	NAI	C2B-C1B-N9A	9.80	137.64	113.30
2	A	1300	NAI	O3-PN-O2N	8.94	137.60	110.70
2	C	3300	NAI	O4B-C1B-C2B	-8.61	88.20	106.62
2	B	2300	NAI	O4B-C1B-C2B	-8.60	88.21	106.62
2	E	5300	NAI	O4B-C1B-C2B	-8.59	88.24	106.62
2	D	4300	NAI	O4B-C1B-C2B	-8.58	88.26	106.62
2	D	4300	NAI	O2A-PA-O5B	8.37	145.51	107.57
2	B	2300	NAI	O2A-PA-O5B	8.36	145.46	107.57
2	C	3300	NAI	O2A-PA-O5B	8.36	145.45	107.57
2	C	3300	NAI	N9A-C8A-N7A	-8.19	102.32	113.94
2	D	4300	NAI	N9A-C8A-N7A	-8.18	102.33	113.94
2	B	2300	NAI	N9A-C8A-N7A	-8.18	102.33	113.94
2	E	5300	NAI	N9A-C8A-N7A	-8.16	102.36	113.94
2	A	1300	NAI	O4B-C4B-C3B	-8.08	89.11	105.15
2	B	2300	NAI	O4B-C4B-C3B	-8.07	89.14	105.15
2	C	3300	NAI	O4B-C4B-C3B	-8.04	89.19	105.15
2	E	5300	NAI	O4B-C4B-C3B	-8.03	89.21	105.15
2	D	4300	NAI	O4B-C4B-C3B	-8.03	89.21	105.15
2	D	4300	NAI	O5B-C5B-C4B	7.86	135.77	108.99
2	B	2300	NAI	O5B-C5B-C4B	7.86	135.75	108.99
2	C	3300	NAI	O5B-C5B-C4B	7.85	135.73	108.99
2	D	4300	NAI	C4B-O4B-C1B	-7.79	92.27	109.47
2	C	3300	NAI	C4B-O4B-C1B	-7.78	92.28	109.47
2	B	2300	NAI	C4B-O4B-C1B	-7.78	92.29	109.47
2	E	5300	NAI	C4B-O4B-C1B	-7.78	92.29	109.47
2	A	1300	NAI	O2A-PA-O5B	7.70	142.46	107.57
2	A	1300	NAI	C4D-O4D-C1D	7.68	126.43	109.47
2	D	4300	NAI	C4D-O4D-C1D	7.67	126.39	109.47
2	B	2300	NAI	C4D-O4D-C1D	7.66	126.38	109.47
2	C	3300	NAI	C4D-O4D-C1D	7.64	126.34	109.47
2	B	2300	NAI	O2A-PA-O3	-7.63	86.65	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3300	NAI	O2A-PA-O3	-7.63	86.66	107.27
2	D	4300	NAI	O2A-PA-O3	-7.62	86.67	107.27
2	A	1300	NAI	C4B-O4B-C1B	-7.53	92.84	109.47
2	A	1300	NAI	O1N-PN-O3	7.31	127.02	107.27
2	A	1300	NAI	C2D-C1D-N1N	7.26	131.15	113.31
2	A	1300	NAI	O2A-PA-O3	-6.91	88.58	107.27
2	D	4300	NAI	O4D-C1D-C2D	-6.69	92.31	106.62
2	A	1300	NAI	O4D-C1D-C2D	-6.68	92.32	106.62
2	B	2300	NAI	O4D-C1D-C2D	-6.68	92.32	106.62
2	C	3300	NAI	O4D-C1D-C2D	-6.68	92.32	106.62
2	C	3300	NAI	C5B-C4B-C3B	6.66	139.20	115.21
2	B	2300	NAI	C5B-C4B-C3B	6.66	139.18	115.21
2	D	4300	NAI	C5B-C4B-C3B	6.66	139.18	115.21
2	E	5300	NAI	O5B-PA-O1A	6.63	135.21	108.94
2	E	5300	NAI	C5D-C4D-C3D	6.55	138.80	115.21
2	E	5300	NAI	O4B-C4B-C5B	-6.43	88.75	109.33
2	E	5300	NAI	O1N-PN-O2N	-6.22	83.50	112.44
2	A	1300	NAI	O4B-C1B-C2B	-6.16	93.44	106.62
2	B	2300	NAI	C4A-N9A-C8A	6.08	112.12	105.74
2	A	1300	NAI	C6A-C5A-C4A	6.08	122.88	116.24
2	C	3300	NAI	C4A-N9A-C8A	6.08	112.12	105.74
2	D	4300	NAI	C4A-N9A-C8A	6.06	112.10	105.74
2	E	5300	NAI	C4A-N9A-C8A	5.99	112.03	105.74
2	B	2300	NAI	C4A-N9A-C1B	-5.71	113.28	126.63
2	C	3300	NAI	C4A-N9A-C1B	-5.70	113.30	126.63
2	D	4300	NAI	C4A-N9A-C1B	-5.69	113.32	126.63
2	E	5300	NAI	PN-O5D-C5D	5.67	153.84	121.35
2	E	5300	NAI	O5B-C5B-C4B	5.44	127.53	108.99
2	A	1300	NAI	C5A-C4A-N3A	-5.40	119.76	127.18
2	E	5300	NAI	O3-PN-O2N	5.29	126.61	110.70
2	C	3300	NAI	C5D-C4D-C3D	5.18	133.84	115.21
2	E	5300	NAI	O1N-PN-O3	5.17	121.26	107.27
2	C	3300	NAI	O2A-PA-O1A	-5.17	88.42	112.44
2	B	2300	NAI	O2A-PA-O1A	-5.16	88.42	112.44
2	D	4300	NAI	O2A-PA-O1A	-5.16	88.43	112.44
2	A	1300	NAI	O2A-PA-O1A	-5.16	88.43	112.44
2	E	5300	NAI	PA-O5B-C5B	-5.15	91.82	121.35
2	D	4300	NAI	O5D-C5D-C4D	-5.12	91.57	108.99
2	D	4300	NAI	C5D-C4D-C3D	5.11	133.60	115.21
2	A	1300	NAI	N9A-C8A-N7A	-5.07	106.75	113.94
2	A	1300	NAI	O4B-C1B-N9A	-5.03	98.43	108.09
2	B	2300	NAI	C5D-C4D-C3D	4.80	132.49	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1300	NAI	O1N-PN-O2N	-4.73	90.44	112.44
2	C	3300	NAI	O5D-C5D-C4D	-4.73	92.90	108.99
2	A	1300	NAI	O5B-PA-O1A	-4.59	90.75	108.94
2	E	5300	NAI	C5B-C4B-C3B	-4.59	98.70	115.21
3	D	4301	GLU	OXT-C-O	-4.53	113.81	124.08
2	A	1300	NAI	O4D-C4D-C5D	4.44	123.57	109.33
2	C	3300	NAI	C6N-N1N-C2N	4.39	124.02	119.32
2	D	4300	NAI	O5B-PA-O1A	-4.37	91.61	108.94
2	C	3300	NAI	O5B-PA-O1A	-4.37	91.63	108.94
2	B	2300	NAI	O5B-PA-O1A	-4.37	91.63	108.94
2	A	1300	NAI	C6A-C5A-N7A	-4.33	123.83	132.97
2	B	2300	NAI	C6N-N1N-C2N	4.32	123.95	119.32
2	B	2300	NAI	O4B-C4B-C5B	-4.30	95.55	109.33
2	D	4300	NAI	O4B-C4B-C5B	-4.30	95.57	109.33
2	C	3300	NAI	O4B-C4B-C5B	-4.29	95.58	109.33
2	D	4300	NAI	C6N-N1N-C2N	4.29	123.92	119.32
2	E	5300	NAI	C6N-N1N-C2N	4.29	123.91	119.32
2	E	5300	NAI	O3-PA-O1A	4.28	123.58	110.70
2	C	3300	NAI	O1N-PN-O5D	4.27	126.93	107.57
2	D	4300	NAI	O1N-PN-O5D	4.27	126.90	107.57
2	B	2300	NAI	O1N-PN-O5D	4.27	126.90	107.57
2	B	2300	NAI	O5D-C5D-C4D	-4.18	94.75	108.99
2	E	5300	NAI	C6A-N1A-C2A	4.16	120.71	115.80
2	D	4300	NAI	O3-PA-O1A	-4.15	98.23	110.70
2	C	3300	NAI	O3-PA-O1A	-4.13	98.29	110.70
2	B	2300	NAI	O3-PA-O1A	-4.13	98.29	110.70
2	E	5300	NAI	O7N-C7N-N7N	-4.05	113.81	122.89
2	B	2300	NAI	O1N-PN-O2N	-3.88	94.41	112.44
2	C	3300	NAI	O1N-PN-O2N	-3.88	94.41	112.44
2	D	4300	NAI	O1N-PN-O2N	-3.87	94.47	112.44
2	A	1300	NAI	C1D-N1N-C2N	-3.86	114.79	121.14
2	E	5300	NAI	C4A-N9A-C1B	3.82	135.56	126.63
2	E	5300	NAI	N1A-C2A-N3A	-3.69	121.06	127.33
2	A	1300	NAI	PA-O5B-C5B	-3.69	100.20	121.35
2	A	1300	NAI	O7N-C7N-C3N	3.54	127.57	120.90
2	A	1300	NAI	O5B-C5B-C4B	3.51	120.96	108.99
2	A	1300	NAI	PN-O5D-C5D	3.45	141.13	121.35
2	E	5300	NAI	O2A-PA-O5B	-3.40	92.14	107.57
2	A	1300	NAI	C5D-C4D-C3D	3.31	127.14	115.21
2	E	5300	NAI	O4D-C4D-C3D	3.17	111.44	105.15
2	A	1300	NAI	C3B-C2B-C1B	3.13	107.39	101.46
2	A	1300	NAI	O3-PA-O1A	-3.13	101.30	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1300	NAI	C5B-C4B-C3B	3.10	126.35	115.21
2	E	5300	NAI	O2A-PA-O1A	3.08	126.79	112.44
2	B	2300	NAI	O4D-C4D-C5D	2.94	118.77	109.33
2	A	1300	NAI	N3A-C4A-N9A	2.91	132.12	127.17
2	C	3300	NAI	C3N-C2N-N1N	-2.90	118.95	123.20
2	D	4300	NAI	C3N-C2N-N1N	-2.87	118.99	123.20
2	B	2300	NAI	C3N-C2N-N1N	-2.87	119.00	123.20
2	C	3300	NAI	C1D-N1N-C6N	-2.85	114.74	120.77
2	B	2300	NAI	C1D-N1N-C6N	-2.85	114.75	120.77
2	E	5300	NAI	C3N-C2N-N1N	-2.84	119.03	123.20
2	D	4300	NAI	C1D-N1N-C6N	-2.82	114.80	120.77
2	B	2300	NAI	C2B-C1B-N9A	-2.77	106.42	113.30
2	C	3300	NAI	C2B-C1B-N9A	-2.75	106.47	113.30
2	D	4300	NAI	C2B-C1B-N9A	-2.75	106.48	113.30
2	A	1300	NAI	O1N-PN-O5D	-2.65	95.56	107.57
2	D	4300	NAI	O4D-C4D-C5D	2.57	117.58	109.33
2	E	5300	NAI	C3D-C2D-C1D	2.54	106.28	101.46
2	C	3300	NAI	O4D-C4D-C5D	2.52	117.41	109.33
2	E	5300	NAI	O7N-C7N-C3N	2.52	125.65	120.90
2	E	5300	NAI	O3D-C3D-C4D	-2.51	103.87	111.08
2	E	5300	NAI	O5D-C5D-C4D	2.50	117.50	108.99
2	E	5300	NAI	O3D-C3D-C2D	2.47	119.73	111.82
2	E	5300	NAI	O2D-C2D-C3D	-2.40	104.11	111.82
2	E	5300	NAI	O2D-C2D-C1D	2.28	117.97	110.10
2	A	1300	NAI	C4A-C5A-N7A	2.19	113.27	109.94
2	C	3300	NAI	O1N-PN-O3	2.08	112.90	107.27
2	E	5300	NAI	C2D-C3D-C4D	2.06	106.60	102.61
2	B	2300	NAI	O1N-PN-O3	2.06	112.83	107.27
2	A	1300	NAI	O4B-C4B-C5B	-2.05	102.76	109.33
2	D	4300	NAI	O1N-PN-O3	2.05	112.82	107.27

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1300	NAI	C1D
2	A	1300	NAI	C4D
2	B	2300	NAI	C4D
2	C	3300	NAI	C4D
2	D	4300	NAI	C4D
2	E	5300	NAI	C1B
2	E	5300	NAI	C1D
2	E	5300	NAI	C4D

All (89) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1300	NAI	C5B-O5B-PA-O2A
2	A	1300	NAI	C5B-O5B-PA-O3
2	A	1300	NAI	O4B-C4B-C5B-O5B
2	A	1300	NAI	C5D-O5D-PN-O1N
2	A	1300	NAI	C4D-C5D-O5D-PN
2	A	1300	NAI	C2D-C1D-N1N-C2N
2	B	2300	NAI	C5B-O5B-PA-O1A
2	B	2300	NAI	C5B-O5B-PA-O2A
2	B	2300	NAI	C4B-C5B-O5B-PA
2	B	2300	NAI	C5D-O5D-PN-O1N
2	B	2300	NAI	C5D-O5D-PN-O2N
2	B	2300	NAI	C4D-C5D-O5D-PN
2	C	3300	NAI	C5B-O5B-PA-O1A
2	C	3300	NAI	C5B-O5B-PA-O2A
2	C	3300	NAI	C4B-C5B-O5B-PA
2	C	3300	NAI	C5D-O5D-PN-O1N
2	C	3300	NAI	C5D-O5D-PN-O2N
2	C	3300	NAI	C4D-C5D-O5D-PN
2	D	4300	NAI	C5B-O5B-PA-O1A
2	D	4300	NAI	C5B-O5B-PA-O2A
2	D	4300	NAI	C4B-C5B-O5B-PA
2	D	4300	NAI	C5D-O5D-PN-O1N
2	D	4300	NAI	C5D-O5D-PN-O2N
2	D	4300	NAI	C4D-C5D-O5D-PN
2	E	5300	NAI	C5B-O5B-PA-O3
2	E	5300	NAI	C4B-C5B-O5B-PA
2	E	5300	NAI	O4B-C1B-N9A-C8A
3	A	1301	GLU	O-C-CA-N
3	A	1301	GLU	CA-CB-CG-CD
3	B	2301	GLU	CA-CB-CG-CD
3	C	3301	GLU	CA-CB-CG-CD
2	A	1300	NAI	O4D-C1D-N1N-C2N
2	B	2300	NAI	O4D-C1D-N1N-C2N
2	C	3300	NAI	O4D-C1D-N1N-C2N
2	D	4300	NAI	O4D-C1D-N1N-C2N
2	A	1300	NAI	C3B-C4B-C5B-O5B
2	A	1300	NAI	C3D-C4D-C5D-O5D
2	B	2300	NAI	C3D-C4D-C5D-O5D
2	C	3300	NAI	C3D-C4D-C5D-O5D
2	D	4300	NAI	C3D-C4D-C5D-O5D
3	B	2301	GLU	OXT-C-CA-N
3	C	3301	GLU	OXT-C-CA-N

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Mol	Chain	Res	Type	Atoms
3	D	4301	GLU	OXT-C-CA-N
3	E	5301	GLU	OXT-C-CA-N
2	A	1300	NAI	C2B-C1B-N9A-C8A
2	E	5300	NAI	C2D-C1D-N1N-C6N
2	E	5300	NAI	O4B-C4B-C5B-O5B
3	A	1301	GLU	OXT-C-CA-N
2	A	1300	NAI	C2D-C1D-N1N-C6N
2	E	5300	NAI	C4D-C5D-O5D-PN
2	B	2300	NAI	O4B-C4B-C5B-O5B
2	C	3300	NAI	O4B-C4B-C5B-O5B
2	D	4300	NAI	O4B-C4B-C5B-O5B
2	E	5300	NAI	O4D-C4D-C5D-O5D
2	E	5300	NAI	C3D-C4D-C5D-O5D
2	E	5300	NAI	O4D-C1D-N1N-C2N
2	A	1300	NAI	C4B-C5B-O5B-PA
2	A	1300	NAI	C2B-C1B-N9A-C4A
2	B	2300	NAI	C2B-C1B-N9A-C8A
2	C	3300	NAI	C2B-C1B-N9A-C8A
2	D	4300	NAI	C2B-C1B-N9A-C8A
2	E	5300	NAI	C2B-C1B-N9A-C8A
2	B	2300	NAI	PN-O3-PA-O2A
2	C	3300	NAI	PN-O3-PA-O2A
2	D	4300	NAI	PN-O3-PA-O2A
2	A	1300	NAI	C5B-O5B-PA-O1A
2	A	1300	NAI	C5D-O5D-PN-O3
2	B	2300	NAI	C5D-O5D-PN-O3
2	C	3300	NAI	C5D-O5D-PN-O3
2	D	4300	NAI	C5D-O5D-PN-O3
2	E	5300	NAI	C5B-O5B-PA-O1A
2	E	5300	NAI	PA-O3-PN-O1N
2	E	5300	NAI	O4B-C1B-N9A-C4A
3	B	2301	GLU	OE2-CD-CG-CB
3	A	1301	GLU	OE2-CD-CG-CB
3	C	3301	GLU	OE2-CD-CG-CB
3	A	1301	GLU	OE1-CD-CG-CB
3	B	2301	GLU	OE1-CD-CG-CB
3	C	3301	GLU	OE1-CD-CG-CB
2	E	5300	NAI	C3B-C4B-C5B-O5B
2	B	2300	NAI	PA-O3-PN-O1N
2	C	3300	NAI	PA-O3-PN-O1N
2	D	4300	NAI	PA-O3-PN-O1N
2	E	5300	NAI	C2B-C1B-N9A-C4A

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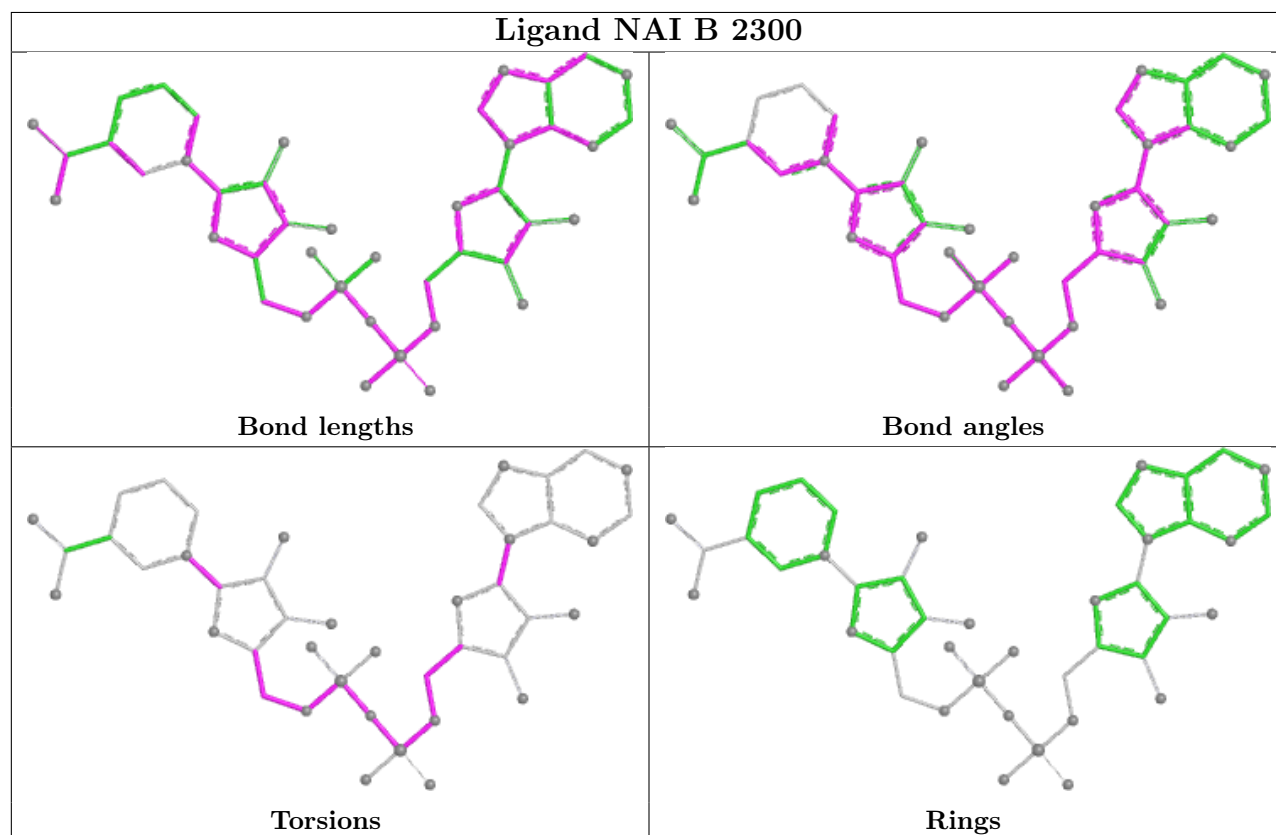
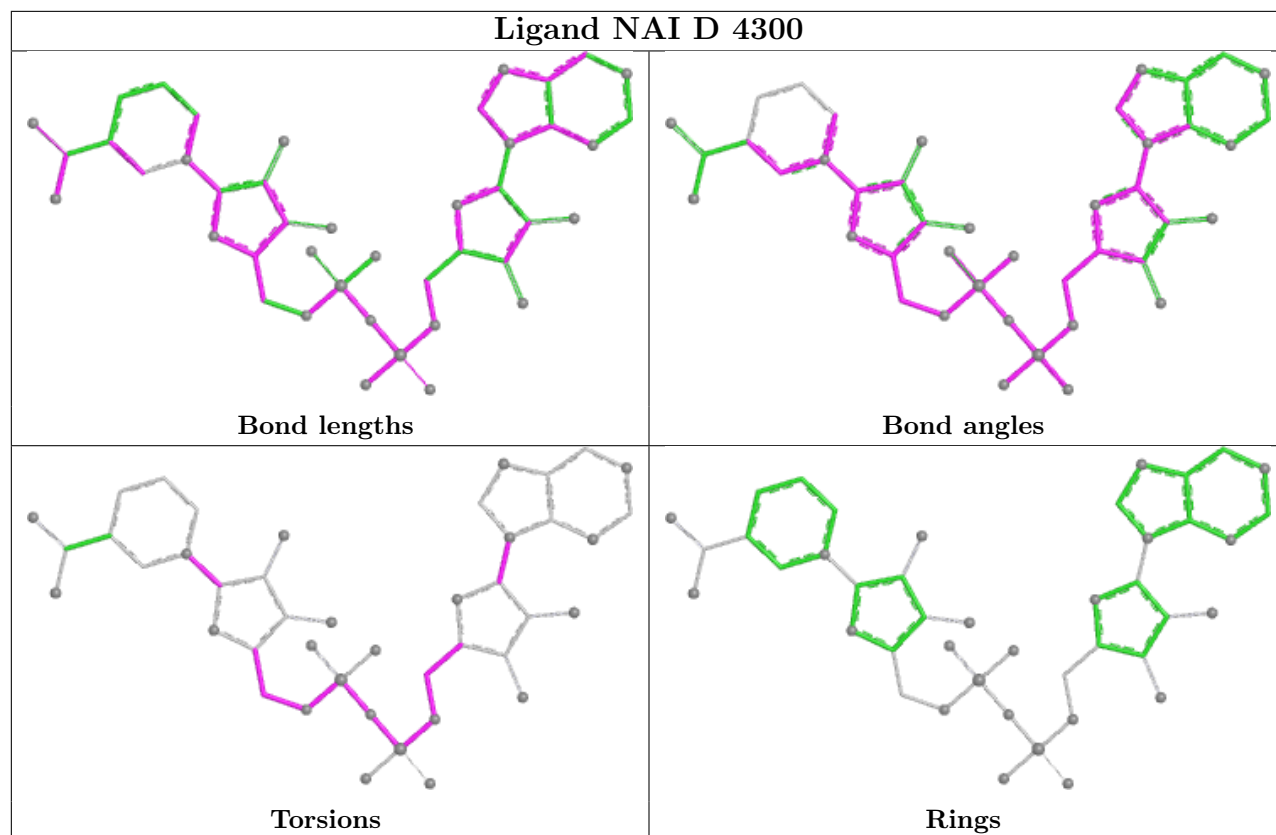
Mol	Chain	Res	Type	Atoms
3	B	2301	GLU	O-C-CA-N
3	C	3301	GLU	O-C-CA-N
3	D	4301	GLU	O-C-CA-N
3	E	5301	GLU	O-C-CA-N
2	E	5300	NAI	PN-O3-PA-O2A

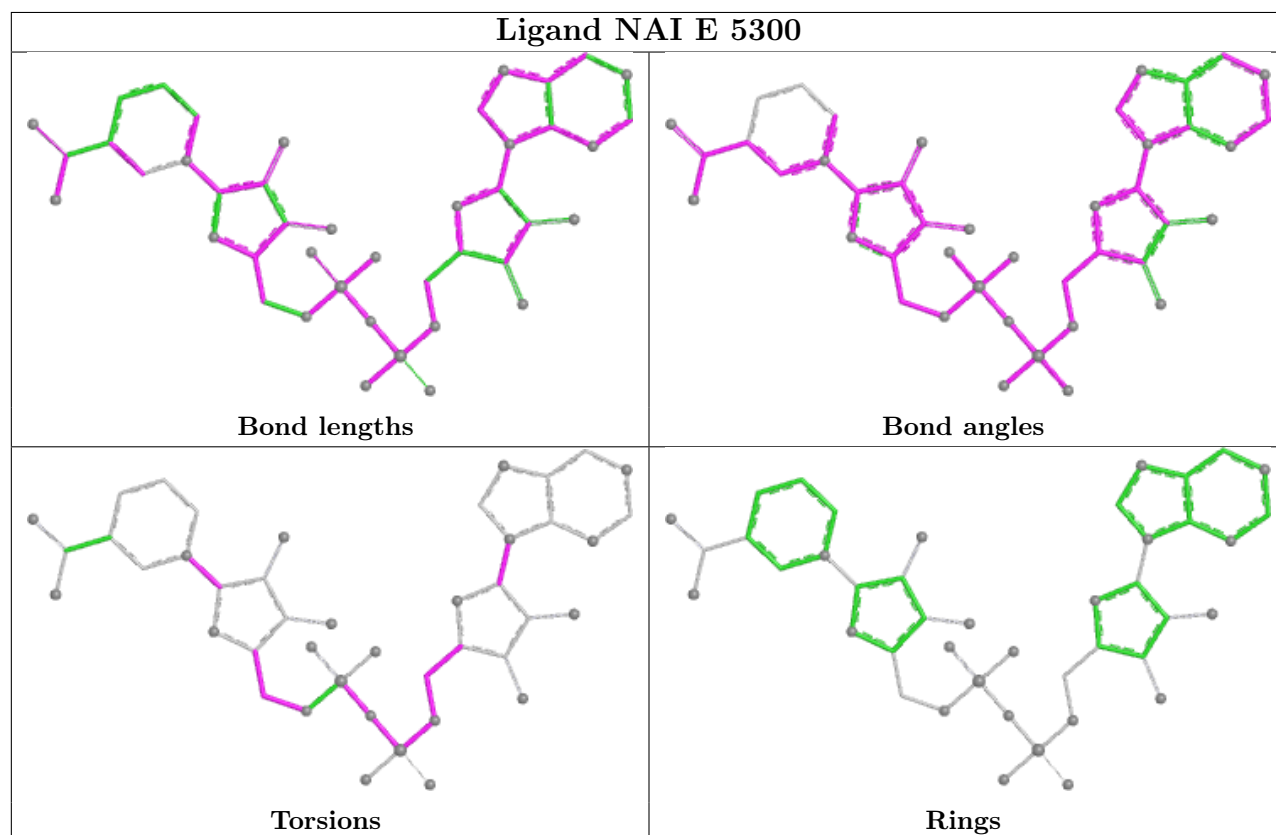
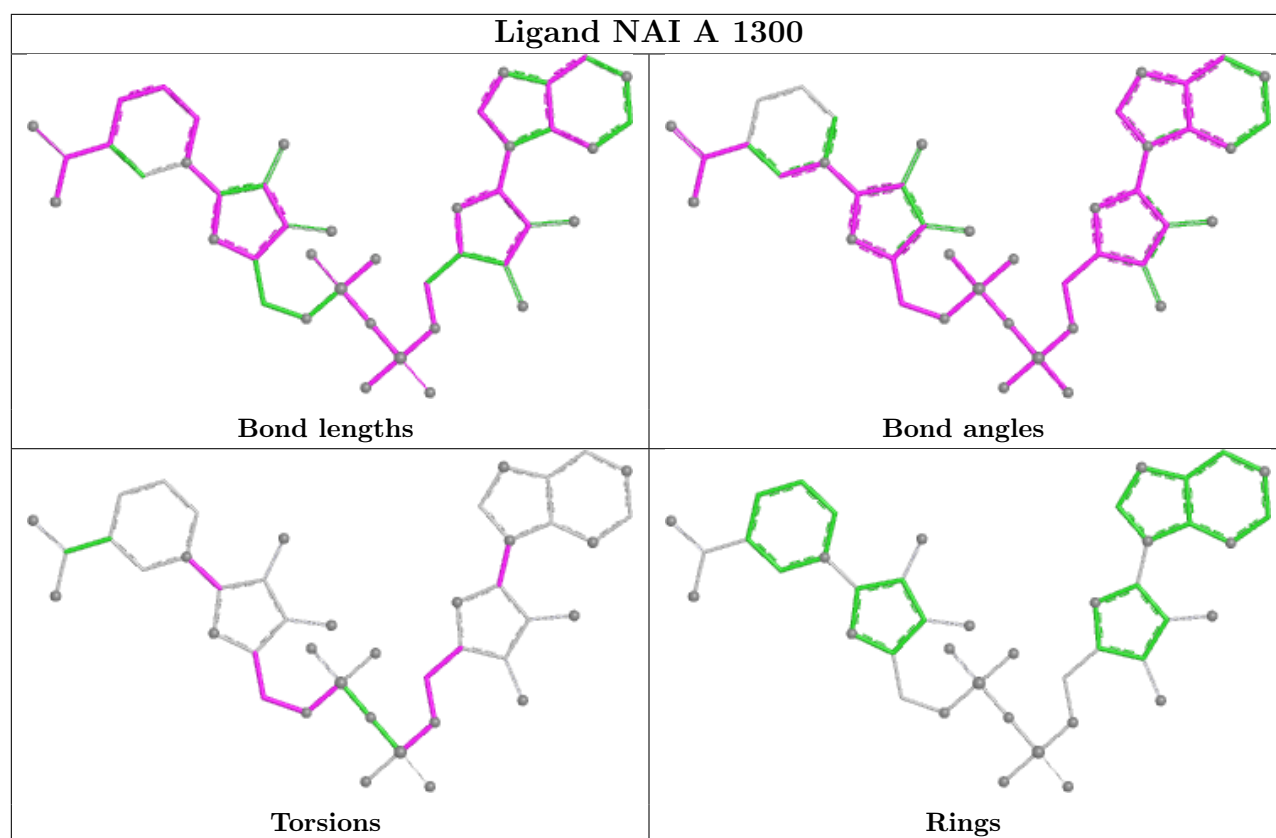
There are no ring outliers.

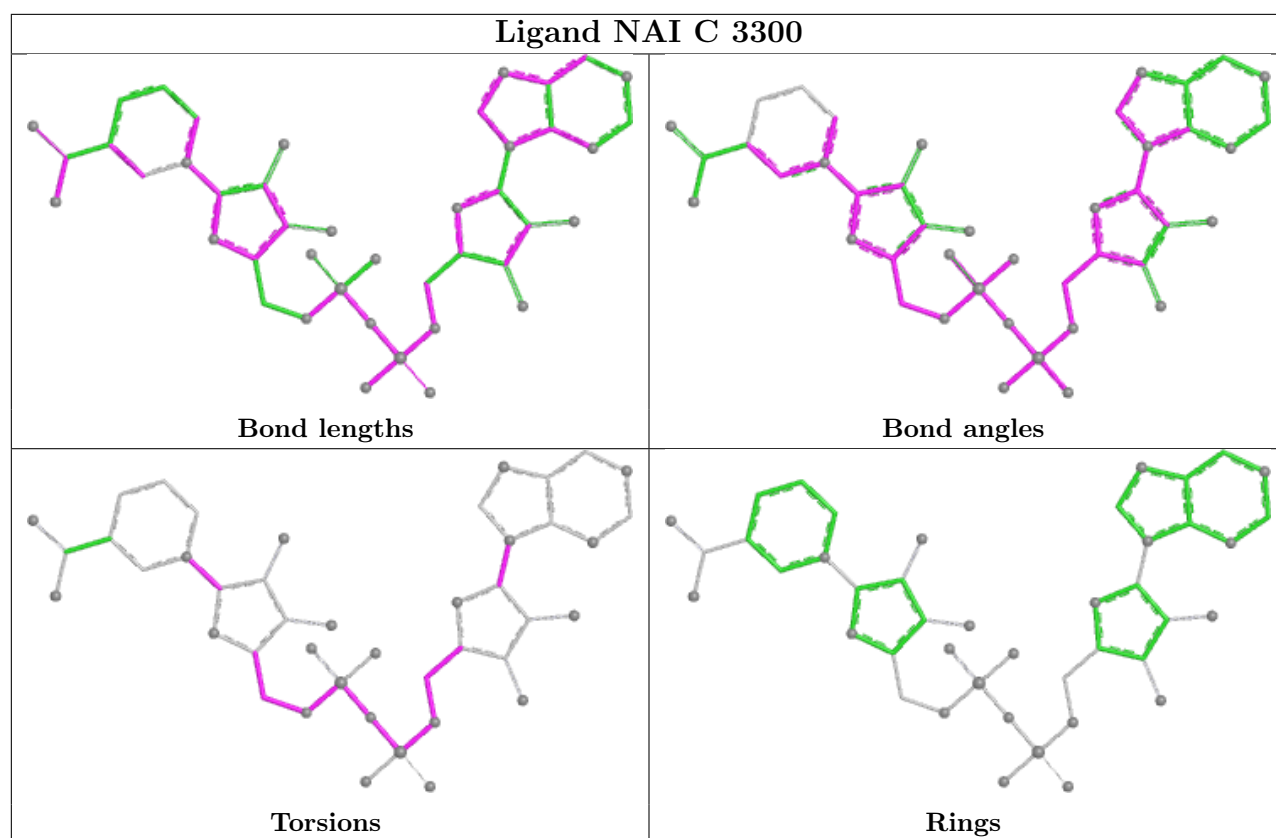
10 monomers are involved in 231 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3301	GLU	12	0
3	A	1301	GLU	8	0
3	B	2301	GLU	17	0
3	D	4301	GLU	21	0
2	D	4300	NAI	40	0
2	B	2300	NAI	68	5
2	A	1300	NAI	26	0
2	E	5300	NAI	32	1
2	C	3300	NAI	38	4
3	E	5301	GLU	11	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	277/277 (100%)	0.06	3 (1%) 78 59	32, 82, 117, 153	0
1	B	276/277 (99%)	0.49	18 (6%) 25 13	39, 129, 183, 200	0
1	C	277/277 (100%)	0.51	24 (8%) 16 9	31, 125, 181, 195	0
1	D	277/277 (100%)	0.02	2 (0%) 84 68	34, 76, 118, 191	0
1	E	277/277 (100%)	0.14	6 (2%) 62 41	24, 80, 128, 142	0
All	All	1384/1385 (99%)	0.24	53 (3%) 44 25	24, 87, 168, 200	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	96	ALA	4.5
1	C	32	ALA	3.8
1	A	8	ALA	3.7
1	C	97	ALA	3.7
1	C	70	VAL	3.6
1	C	64	ASP	3.4
1	B	98	GLY	3.4
1	B	162	VAL	3.3
1	B	92	VAL	3.3
1	C	39	LEU	3.1
1	B	204	ARG	3.0
1	C	35	PRO	3.0
1	A	204	ARG	2.9
1	C	92	VAL	2.9
1	E	73	HIS	2.8
1	C	52	LEU	2.8
1	E	98	GLY	2.7
1	B	32	ALA	2.6
1	B	13	PHE	2.6
1	B	146	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	39	LEU	2.6
1	B	136	ALA	2.5
1	B	152	LEU	2.5
1	B	220	SER	2.5
1	C	107	LYS	2.5
1	D	200	ARG	2.4
1	C	25	LEU	2.4
1	C	148	LEU	2.4
1	E	272	ALA	2.4
1	B	139	THR	2.3
1	C	118	ILE	2.3
1	C	24	VAL	2.3
1	B	148	LEU	2.3
1	C	78	ILE	2.3
1	C	145	ASP	2.3
1	B	221	GLU	2.3
1	B	14	ALA	2.3
1	C	14	ALA	2.3
1	B	50	VAL	2.2
1	C	94	SER	2.2
1	B	90	HIS	2.2
1	C	146	GLY	2.2
1	D	268	LEU	2.2
1	C	110	ALA	2.1
1	C	11	LEU	2.1
1	A	224	PRO	2.1
1	B	24	VAL	2.1
1	B	-1	ARG	2.1
1	E	10	GLN	2.1
1	C	6	ILE	2.0
1	C	10	GLN	2.0
1	C	45	LEU	2.0
1	E	95	CYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

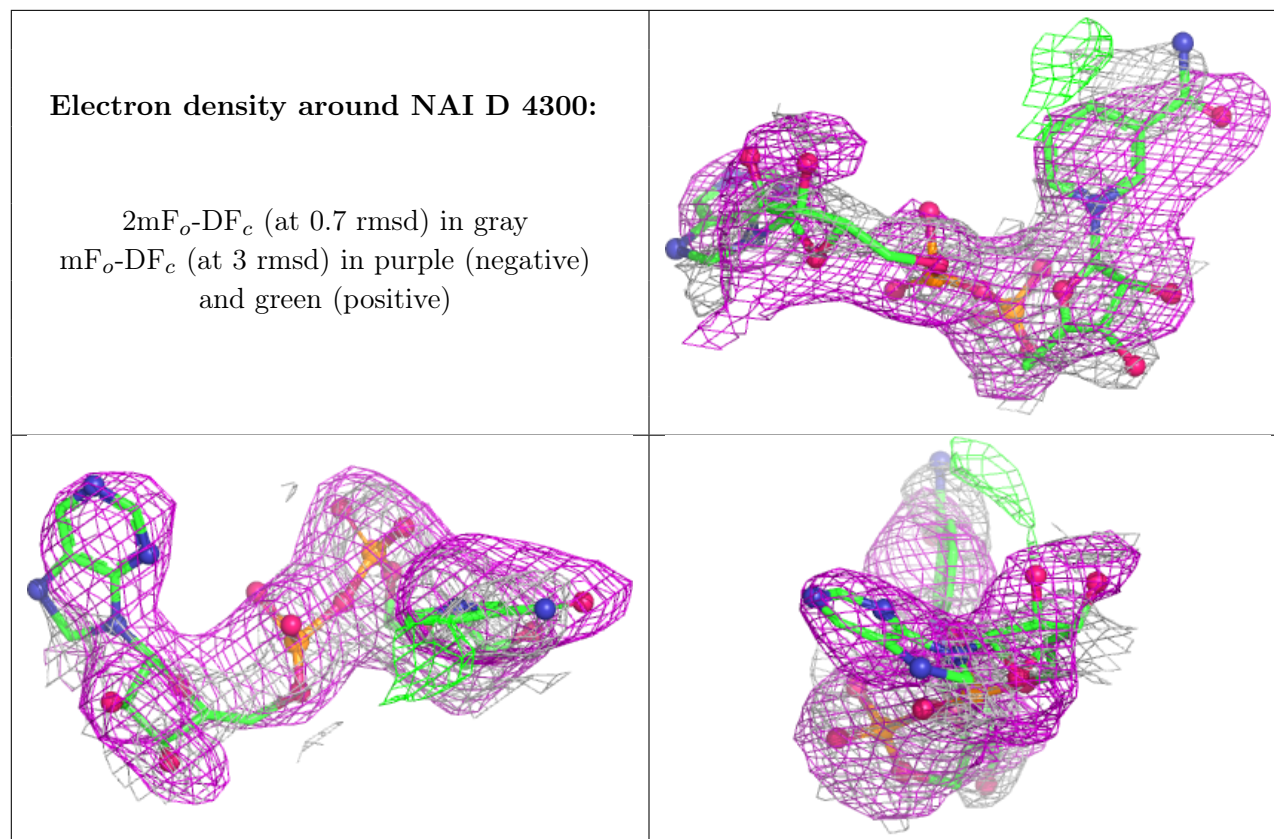
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

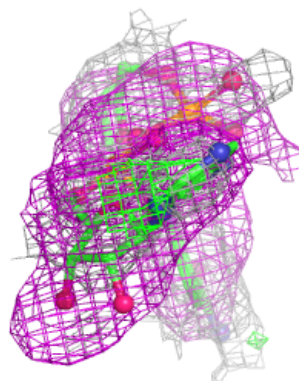
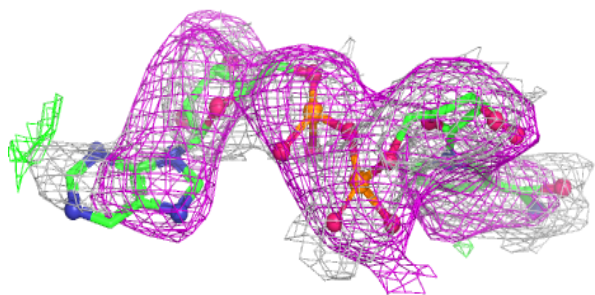
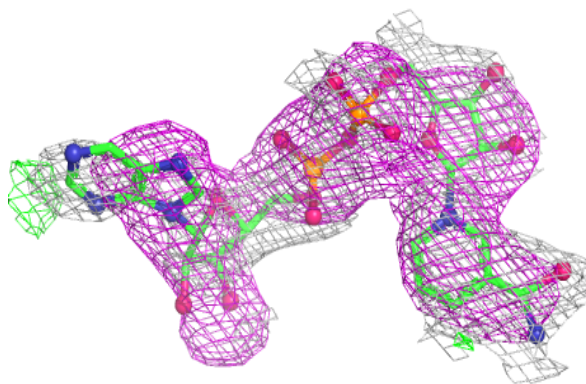
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GLU	C	3301	10/10	0.13	0.20	200,200,200,200	0
3	GLU	A	1301	10/10	0.16	0.20	120,131,140,140	0
3	GLU	B	2301	10/10	0.26	0.19	192,200,200,200	0
3	GLU	E	5301	10/10	0.34	0.28	195,200,200,200	0
2	NAI	D	4300	43/44	0.44	0.23	81,91,95,95	0
2	NAI	A	1300	43/44	0.52	0.19	63,93,95,95	0
2	NAI	E	5300	43/44	0.52	0.21	69,94,95,95	0
2	NAI	C	3300	43/44	0.55	0.26	189,195,195,195	0
3	GLU	D	4301	10/10	0.58	0.21	182,193,196,198	0
2	NAI	B	2300	43/44	0.63	0.19	192,195,195,195	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

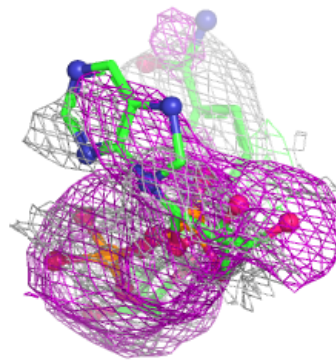
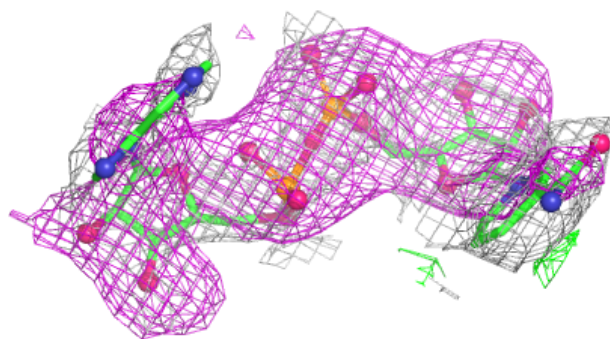
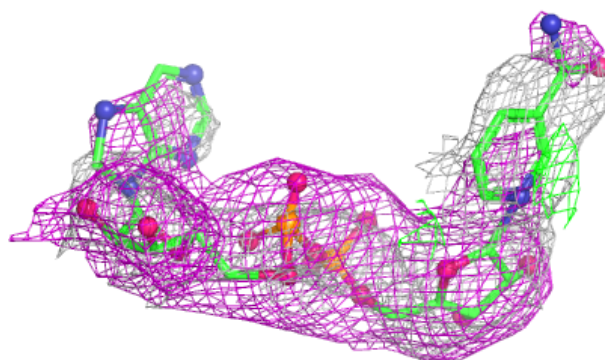


Electron density around NAI A 1300:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

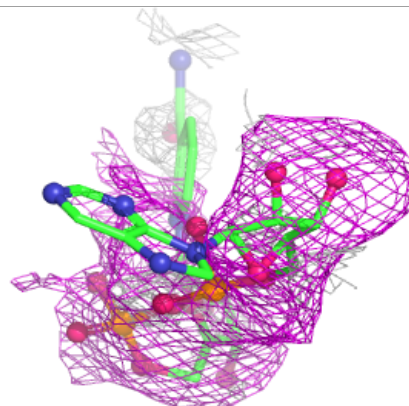
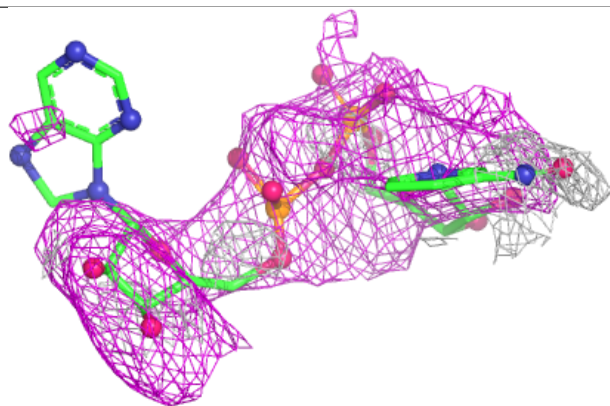
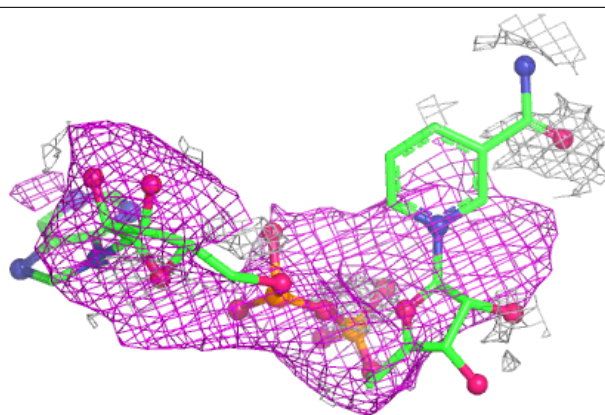
**Electron density around NAI E 5300:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

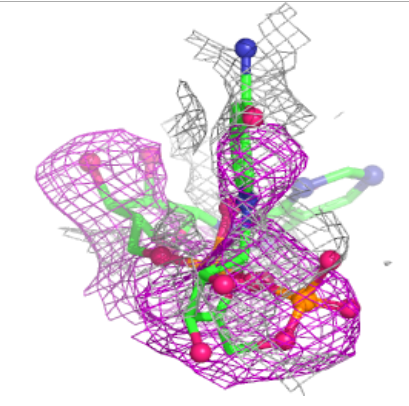
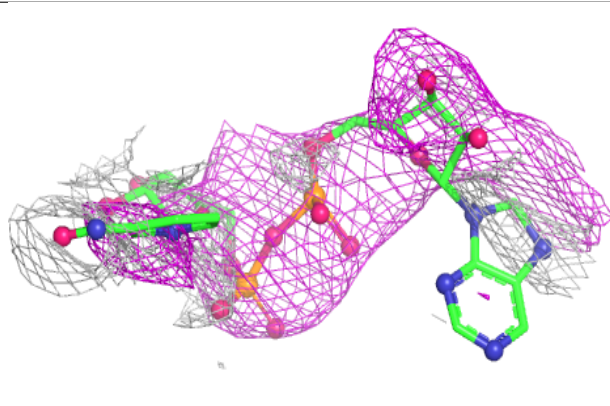
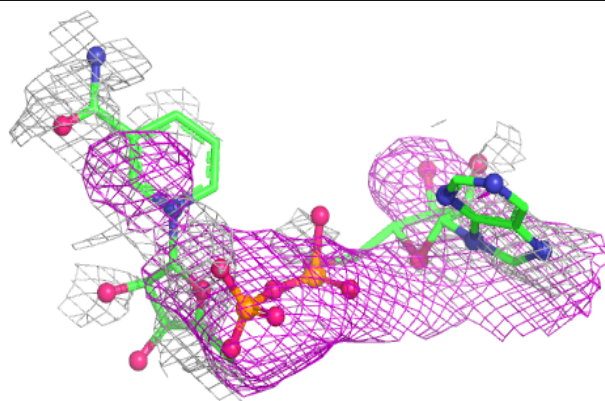


Electron density around NAI C 3300:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around NAI B 2300:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.