



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:00 AM UTC

PDB ID : 2BMA / pdb_00002bma
Title : The crystal structure of Plasmodium falciparum glutamate dehydrogenase, a putative target for novel antimalarial drugs
Authors : Werner, C.; Stubbs, M.T.; Krauth-Siege, R.L.; Klebe, G.
Deposited on : 2005-03-10
Resolution : 2.70 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

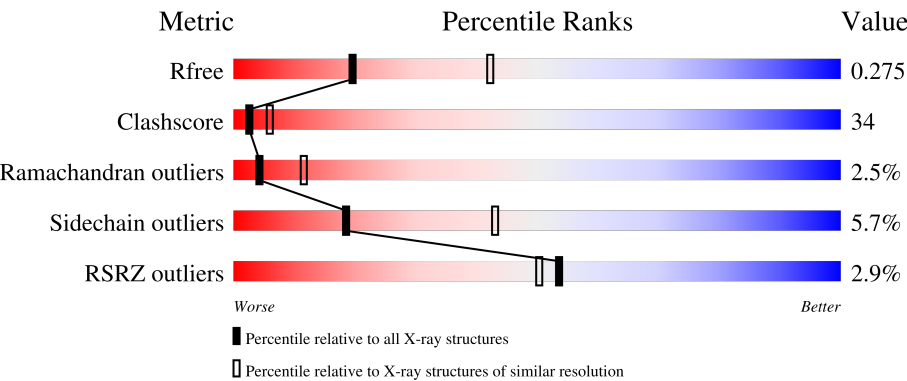
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	470	5% 38% 54% 7% ..
1	B	470	% 54% 39% 6% .
1	C	470	4% 40% 52% 7% ..
1	D	470	% 55% 39% 6% .
1	E	470	% 56% 38% 6% .

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Mol	Chain	Length	Quality of chain
1	F	470	4% 39% 52% 7% ..

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 22068 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 GLUTAMATE DEHYDROGENASE (NADP+).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	0	0
			3678	2350	619	690	19			
1	B	467	Total	C	N	O	S	0	0	0
			3678	2350	619	690	19			
1	C	467	Total	C	N	O	S	0	0	0
			3678	2350	619	690	19			
1	D	467	Total	C	N	O	S	0	0	0
			3678	2350	619	690	19			
1	E	467	Total	C	N	O	S	0	0	0
			3678	2350	619	690	19			
1	F	467	Total	C	N	O	S	0	0	0
			3678	2350	619	690	19			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	325	ASP	GLU	conflict	UNP O96940
A	326	VAL	ILE	conflict	UNP O96940
A	327	ASP	ASN	conflict	UNP O96940
A	329	ASP	GLU	conflict	UNP O96940
A	330	GLN	ASP	conflict	UNP O96940
B	325	ASP	GLU	conflict	UNP O96940
B	326	VAL	ILE	conflict	UNP O96940
B	327	ASP	ASN	conflict	UNP O96940
B	329	ASP	GLU	conflict	UNP O96940
B	330	GLN	ASP	conflict	UNP O96940
C	325	ASP	GLU	conflict	UNP O96940
C	326	VAL	ILE	conflict	UNP O96940
C	327	ASP	ASN	conflict	UNP O96940
C	329	ASP	GLU	conflict	UNP O96940
C	330	GLN	ASP	conflict	UNP O96940
D	325	ASP	GLU	conflict	UNP O96940
D	326	VAL	ILE	conflict	UNP O96940

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Chain	Residue	Modelled	Actual	Comment	Reference
D	327	ASP	ASN	conflict	UNP O96940
D	329	ASP	GLU	conflict	UNP O96940
D	330	GLN	ASP	conflict	UNP O96940
E	325	ASP	GLU	conflict	UNP O96940
E	326	VAL	ILE	conflict	UNP O96940
E	327	ASP	ASN	conflict	UNP O96940
E	329	ASP	GLU	conflict	UNP O96940
E	330	GLN	ASP	conflict	UNP O96940
F	325	ASP	GLU	conflict	UNP O96940
F	326	VAL	ILE	conflict	UNP O96940
F	327	ASP	ASN	conflict	UNP O96940
F	329	ASP	GLU	conflict	UNP O96940
F	330	GLN	ASP	conflict	UNP O96940

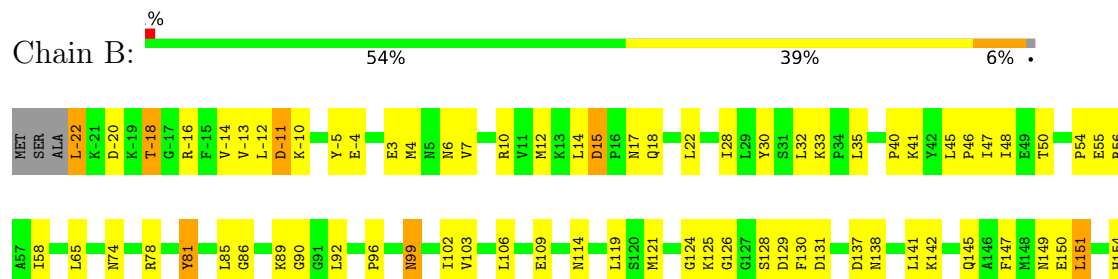
3 Residue-property plots

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.

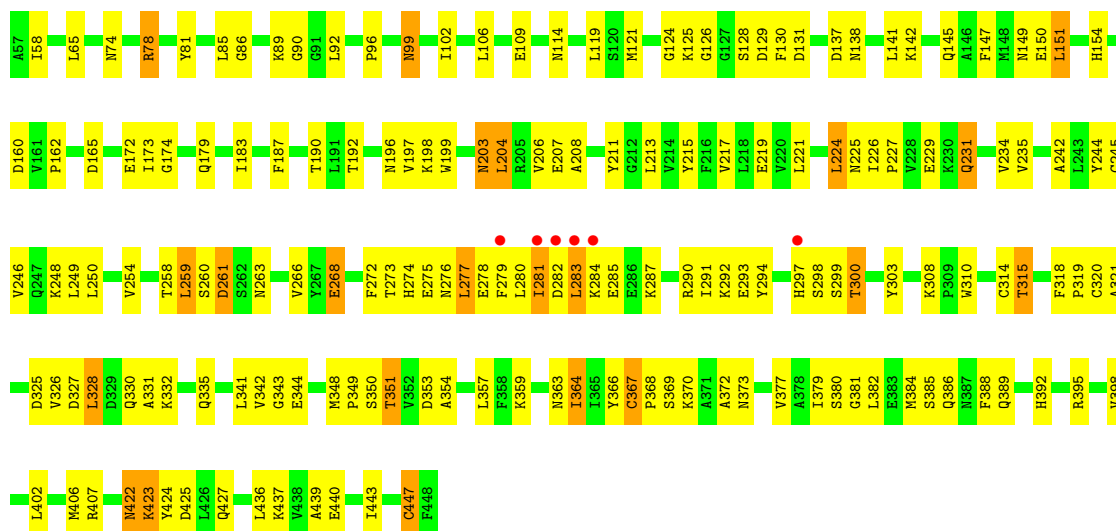
• Molecule 1: GLUTAMATE DEHYDROGENASE (NADP+)



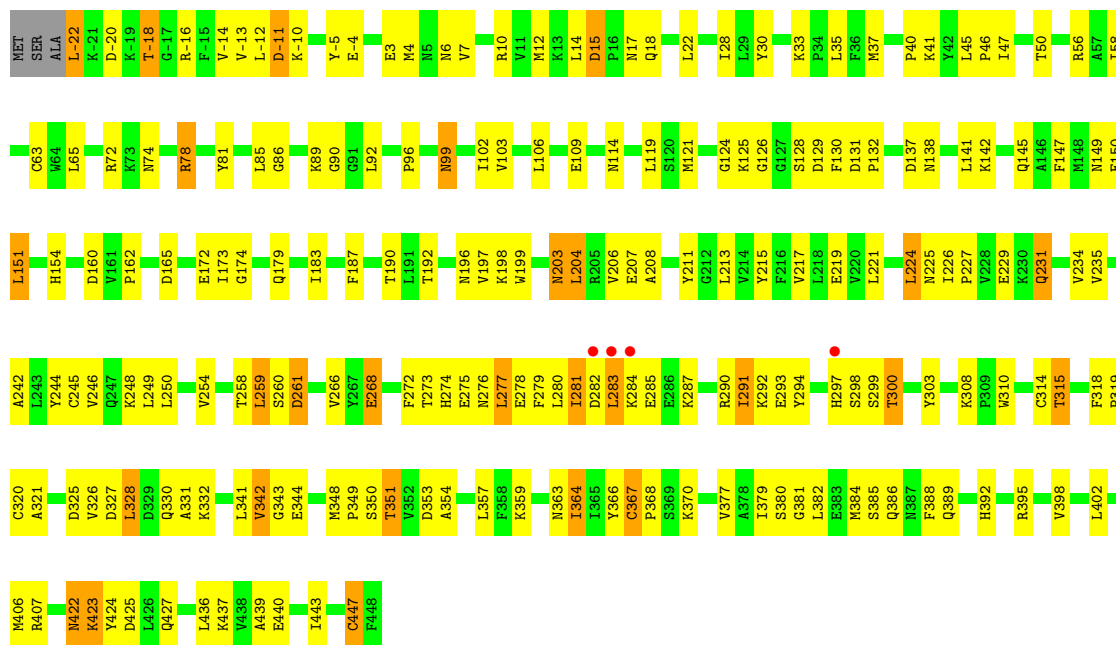
• Molecule 1: GLUTAMATE DEHYDROGENASE (NADP+)



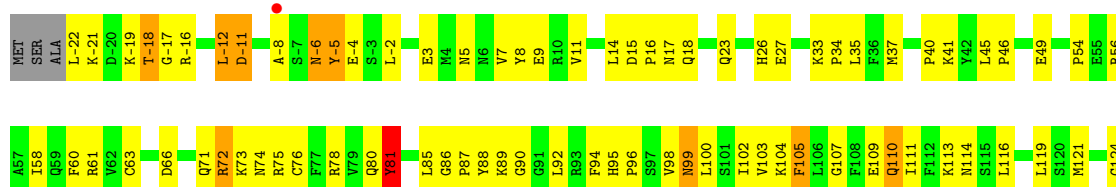


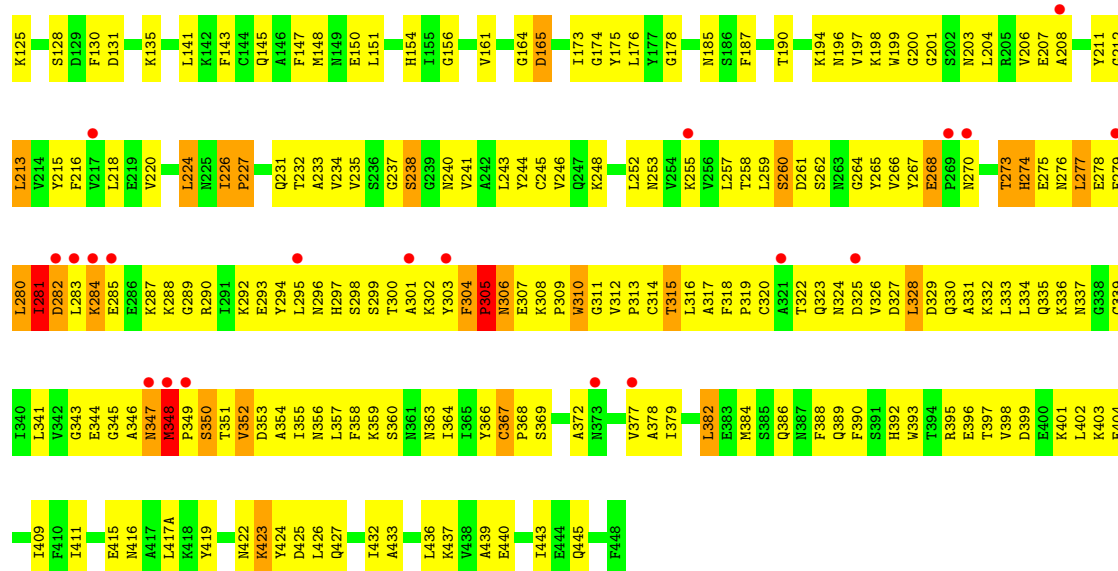


• Molecule 1: GLUTAMATE DEHYDROGENASE (NADP+)



• Molecule 1: GLUTAMATE DEHYDROGENASE (NADP+)





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	167.61Å 96.85Å 196.19Å 90.00° 91.72° 90.00°	Depositor
Resolution (Å)	100.00 – 2.70 100.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.2 (100.00-2.70) 91.2 (100.00-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 2.71Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.249 , 0.277 0.246 , 0.275	Depositor DCC
R_{free} test set	8223 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å ²)	38.8	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.013 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.078 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.065 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.016 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	22068	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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

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	0/3756	1.05	25/5070 (0.5%)
1	B	0.55	0/3756	1.02	22/5070 (0.4%)
1	C	0.53	0/3756	1.05	25/5070 (0.5%)
1	D	0.55	0/3756	1.02	22/5070 (0.4%)
1	E	0.56	0/3756	1.02	20/5070 (0.4%)
1	F	0.53	0/3756	1.05	23/5070 (0.5%)
All	All	0.54	0/22536	1.04	137/30420 (0.5%)

There are no bond length outliers.

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	245	CYS	N-CA-C	-10.14	100.22	111.07
1	A	245	CYS	N-CA-C	-10.02	100.35	111.07
1	F	245	CYS	N-CA-C	-9.97	100.40	111.07
1	F	81	TYR	N-CA-C	9.71	121.63	111.14
1	C	81	TYR	N-CA-C	9.30	121.18	111.14
1	A	81	TYR	N-CA-C	9.28	121.16	111.14
1	B	367	CYS	CA-C-N	8.73	129.26	119.83
1	B	367	CYS	C-N-CA	8.73	129.26	119.83
1	D	367	CYS	CA-C-N	8.70	129.22	119.83
1	D	367	CYS	C-N-CA	8.70	129.22	119.83
1	B	315	THR	N-CA-C	-8.61	103.29	113.88
1	E	367	CYS	CA-C-N	8.51	129.02	119.83
1	E	367	CYS	C-N-CA	8.51	129.02	119.83
1	D	315	THR	N-CA-C	-8.38	103.57	113.88
1	E	315	THR	N-CA-C	-8.37	103.59	113.88
1	F	348	MET	CA-C-N	7.61	127.14	118.85
1	F	348	MET	C-N-CA	7.61	127.14	118.85
1	C	348	MET	CA-C-N	7.53	127.06	118.85
1	C	348	MET	C-N-CA	7.53	127.06	118.85
1	A	367	CYS	CA-C-N	7.44	128.61	119.98
1	A	367	CYS	C-N-CA	7.44	128.61	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	348	MET	CA-C-N	7.41	126.93	118.85
1	A	348	MET	C-N-CA	7.41	126.93	118.85
1	C	367	CYS	CA-C-N	7.40	128.56	119.98
1	C	367	CYS	C-N-CA	7.40	128.56	119.98
1	F	367	CYS	CA-C-N	7.24	128.38	119.98
1	F	367	CYS	C-N-CA	7.24	128.38	119.98
1	F	425	ASP	N-CA-C	-6.96	99.17	109.62
1	C	425	ASP	N-CA-C	-6.84	99.36	109.62
1	A	258	THR	N-CA-C	6.80	119.27	109.14
1	C	258	THR	N-CA-C	6.77	119.22	109.14
1	A	425	ASP	N-CA-C	-6.76	99.47	109.62
1	F	258	THR	N-CA-C	6.66	119.07	109.14
1	B	245	CYS	N-CA-C	-6.65	103.96	111.14
1	E	245	CYS	N-CA-C	-6.61	104.00	111.14
1	B	137	ASP	N-CA-C	-6.58	104.19	111.36
1	F	260	SER	N-CA-C	6.55	119.39	109.95
1	A	260	SER	N-CA-C	6.52	119.34	109.95
1	D	245	CYS	N-CA-C	-6.50	104.12	111.14
1	A	299	SER	N-CA-C	-6.49	105.22	113.01
1	C	260	SER	N-CA-C	6.48	119.28	109.95
1	D	17	ASN	N-CA-C	6.38	119.99	112.72
1	E	137	ASP	N-CA-C	-6.36	104.43	111.36
1	D	137	ASP	N-CA-C	-6.31	104.48	111.36
1	C	299	SER	N-CA-C	-6.30	105.45	113.01
1	A	156	GLY	CA-C-N	6.29	127.70	119.84
1	A	156	GLY	C-N-CA	6.29	127.70	119.84
1	E	17	ASN	N-CA-C	6.28	119.87	112.72
1	B	15	ASP	CA-C-N	6.24	125.72	119.24
1	B	15	ASP	C-N-CA	6.24	125.72	119.24
1	F	299	SER	N-CA-C	-6.21	105.55	113.01
1	D	129	ASP	N-CA-C	-6.20	106.08	113.21
1	E	15	ASP	CA-C-N	6.13	125.62	119.24
1	E	15	ASP	C-N-CA	6.13	125.62	119.24
1	D	15	ASP	CA-C-N	6.13	125.61	119.24
1	D	15	ASP	C-N-CA	6.13	125.61	119.24
1	F	156	GLY	CA-C-N	6.11	127.47	119.84
1	F	156	GLY	C-N-CA	6.11	127.47	119.84
1	E	129	ASP	N-CA-C	-6.07	106.23	113.21
1	B	203	ASN	N-CA-C	-6.03	102.41	110.55
1	C	304	PHE	CA-C-N	6.03	127.37	119.84
1	C	304	PHE	C-N-CA	6.03	127.37	119.84
1	D	258	THR	N-CA-C	6.02	117.93	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	258	THR	N-CA-C	6.02	117.93	108.96
1	A	-8	ALA	N-CA-C	-6.02	100.38	109.95
1	B	258	THR	N-CA-C	6.01	117.91	108.96
1	B	129	ASP	N-CA-C	-6.00	106.31	113.21
1	C	156	GLY	CA-C-N	6.00	127.34	119.84
1	C	156	GLY	C-N-CA	6.00	127.34	119.84
1	B	425	ASP	N-CA-C	-5.98	100.65	109.62
1	A	304	PHE	CA-C-N	5.98	127.31	119.84
1	A	304	PHE	C-N-CA	5.98	127.31	119.84
1	B	17	ASN	N-CA-C	5.97	119.53	112.72
1	F	-8	ALA	N-CA-C	-5.87	100.62	109.95
1	B	259	LEU	N-CA-C	-5.87	100.04	108.60
1	C	-8	ALA	N-CA-C	-5.85	100.64	109.95
1	E	268	GLU	CA-C-N	5.82	127.12	119.84
1	E	268	GLU	C-N-CA	5.82	127.12	119.84
1	D	203	ASN	N-CA-C	-5.80	102.72	110.55
1	E	425	ASP	N-CA-C	-5.79	100.93	109.62
1	F	304	PHE	CA-C-N	5.77	127.05	119.84
1	F	304	PHE	C-N-CA	5.77	127.05	119.84
1	C	274	HIS	N-CA-C	-5.76	104.20	111.11
1	A	274	HIS	N-CA-C	-5.73	104.24	111.11
1	D	268	GLU	CA-C-N	5.71	126.98	119.84
1	D	268	GLU	C-N-CA	5.71	126.98	119.84
1	D	259	LEU	N-CA-C	-5.71	100.26	108.60
1	A	17	ASN	N-CA-C	5.69	119.81	112.41
1	E	203	ASN	N-CA-C	-5.69	102.86	110.55
1	F	17	ASN	N-CA-C	5.69	119.81	112.41
1	B	268	GLU	CA-C-N	5.67	126.93	119.84
1	B	268	GLU	C-N-CA	5.67	126.93	119.84
1	F	274	HIS	N-CA-C	-5.64	104.34	111.11
1	D	447	CYS	N-CA-C	5.62	117.39	108.67
1	E	447	CYS	N-CA-C	5.62	117.38	108.67
1	D	425	ASP	N-CA-C	-5.61	101.20	109.62
1	D	299	SER	N-CA-C	-5.61	106.39	113.18
1	D	151	LEU	N-CA-C	5.56	117.34	111.28
1	C	382	LEU	N-CA-C	-5.56	105.38	111.82
1	A	382	LEU	N-CA-C	-5.54	105.39	111.82
1	B	151	LEU	N-CA-C	5.53	117.31	111.28
1	C	268	GLU	CA-C-N	5.53	124.99	119.24
1	C	268	GLU	C-N-CA	5.53	124.99	119.24
1	B	310	TRP	N-CA-C	5.50	119.49	112.34
1	C	17	ASN	N-CA-C	5.50	119.56	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	260	SER	N-CA-C	5.49	116.62	108.60
1	E	310	TRP	N-CA-C	5.49	119.48	112.34
1	E	259	LEU	N-CA-C	-5.49	100.39	108.79
1	D	310	TRP	N-CA-C	5.48	119.46	112.34
1	B	299	SER	N-CA-C	-5.46	106.57	113.18
1	E	151	LEU	N-CA-C	5.46	117.23	111.28
1	A	98	VAL	N-CA-C	5.43	117.28	109.51
1	B	260	SER	N-CA-C	5.40	117.05	108.79
1	B	447	CYS	N-CA-C	5.40	117.03	108.67
1	E	299	SER	N-CA-C	-5.38	106.67	113.18
1	F	226	ILE	CA-C-N	5.36	126.54	119.84
1	F	226	ILE	C-N-CA	5.36	126.54	119.84
1	F	382	LEU	N-CA-C	-5.34	105.63	111.82
1	C	98	VAL	N-CA-C	5.31	117.11	109.51
1	D	260	SER	N-CA-C	5.29	116.83	108.96
1	A	268	GLU	CA-C-N	5.28	124.73	119.24
1	A	268	GLU	C-N-CA	5.28	124.73	119.24
1	A	226	ILE	CA-C-N	5.23	126.38	119.84
1	A	226	ILE	C-N-CA	5.23	126.38	119.84
1	F	268	GLU	CA-C-N	5.23	124.67	119.24
1	F	268	GLU	C-N-CA	5.23	124.67	119.24
1	B	287	LYS	N-CA-C	-5.20	107.60	114.31
1	C	226	ILE	CA-C-N	5.13	126.25	119.84
1	C	226	ILE	C-N-CA	5.13	126.25	119.84
1	C	436	LEU	N-CA-C	5.11	117.25	111.11
1	B	372	ALA	N-CA-C	5.07	116.81	111.28
1	D	-15	PHE	N-CA-C	5.06	117.31	108.76
1	F	98	VAL	N-CA-C	5.06	116.75	109.51
1	D	372	ALA	N-CA-C	5.03	116.76	111.28
1	C	296	ASN	N-CA-C	-5.01	106.47	112.59
1	A	53	GLU	CA-C-N	5.00	125.00	119.90
1	A	53	GLU	C-N-CA	5.00	125.00	119.90

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	3678	0	3656	316	0
1	B	3678	0	3656	209	0
1	C	3678	0	3656	312	0
1	D	3678	0	3656	210	0
1	E	3678	0	3656	209	0
1	F	3678	0	3656	316	0
All	All	22068	0	21936	1501	0

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 34.

All (1501) 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)
1:E:281:ILE:HG23	1:E:282:ASP:H	1.14	1.11
1:D:281:ILE:HG23	1:D:282:ASP:H	1.14	1.08
1:B:281:ILE:HG23	1:B:282:ASP:H	1.13	1.06
1:A:277:LEU:O	1:A:281:ILE:HG22	1.62	0.99
1:C:277:LEU:O	1:C:281:ILE:HG22	1.62	0.99
1:C:246:VAL:HG21	1:C:259:LEU:HD21	1.44	0.98
1:A:246:VAL:HG21	1:A:259:LEU:HD21	1.44	0.98
1:F:277:LEU:O	1:F:281:ILE:HG22	1.64	0.97
1:E:6:ASN:HB3	1:E:10:ARG:HH12	1.31	0.96
1:D:327:ASP:H	1:D:330:GLN:NE2	1.63	0.96
1:B:6:ASN:HB3	1:B:10:ARG:HH12	1.31	0.95
1:B:327:ASP:H	1:B:330:GLN:NE2	1.63	0.95
1:D:6:ASN:HB3	1:D:10:ARG:HH12	1.31	0.94
1:F:246:VAL:HG21	1:F:259:LEU:HD21	1.44	0.94
1:E:327:ASP:H	1:E:330:GLN:NE2	1.65	0.93
1:B:-18:THR:HG23	1:B:-16:ARG:H	1.32	0.93
1:D:-18:THR:HG23	1:D:-16:ARG:H	1.31	0.93
1:B:208:ALA:HB2	1:B:379:ILE:HG13	1.51	0.93
1:D:208:ALA:HB2	1:D:379:ILE:HG13	1.51	0.93
1:B:259:LEU:HD12	1:B:280:LEU:HD13	1.50	0.92
1:E:208:ALA:HB2	1:E:379:ILE:HG13	1.53	0.90
1:E:-18:THR:HG23	1:E:-16:ARG:H	1.34	0.90
1:E:259:LEU:HD12	1:E:280:LEU:HD13	1.51	0.90
1:F:90:GLY:HA3	1:F:124:GLY:O	1.72	0.89
1:D:259:LEU:HD12	1:D:280:LEU:HD13	1.52	0.89
1:A:90:GLY:HA3	1:A:124:GLY:O	1.74	0.88
1:B:281:ILE:HG23	1:B:282:ASP:N	1.88	0.87
1:C:90:GLY:HA3	1:C:124:GLY:O	1.72	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:281:ILE:HG23	1:D:282:ASP:N	1.89	0.86
1:C:359:LYS:HZ3	1:C:427:GLN:HB3	1.40	0.86
1:A:266:VAL:HG21	1:A:294:TYR:HD1	1.40	0.85
1:A:417(A):LEU:HD13	1:A:423:LYS:HB2	1.58	0.85
1:E:281:ILE:HG23	1:E:282:ASP:N	1.89	0.85
1:F:266:VAL:HG21	1:F:294:TYR:HD1	1.42	0.85
1:F:313:PRO:HG3	1:F:337:ASN:HD22	1.42	0.85
1:A:259:LEU:HD12	1:A:280:LEU:HD13	1.59	0.85
1:F:417(A):LEU:HD13	1:F:423:LYS:HB2	1.57	0.84
1:C:313:PRO:HG3	1:C:337:ASN:HD22	1.42	0.84
1:A:313:PRO:HG3	1:A:337:ASN:HD22	1.43	0.84
1:A:379:ILE:HD13	1:A:382:LEU:HD12	1.59	0.84
1:F:351:THR:HG22	1:F:353:ASP:H	1.43	0.84
1:F:259:LEU:HD12	1:F:280:LEU:HD13	1.60	0.84
1:F:99:ASN:ND2	1:F:102:ILE:H	1.76	0.84
1:C:7:VAL:HG13	1:C:49:GLU:HG3	1.60	0.83
1:F:99:ASN:HD22	1:F:99:ASN:C	1.87	0.83
1:A:99:ASN:ND2	1:A:102:ILE:H	1.76	0.83
1:C:417(A):LEU:HD13	1:C:423:LYS:HB2	1.58	0.83
1:C:99:ASN:ND2	1:C:102:ILE:H	1.76	0.83
1:F:7:VAL:HG13	1:F:49:GLU:HG3	1.60	0.83
1:C:266:VAL:HG21	1:C:294:TYR:HD1	1.43	0.82
1:A:283:LEU:O	1:A:287:LYS:HB3	1.78	0.82
1:F:99:ASN:HD21	1:F:102:ILE:H	1.27	0.82
1:C:259:LEU:HD12	1:C:280:LEU:HD13	1.60	0.82
1:C:308:LYS:HD2	1:C:330:GLN:OE1	1.80	0.82
1:C:351:THR:HG22	1:C:353:ASP:H	1.44	0.82
1:F:5:ASN:O	1:F:9:GLU:HG2	1.78	0.82
1:A:5:ASN:O	1:A:9:GLU:HG2	1.80	0.82
1:A:351:THR:HG22	1:A:353:ASP:H	1.45	0.82
1:F:283:LEU:O	1:F:287:LYS:HB3	1.80	0.82
1:F:308:LYS:HD2	1:F:330:GLN:OE1	1.79	0.81
1:C:99:ASN:HD21	1:C:102:ILE:H	1.29	0.81
1:A:7:VAL:HG13	1:A:49:GLU:HG3	1.62	0.81
1:A:266:VAL:HG21	1:A:294:TYR:CD1	2.14	0.81
1:F:379:ILE:HD13	1:F:382:LEU:HD12	1.60	0.81
1:C:5:ASN:O	1:C:9:GLU:HG2	1.79	0.81
1:C:283:LEU:O	1:C:287:LYS:HB3	1.81	0.81
1:E:266:VAL:HG21	1:E:294:TYR:HD1	1.45	0.81
1:F:280:LEU:HA	1:F:284:LYS:NZ	1.95	0.81
1:B:266:VAL:HG21	1:B:294:TYR:HD1	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:LEU:HA	1:C:284:LYS:CE	2.11	0.80
1:F:280:LEU:HA	1:F:284:LYS:CE	2.11	0.80
1:A:99:ASN:C	1:A:99:ASN:HD22	1.87	0.80
1:C:266:VAL:HG21	1:C:294:TYR:CD1	2.16	0.80
1:F:96:PRO:HG3	1:F:131:ASP:HB2	1.62	0.80
1:A:280:LEU:HA	1:A:284:LYS:CE	2.12	0.80
1:C:96:PRO:HG3	1:C:131:ASP:HB2	1.63	0.80
1:A:99:ASN:HD21	1:A:102:ILE:H	1.29	0.80
1:A:280:LEU:HA	1:A:284:LYS:NZ	1.94	0.80
1:C:280:LEU:HA	1:C:284:LYS:NZ	1.96	0.80
1:F:266:VAL:HG21	1:F:294:TYR:CD1	2.15	0.80
1:C:379:ILE:HD13	1:C:382:LEU:HD12	1.62	0.80
1:A:308:LYS:HD2	1:A:330:GLN:OE1	1.81	0.79
1:A:96:PRO:HG3	1:A:131:ASP:HB2	1.65	0.79
1:D:266:VAL:HG21	1:D:294:TYR:HD1	1.46	0.79
1:E:351:THR:HG22	1:E:354:ALA:H	1.48	0.79
1:A:292:LYS:HG2	1:A:303:TYR:CE1	2.18	0.79
1:A:328:LEU:HG	1:A:353:ASP:HB3	1.65	0.78
1:C:292:LYS:HG2	1:C:303:TYR:CE1	2.18	0.78
1:A:15:ASP:HB3	1:A:18:GLN:HG3	1.66	0.78
1:C:328:LEU:HG	1:C:353:ASP:HB3	1.63	0.78
1:F:292:LYS:HG2	1:F:303:TYR:CE1	2.18	0.78
1:F:328:LEU:HG	1:F:353:ASP:HB3	1.64	0.78
1:B:351:THR:HG22	1:B:354:ALA:H	1.48	0.78
1:C:15:ASP:HB3	1:C:18:GLN:HG3	1.64	0.78
1:C:99:ASN:C	1:C:99:ASN:HD22	1.87	0.78
1:A:379:ILE:HD11	1:A:398:VAL:CG1	2.14	0.78
1:D:351:THR:HG22	1:D:354:ALA:H	1.48	0.78
1:F:379:ILE:HD11	1:F:398:VAL:CG1	2.15	0.77
1:F:15:ASP:HB3	1:F:18:GLN:HG3	1.66	0.76
1:D:266:VAL:HG21	1:D:294:TYR:CD1	2.21	0.76
1:C:379:ILE:HD11	1:C:398:VAL:CG1	2.15	0.76
1:C:333:LEU:HA	1:C:336:LYS:HE2	1.68	0.76
1:E:422:ASN:O	1:E:423:LYS:HB3	1.85	0.75
1:A:343:GLY:HA2	1:A:367:CYS:HB2	1.68	0.75
1:C:196:ASN:HD21	1:C:198:LYS:NZ	1.85	0.75
1:E:266:VAL:HG21	1:E:294:TYR:CD1	2.21	0.75
1:D:281:ILE:CG2	1:D:282:ASP:H	1.98	0.75
1:C:273:THR:HG22	1:C:275:GLU:H	1.52	0.74
1:F:204:LEU:HA	1:F:207:GLU:OE2	1.87	0.74
1:A:196:ASN:HD21	1:A:198:LYS:NZ	1.85	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:ASN:HD21	1:A:198:LYS:HZ3	1.32	0.74
1:B:281:ILE:CG2	1:B:282:ASP:H	1.97	0.74
1:B:266:VAL:HG21	1:B:294:TYR:CD1	2.21	0.74
1:E:281:ILE:CG2	1:E:282:ASP:H	1.97	0.74
1:F:333:LEU:HA	1:F:336:LYS:HE2	1.68	0.74
1:B:422:ASN:O	1:B:423:LYS:HB3	1.87	0.74
1:D:114:ASN:ND2	1:D:377:VAL:HG11	2.03	0.74
1:D:284:LYS:HD3	1:D:293:GLU:HB2	1.70	0.74
1:A:333:LEU:HA	1:A:336:LYS:HE2	1.70	0.74
1:C:204:LEU:HA	1:C:207:GLU:OE2	1.87	0.74
1:B:234:VAL:HG23	1:B:314:CYS:HB3	1.70	0.73
1:C:390:PHE:HB2	1:F:388:PHE:HD1	1.53	0.73
1:E:284:LYS:HD3	1:E:293:GLU:HB2	1.70	0.73
1:F:41:LYS:O	1:F:46:PRO:HD2	1.88	0.73
1:F:273:THR:HG22	1:F:275:GLU:H	1.52	0.73
1:F:326:VAL:HA	1:F:330:GLN:NE2	2.04	0.73
1:D:422:ASN:O	1:D:423:LYS:HB3	1.86	0.73
1:A:390:PHE:HB2	1:C:388:PHE:HD1	1.53	0.73
1:C:273:THR:HG22	1:C:275:GLU:N	2.03	0.73
1:A:41:LYS:O	1:A:46:PRO:HD2	1.89	0.73
1:F:114:ASN:ND2	1:F:377:VAL:HG11	2.03	0.73
1:A:204:LEU:HA	1:A:207:GLU:OE2	1.87	0.73
1:F:343:GLY:HA2	1:F:367:CYS:HB2	1.68	0.73
1:B:284:LYS:HD3	1:B:293:GLU:HB2	1.71	0.73
1:F:273:THR:HG22	1:F:275:GLU:N	2.03	0.73
1:A:273:THR:HG22	1:A:275:GLU:H	1.53	0.72
1:C:343:GLY:HA2	1:C:367:CYS:HB2	1.69	0.72
1:C:41:LYS:O	1:C:46:PRO:HD2	1.90	0.72
1:C:235:VAL:HG22	1:C:318:PHE:HB2	1.71	0.72
1:E:234:VAL:HG23	1:E:314:CYS:HB3	1.71	0.72
1:F:196:ASN:HD21	1:F:198:LYS:NZ	1.85	0.72
1:F:148:MET:HE2	1:F:176:LEU:HD22	1.70	0.72
1:A:284:LYS:HZ3	1:A:284:LYS:H	1.37	0.72
1:D:277:LEU:O	1:D:281:ILE:HG22	1.88	0.72
1:C:208:ALA:HB2	1:C:379:ILE:HG13	1.70	0.72
1:E:282:ASP:O	1:E:283:LEU:HG	1.90	0.72
1:A:92:LEU:O	1:A:165:ASP:HB3	1.90	0.72
1:B:114:ASN:ND2	1:B:377:VAL:HG11	2.04	0.72
1:B:282:ASP:O	1:B:283:LEU:HG	1.90	0.72
1:A:273:THR:HG22	1:A:275:GLU:N	2.04	0.71
1:C:274:HIS:O	1:C:278:GLU:HG2	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:326:VAL:HA	1:C:330:GLN:NE2	2.05	0.71
1:C:114:ASN:ND2	1:C:377:VAL:HG11	2.04	0.71
1:F:196:ASN:HD21	1:F:198:LYS:HZ3	1.37	0.71
1:F:273:THR:H	1:F:276:ASN:HB2	1.55	0.71
1:B:277:LEU:O	1:B:281:ILE:HG22	1.91	0.71
1:B:348:MET:HG3	1:B:348:MET:O	1.90	0.71
1:F:241:VAL:HG11	1:F:345:GLY:O	1.90	0.71
1:F:8:TYR:CE1	1:F:26:HIS:HB2	2.26	0.71
1:A:326:VAL:HA	1:A:330:GLN:NE2	2.05	0.71
1:C:148:MET:HE2	1:C:176:LEU:HD22	1.72	0.71
1:D:282:ASP:O	1:D:283:LEU:HG	1.90	0.71
1:C:273:THR:H	1:C:276:ASN:HB2	1.56	0.71
1:F:284:LYS:HZ3	1:F:284:LYS:H	1.39	0.71
1:F:423:LYS:HG3	1:F:424:TYR:CE1	2.26	0.71
1:A:208:ALA:HB2	1:A:379:ILE:HG13	1.72	0.71
1:C:241:VAL:HG11	1:C:345:GLY:O	1.90	0.71
1:A:121:MET:HE1	1:A:377:VAL:HG12	1.73	0.71
1:A:423:LYS:HG3	1:A:424:TYR:CE1	2.25	0.71
1:C:33:LYS:O	1:C:37:MET:HG2	1.91	0.71
1:E:114:ASN:ND2	1:E:377:VAL:HG11	2.05	0.71
1:F:208:ALA:HB2	1:F:379:ILE:HG13	1.72	0.71
1:A:241:VAL:HG11	1:A:345:GLY:O	1.91	0.70
1:B:6:ASN:HB3	1:B:10:ARG:NH1	2.05	0.70
1:A:148:MET:HE2	1:A:176:LEU:HD22	1.73	0.70
1:A:388:PHE:HD1	1:F:390:PHE:HB2	1.56	0.70
1:A:114:ASN:ND2	1:A:377:VAL:HG11	2.07	0.70
1:C:284:LYS:H	1:C:284:LYS:HZ3	1.37	0.70
1:C:423:LYS:HG3	1:C:424:TYR:CE1	2.26	0.70
1:A:274:HIS:O	1:A:278:GLU:HG2	1.92	0.70
1:E:277:LEU:O	1:E:281:ILE:HG22	1.91	0.70
1:C:344:GLU:OE2	1:C:369:SER:HB2	1.92	0.70
1:D:6:ASN:HB3	1:D:10:ARG:NH1	2.05	0.70
1:E:348:MET:O	1:E:348:MET:HG3	1.91	0.70
1:F:92:LEU:O	1:F:165:ASP:HB3	1.92	0.70
1:F:280:LEU:HD23	1:F:284:LYS:CE	2.22	0.70
1:C:313:PRO:HB3	1:C:337:ASN:HB3	1.74	0.69
1:B:278:GLU:HA	1:B:281:ILE:CG2	2.23	0.69
1:A:273:THR:H	1:A:276:ASN:HB2	1.57	0.69
1:D:234:VAL:HG23	1:D:314:CYS:HB3	1.74	0.69
1:F:326:VAL:HA	1:F:330:GLN:HE22	1.55	0.69
1:B:114:ASN:HD22	1:B:377:VAL:HG11	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:VAL:HG21	1:B:259:LEU:HD21	1.75	0.69
1:C:326:VAL:HA	1:C:330:GLN:HE22	1.55	0.69
1:D:246:VAL:HG21	1:D:259:LEU:HD21	1.74	0.69
1:E:-10:LYS:HG3	1:E:-5:TYR:CE2	2.28	0.69
1:A:344:GLU:OE2	1:A:369:SER:HB2	1.92	0.69
1:C:196:ASN:HD21	1:C:198:LYS:HZ3	1.39	0.69
1:C:273:THR:HB	1:C:276:ASN:CG	2.18	0.69
1:D:327:ASP:N	1:D:330:GLN:NE2	2.40	0.69
1:D:348:MET:O	1:D:348:MET:HG3	1.91	0.69
1:C:8:TYR:CE1	1:C:26:HIS:HB2	2.27	0.69
1:A:280:LEU:HD23	1:A:284:LYS:CE	2.23	0.69
1:F:33:LYS:O	1:F:37:MET:HG2	1.93	0.69
1:F:273:THR:HB	1:F:276:ASN:CG	2.17	0.69
1:F:313:PRO:HG3	1:F:337:ASN:ND2	2.07	0.69
1:F:344:GLU:OE2	1:F:369:SER:HB2	1.93	0.69
1:C:121:MET:HE1	1:C:377:VAL:HG12	1.74	0.69
1:C:313:PRO:HG3	1:C:337:ASN:ND2	2.07	0.69
1:C:280:LEU:HD23	1:C:284:LYS:CE	2.23	0.68
1:F:121:MET:HE1	1:F:377:VAL:HG12	1.75	0.68
1:A:235:VAL:HG22	1:A:318:PHE:HB2	1.74	0.68
1:D:-5:TYR:OH	1:D:40:PRO:HG3	1.93	0.68
1:D:278:GLU:HA	1:D:281:ILE:CG2	2.23	0.68
1:E:278:GLU:HA	1:E:281:ILE:CG2	2.23	0.68
1:E:114:ASN:HD22	1:E:377:VAL:HG11	1.58	0.68
1:A:273:THR:HB	1:A:276:ASN:CG	2.19	0.68
1:F:148:MET:HB2	1:F:176:LEU:HD23	1.75	0.68
1:F:235:VAL:HG22	1:F:318:PHE:HB2	1.75	0.68
1:F:313:PRO:HB3	1:F:337:ASN:HB3	1.75	0.68
1:E:351:THR:CG2	1:E:354:ALA:H	2.06	0.68
1:F:274:HIS:O	1:F:278:GLU:HG2	1.94	0.68
1:C:23:GLN:O	1:C:27:GLU:HB2	1.94	0.68
1:C:284:LYS:NZ	1:C:284:LYS:H	1.91	0.68
1:D:351:THR:CG2	1:D:354:ALA:H	2.06	0.68
1:E:-5:TYR:OH	1:E:40:PRO:HG3	1.94	0.68
1:F:280:LEU:HD23	1:F:284:LYS:HE3	1.74	0.68
1:A:33:LYS:O	1:A:37:MET:HG2	1.93	0.68
1:A:280:LEU:HD23	1:A:284:LYS:HE3	1.75	0.68
1:C:265:TYR:CG	1:C:309:PRO:HG3	2.28	0.68
1:E:6:ASN:HB3	1:E:10:ARG:NH1	2.06	0.68
1:F:265:TYR:CE2	1:F:304:PHE:HB2	2.29	0.68
1:F:73:LYS:HG2	1:F:74:ASN:N	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:-5:TYR:OH	1:B:40:PRO:HG3	1.94	0.67
1:C:234:VAL:HG23	1:C:314:CYS:HB3	1.76	0.67
1:A:8:TYR:CE1	1:A:26:HIS:HB2	2.28	0.67
1:C:280:LEU:HD23	1:C:284:LYS:HE3	1.76	0.67
1:A:326:VAL:HA	1:A:330:GLN:HE22	1.57	0.67
1:D:114:ASN:HD22	1:D:377:VAL:HG11	1.57	0.67
1:D:327:ASP:H	1:D:330:GLN:HE21	1.43	0.67
1:E:246:VAL:HG21	1:E:259:LEU:HD21	1.75	0.67
1:F:-18:THR:HG22	1:F:-16:ARG:HB2	1.77	0.67
1:C:73:LYS:HG2	1:C:74:ASN:N	2.08	0.67
1:C:92:LEU:O	1:C:165:ASP:HB3	1.94	0.67
1:A:313:PRO:HG3	1:A:337:ASN:ND2	2.08	0.67
1:B:235:VAL:HG22	1:B:318:PHE:HB2	1.77	0.67
1:B:351:THR:CG2	1:B:354:ALA:H	2.06	0.67
1:C:266:VAL:HG22	1:C:267:TYR:N	2.10	0.67
1:F:234:VAL:HG23	1:F:314:CYS:HB3	1.77	0.67
1:F:265:TYR:CG	1:F:309:PRO:HG3	2.30	0.67
1:F:284:LYS:NZ	1:F:284:LYS:H	1.93	0.67
1:A:265:TYR:CG	1:A:309:PRO:HG3	2.29	0.67
1:B:279:PHE:O	1:B:283:LEU:HB2	1.95	0.67
1:C:265:TYR:CE2	1:C:304:PHE:HB2	2.30	0.67
1:F:310:TRP:HB3	1:F:334:LEU:HD11	1.76	0.67
1:A:310:TRP:HB3	1:A:334:LEU:HD11	1.77	0.67
1:B:381:GLY:HA2	1:B:384:MET:HE3	1.77	0.67
1:C:148:MET:HB2	1:C:176:LEU:HD23	1.76	0.67
1:A:73:LYS:HG2	1:A:74:ASN:N	2.10	0.66
1:D:90:GLY:HA3	1:D:124:GLY:O	1.95	0.66
1:F:23:GLN:O	1:F:27:GLU:HB2	1.93	0.66
1:A:23:GLN:O	1:A:27:GLU:HB2	1.95	0.66
1:C:-18:THR:HG22	1:C:-16:ARG:HB2	1.77	0.66
1:F:215:TYR:OH	1:F:248:LYS:HE2	1.95	0.66
1:A:148:MET:HB2	1:A:176:LEU:HD23	1.76	0.66
1:C:119:LEU:HB2	1:C:121:MET:HE2	1.77	0.66
1:D:377:VAL:O	1:D:380:SER:HB3	1.95	0.66
1:A:313:PRO:HB3	1:A:337:ASN:HB3	1.75	0.66
1:A:284:LYS:NZ	1:A:284:LYS:H	1.93	0.66
1:B:327:ASP:H	1:B:330:GLN:HE21	1.44	0.66
1:D:-10:LYS:HG3	1:D:-5:TYR:CE2	2.29	0.66
1:B:-10:LYS:HG3	1:B:-5:TYR:CE2	2.30	0.66
1:C:-18:THR:CG2	1:C:-16:ARG:HB2	2.26	0.66
1:F:327:ASP:O	1:F:354:ALA:HB2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:ASP:O	1:C:354:ALA:HB2	1.96	0.66
1:A:234:VAL:HG23	1:A:314:CYS:HB3	1.78	0.66
1:E:235:VAL:HG22	1:E:318:PHE:HB2	1.78	0.66
1:B:208:ALA:CB	1:B:379:ILE:HG13	2.26	0.65
1:F:119:LEU:HB2	1:F:121:MET:HE2	1.76	0.65
1:A:119:LEU:HB2	1:A:121:MET:HE2	1.78	0.65
1:B:90:GLY:HA3	1:B:124:GLY:O	1.95	0.65
1:B:327:ASP:N	1:B:330:GLN:NE2	2.40	0.65
1:C:215:TYR:OH	1:C:248:LYS:HE2	1.96	0.65
1:B:149:ASN:ND2	1:B:183:ILE:HD11	2.12	0.65
1:D:235:VAL:HG22	1:D:318:PHE:HB2	1.79	0.65
1:F:266:VAL:HG22	1:F:267:TYR:N	2.10	0.65
1:C:206:VAL:HG13	1:C:240:ASN:OD1	1.96	0.65
1:E:279:PHE:O	1:E:283:LEU:HB2	1.97	0.65
1:E:290:ARG:HB3	1:E:292:LYS:HZ3	1.59	0.65
1:A:206:VAL:HG13	1:A:240:ASN:OD1	1.97	0.65
1:A:266:VAL:HG22	1:A:267:TYR:N	2.12	0.65
1:B:422:ASN:C	1:B:422:ASN:HD22	2.05	0.65
1:E:90:GLY:HA3	1:E:124:GLY:O	1.97	0.65
1:A:215:TYR:OH	1:A:248:LYS:HE2	1.97	0.65
1:C:310:TRP:HB3	1:C:334:LEU:HD11	1.77	0.65
1:D:215:TYR:OH	1:D:248:LYS:HE2	1.97	0.65
1:E:377:VAL:O	1:E:380:SER:HB3	1.97	0.65
1:A:-18:THR:HG22	1:A:-16:ARG:HB2	1.78	0.64
1:A:327:ASP:O	1:A:354:ALA:HB2	1.96	0.64
1:B:259:LEU:CD1	1:B:280:LEU:HD13	2.27	0.64
1:C:266:VAL:HG22	1:C:267:TYR:H	1.62	0.64
1:C:237:GLY:N	1:C:260:SER:OG	2.31	0.64
1:D:279:PHE:O	1:D:283:LEU:HB2	1.97	0.64
1:D:422:ASN:C	1:D:422:ASN:HD22	2.06	0.64
1:A:196:ASN:ND2	1:A:198:LYS:NZ	2.45	0.64
1:D:149:ASN:ND2	1:D:183:ILE:HD11	2.12	0.64
1:F:330:GLN:O	1:F:334:LEU:HD12	1.97	0.64
1:A:-18:THR:CG2	1:A:-16:ARG:HB2	2.28	0.64
1:C:196:ASN:ND2	1:C:198:LYS:NZ	2.45	0.64
1:E:149:ASN:ND2	1:E:183:ILE:HD11	2.12	0.64
1:F:-18:THR:CG2	1:F:-16:ARG:HB2	2.26	0.64
1:B:377:VAL:O	1:B:380:SER:HB3	1.97	0.64
1:F:206:VAL:HG13	1:F:240:ASN:OD1	1.98	0.64
1:D:326:VAL:HA	1:D:330:GLN:NE2	2.13	0.64
1:E:74:ASN:ND2	1:E:130:PHE:HA	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:119:LEU:HB2	1:E:121:MET:HE2	1.80	0.63
1:B:279:PHE:HB3	1:B:297:HIS:CD2	2.34	0.63
1:E:215:TYR:OH	1:E:248:LYS:HE2	1.99	0.63
1:D:208:ALA:CB	1:D:379:ILE:HG13	2.26	0.63
1:E:326:VAL:HA	1:E:330:GLN:NE2	2.14	0.63
1:E:344:GLU:OE1	1:E:349:PRO:HD2	1.99	0.63
1:E:381:GLY:HA2	1:E:384:MET:HE3	1.80	0.63
1:A:237:GLY:N	1:A:260:SER:OG	2.31	0.63
1:A:265:TYR:CE2	1:A:304:PHE:HB2	2.33	0.63
1:A:423:LYS:HG3	1:A:424:TYR:CD1	2.32	0.63
1:F:196:ASN:ND2	1:F:198:LYS:NZ	2.46	0.63
1:F:266:VAL:HG22	1:F:267:TYR:H	1.62	0.63
1:B:119:LEU:HB2	1:B:121:MET:HE2	1.79	0.63
1:B:326:VAL:HA	1:B:330:GLN:NE2	2.13	0.63
1:D:47:ILE:HD11	1:D:443:ILE:HD11	1.80	0.63
1:D:99:ASN:ND2	1:D:102:ILE:H	1.96	0.63
1:E:196:ASN:ND2	1:E:198:LYS:HZ3	1.96	0.63
1:F:423:LYS:HG3	1:F:424:TYR:CD1	2.34	0.63
1:A:327:ASP:H	1:A:330:GLN:NE2	1.97	0.63
1:B:215:TYR:OH	1:B:248:LYS:HE2	1.99	0.63
1:E:279:PHE:HB3	1:E:297:HIS:CD2	2.34	0.63
1:F:341:LEU:HD23	1:F:341:LEU:C	2.24	0.63
1:D:-10:LYS:HA	1:D:-5:TYR:CD1	2.34	0.63
1:D:119:LEU:HB2	1:D:121:MET:HE2	1.80	0.63
1:F:237:GLY:N	1:F:260:SER:OG	2.32	0.63
1:D:278:GLU:HA	1:D:281:ILE:HG22	1.81	0.63
1:E:327:ASP:H	1:E:330:GLN:HE21	1.46	0.62
1:B:74:ASN:ND2	1:B:130:PHE:HA	2.13	0.62
1:B:99:ASN:ND2	1:B:102:ILE:H	1.97	0.62
1:B:278:GLU:HA	1:B:281:ILE:HG22	1.80	0.62
1:C:341:LEU:C	1:C:341:LEU:HD23	2.24	0.62
1:E:422:ASN:HD22	1:E:422:ASN:C	2.07	0.62
1:C:368:PRO:CG	1:C:427:GLN:HA	2.30	0.62
1:E:327:ASP:N	1:E:330:GLN:NE2	2.42	0.62
1:A:287:LYS:HG2	1:A:287:LYS:O	1.99	0.62
1:B:-10:LYS:HA	1:B:-5:TYR:CD1	2.34	0.62
1:E:-10:LYS:HA	1:E:-5:TYR:CD1	2.34	0.62
1:F:282:ASP:O	1:F:283:LEU:HD23	1.99	0.62
1:C:331:ALA:O	1:C:335:GLN:HB2	1.99	0.62
1:A:368:PRO:CG	1:A:427:GLN:HA	2.29	0.62
1:E:259:LEU:CD1	1:E:280:LEU:HD13	2.27	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:VAL:HG22	1:A:267:TYR:H	1.63	0.62
1:C:282:ASP:O	1:C:283:LEU:HD23	1.99	0.62
1:C:327:ASP:H	1:C:330:GLN:NE2	1.97	0.62
1:E:74:ASN:HD21	1:E:130:PHE:HA	1.65	0.62
1:E:278:GLU:HA	1:E:281:ILE:HG22	1.81	0.62
1:D:344:GLU:OE1	1:D:349:PRO:HD2	1.98	0.62
1:F:287:LYS:O	1:F:287:LYS:HG2	2.00	0.62
1:A:282:ASP:O	1:A:283:LEU:HD23	1.99	0.62
1:C:423:LYS:HG3	1:C:424:TYR:CD1	2.35	0.62
1:A:313:PRO:CG	1:A:337:ASN:HD22	2.11	0.61
1:C:287:LYS:O	1:C:287:LYS:HG2	2.00	0.61
1:E:99:ASN:ND2	1:E:102:ILE:H	1.98	0.61
1:C:330:GLN:O	1:C:334:LEU:HD12	1.98	0.61
1:D:231:GLN:HG3	1:D:315:THR:OG1	2.00	0.61
1:A:341:LEU:HD23	1:A:341:LEU:C	2.24	0.61
1:D:284:LYS:HE3	1:D:291:ILE:HA	1.81	0.61
1:C:284:LYS:NZ	1:C:284:LYS:HB2	2.15	0.61
1:B:47:ILE:HD11	1:B:443:ILE:HD11	1.81	0.61
1:B:402:LEU:O	1:B:406:MET:HG2	2.00	0.61
1:D:74:ASN:ND2	1:D:130:PHE:HA	2.16	0.61
1:D:279:PHE:HB3	1:D:297:HIS:CD2	2.35	0.61
1:F:313:PRO:CG	1:F:337:ASN:HD22	2.10	0.61
1:B:284:LYS:HE3	1:B:291:ILE:HA	1.81	0.61
1:D:381:GLY:HA2	1:D:384:MET:HE3	1.80	0.61
1:D:402:LEU:O	1:D:406:MET:HG2	2.01	0.61
1:F:277:LEU:HA	1:F:280:LEU:HD12	1.82	0.61
1:F:368:PRO:CG	1:F:427:GLN:HA	2.30	0.61
1:A:150:GLU:OE1	1:E:56:ARG:HD3	2.00	0.61
1:A:110:GLN:HE22	1:A:114:ASN:HD21	1.49	0.61
1:A:331:ALA:O	1:A:335:GLN:HB2	2.00	0.61
1:A:379:ILE:HD11	1:A:398:VAL:HG13	1.81	0.61
1:D:196:ASN:ND2	1:D:198:LYS:HZ3	1.99	0.61
1:E:47:ILE:HD11	1:E:443:ILE:HD11	1.82	0.61
1:E:231:GLN:HG3	1:E:315:THR:OG1	2.00	0.61
1:E:279:PHE:CD1	1:E:297:HIS:HB3	2.36	0.61
1:B:196:ASN:ND2	1:B:198:LYS:HZ3	1.99	0.61
1:C:284:LYS:NZ	1:C:284:LYS:N	2.49	0.61
1:D:279:PHE:CD1	1:D:297:HIS:HB3	2.35	0.61
1:C:313:PRO:CG	1:C:337:ASN:HD22	2.11	0.60
1:F:331:ALA:O	1:F:335:GLN:HB2	2.01	0.60
1:B:279:PHE:CD1	1:B:297:HIS:HB3	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ARG:HD3	1:E:150:GLU:OE1	2.01	0.60
1:F:327:ASP:H	1:F:330:GLN:NE2	1.98	0.60
1:A:110:GLN:HE22	1:A:114:ASN:ND2	2.00	0.60
1:C:259:LEU:CD1	1:C:280:LEU:HD13	2.32	0.60
1:E:402:LEU:O	1:E:406:MET:HG2	2.00	0.60
1:D:-16:ARG:HB3	1:F:71:GLN:HB2	1.84	0.60
1:D:287:LYS:O	1:D:287:LYS:HG2	2.01	0.60
1:F:333:LEU:HD23	1:F:336:LYS:CE	2.31	0.60
1:A:35:LEU:HD11	1:A:436:LEU:HD21	1.84	0.60
1:A:330:GLN:O	1:A:334:LEU:HD12	2.02	0.60
1:B:273:THR:HG22	1:B:275:GLU:H	1.66	0.60
1:C:368:PRO:HG3	1:C:427:GLN:HA	1.83	0.60
1:A:333:LEU:HD23	1:A:336:LYS:CE	2.31	0.60
1:A:389:GLN:HG2	1:C:389:GLN:HG2	1.82	0.60
1:C:333:LEU:HD23	1:C:336:LYS:CE	2.32	0.60
1:A:71:GLN:HB2	1:E:-16:ARG:HB3	1.84	0.59
1:C:379:ILE:HD11	1:C:398:VAL:HG13	1.84	0.59
1:B:150:GLU:OE1	1:C:56:ARG:HD3	2.02	0.59
1:C:277:LEU:HA	1:C:280:LEU:HD12	1.85	0.59
1:F:218:LEU:HD22	1:F:252:LEU:HD11	1.85	0.59
1:F:379:ILE:HD11	1:F:398:VAL:HG13	1.83	0.59
1:B:106:LEU:HB2	1:B:125:LYS:HG2	1.84	0.59
1:F:35:LEU:HD11	1:F:436:LEU:HD21	1.84	0.59
1:F:110:GLN:HE22	1:F:114:ASN:HD21	1.50	0.59
1:E:273:THR:HG22	1:E:275:GLU:H	1.67	0.59
1:E:284:LYS:HE3	1:E:291:ILE:HA	1.83	0.59
1:B:231:GLN:HG3	1:B:315:THR:OG1	2.01	0.59
1:E:106:LEU:HB2	1:E:125:LYS:HG2	1.85	0.59
1:B:351:THR:HG23	1:B:353:ASP:H	1.68	0.59
1:F:333:LEU:HD23	1:F:336:LYS:HE2	1.85	0.59
1:A:440:GLU:HB2	1:F:198:LYS:HE3	1.85	0.59
1:B:344:GLU:OE1	1:B:349:PRO:HD2	2.01	0.59
1:C:218:LEU:HD22	1:C:252:LEU:HD11	1.85	0.59
1:D:106:LEU:HB2	1:D:125:LYS:HG2	1.84	0.59
1:A:86:GLY:HA2	1:F:187:PHE:CD2	2.38	0.59
1:D:99:ASN:C	1:D:99:ASN:HD22	2.09	0.59
1:D:259:LEU:CD1	1:D:280:LEU:HD13	2.27	0.59
1:D:273:THR:HG22	1:D:275:GLU:H	1.66	0.59
1:E:351:THR:HG23	1:E:353:ASP:H	1.66	0.59
1:F:259:LEU:CD1	1:F:280:LEU:HD13	2.31	0.59
1:F:350:SER:HB2	1:F:366:TYR:OH	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:ASN:HD21	1:B:130:PHE:HA	1.67	0.59
1:A:368:PRO:HG3	1:A:427:GLN:HA	1.85	0.59
1:A:350:SER:HB2	1:A:366:TYR:OH	2.03	0.58
1:A:389:GLN:HG2	1:F:389:GLN:HG2	1.85	0.58
1:B:99:ASN:C	1:B:99:ASN:HD22	2.11	0.58
1:C:261:ASP:OD2	1:C:262:SER:N	2.36	0.58
1:E:203:ASN:O	1:E:204:LEU:HB2	2.03	0.58
1:A:218:LEU:HD22	1:A:252:LEU:HD11	1.84	0.58
1:A:277:LEU:HA	1:A:280:LEU:HD12	1.86	0.58
1:B:287:LYS:O	1:B:287:LYS:HG2	2.03	0.58
1:D:150:GLU:OE1	1:F:56:ARG:HD3	2.02	0.58
1:E:208:ALA:CB	1:E:379:ILE:HG13	2.28	0.58
1:F:284:LYS:NZ	1:F:284:LYS:HB2	2.18	0.58
1:F:368:PRO:HG3	1:F:427:GLN:HA	1.85	0.58
1:A:259:LEU:CD1	1:A:280:LEU:HD13	2.31	0.58
1:A:261:ASP:OD2	1:A:262:SER:N	2.36	0.58
1:C:35:LEU:HD11	1:C:436:LEU:HD21	1.84	0.58
1:A:294:TYR:CZ	1:A:298:SER:HB2	2.38	0.58
1:C:110:GLN:HE22	1:C:114:ASN:ND2	2.01	0.58
1:A:284:LYS:NZ	1:A:284:LYS:N	2.51	0.58
1:C:422:ASN:O	1:C:424:TYR:N	2.36	0.58
1:D:351:THR:HG23	1:D:353:ASP:H	1.68	0.58
1:F:279:PHE:O	1:F:283:LEU:HB2	2.03	0.58
1:A:284:LYS:NZ	1:A:284:LYS:HB2	2.18	0.58
1:F:284:LYS:NZ	1:F:284:LYS:N	2.51	0.58
1:B:-5:TYR:OH	1:B:40:PRO:CG	2.52	0.58
1:C:110:GLN:HE22	1:C:114:ASN:HD21	1.52	0.58
1:C:279:PHE:O	1:C:283:LEU:HB2	2.04	0.58
1:F:45:LEU:HB2	1:F:46:PRO:HD3	1.85	0.58
1:F:110:GLN:HE22	1:F:114:ASN:ND2	2.00	0.58
1:F:261:ASP:OD2	1:F:262:SER:N	2.37	0.58
1:A:3:GLU:HA	1:A:3:GLU:OE2	2.04	0.58
1:D:203:ASN:O	1:D:204:LEU:HB2	2.02	0.58
1:B:-18:THR:CG2	1:B:-16:ARG:H	2.13	0.58
1:B:204:LEU:HA	1:B:207:GLU:OE2	2.04	0.58
1:B:290:ARG:HB3	1:B:292:LYS:HZ3	1.69	0.57
1:D:-5:TYR:OH	1:D:40:PRO:CG	2.52	0.57
1:E:99:ASN:C	1:E:99:ASN:HD22	2.11	0.57
1:A:329:ASP:O	1:A:332:LYS:HB2	2.05	0.57
1:F:329:ASP:O	1:F:332:LYS:HB2	2.03	0.57
1:B:56:ARG:HD3	1:C:150:GLU:OE1	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:VAL:HG13	1:C:240:ASN:CG	2.30	0.57
1:C:329:ASP:O	1:C:332:LYS:HB2	2.03	0.57
1:F:294:TYR:CZ	1:F:298:SER:HB2	2.39	0.57
1:A:-12:LEU:O	1:A:-11:ASP:CB	2.52	0.57
1:A:333:LEU:HD23	1:A:336:LYS:HE2	1.86	0.57
1:C:45:LEU:HB2	1:C:46:PRO:HD3	1.85	0.57
1:D:47:ILE:CD1	1:D:443:ILE:HD11	2.33	0.57
1:A:187:PHE:CD2	1:C:86:GLY:HA2	2.39	0.57
1:B:203:ASN:O	1:B:204:LEU:HB2	2.04	0.57
1:C:333:LEU:HD23	1:C:336:LYS:HE2	1.86	0.57
1:E:328:LEU:HD22	1:E:332:LYS:HE3	1.87	0.57
1:D:219:GLU:OE2	1:D:407:ARG:NH1	2.38	0.57
1:A:45:LEU:HB2	1:A:46:PRO:HD3	1.85	0.57
1:C:265:TYR:CB	1:C:309:PRO:HG3	2.34	0.57
1:E:287:LYS:NZ	1:E:293:GLU:OE1	2.33	0.57
1:A:99:ASN:ND2	1:A:99:ASN:C	2.60	0.57
1:D:290:ARG:HB3	1:D:292:LYS:HZ3	1.69	0.57
1:A:359:LYS:HZ3	1:A:427:GLN:HB3	1.69	0.56
1:B:47:ILE:CD1	1:B:443:ILE:HD11	2.35	0.56
1:E:173:ILE:HD13	1:E:192:THR:O	2.05	0.56
1:A:206:VAL:HG13	1:A:240:ASN:CG	2.30	0.56
1:D:283:LEU:O	1:D:287:LYS:HB3	2.06	0.56
1:D:287:LYS:NZ	1:D:293:GLU:OE1	2.34	0.56
1:E:-5:TYR:OH	1:E:40:PRO:CG	2.54	0.56
1:E:219:GLU:OE2	1:E:407:ARG:NH1	2.38	0.56
1:A:311:GLY:O	1:A:312:VAL:C	2.48	0.56
1:A:422:ASN:O	1:A:424:TYR:N	2.37	0.56
1:B:-16:ARG:HB3	1:C:71:GLN:HB2	1.86	0.56
1:E:128:SER:C	1:E:130:PHE:H	2.13	0.56
1:A:279:PHE:O	1:A:283:LEU:HB2	2.05	0.56
1:C:-12:LEU:O	1:C:-11:ASP:CB	2.52	0.56
1:C:294:TYR:CZ	1:C:298:SER:HB2	2.40	0.56
1:A:423:LYS:HD2	1:A:423:LYS:O	2.05	0.56
1:C:85:LEU:HD22	1:C:437:LYS:HG2	1.87	0.56
1:C:196:ASN:ND2	1:C:198:LYS:HZ1	2.03	0.56
1:C:389:GLN:HG2	1:F:389:GLN:HG2	1.88	0.56
1:F:3:GLU:OE2	1:F:3:GLU:HA	2.06	0.56
1:C:141:LEU:O	1:C:145:GLN:HG3	2.05	0.56
1:C:311:GLY:O	1:C:312:VAL:C	2.48	0.56
1:C:344:GLU:CD	1:C:349:PRO:HD2	2.30	0.56
1:D:74:ASN:HD21	1:D:130:PHE:HA	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:280:LEU:HD23	1:D:284:LYS:NZ	2.20	0.56
1:F:423:LYS:HD2	1:F:423:LYS:O	2.05	0.56
1:D:-18:THR:HG23	1:D:-16:ARG:N	2.13	0.56
1:C:3:GLU:HA	1:C:3:GLU:OE2	2.05	0.56
1:F:422:ASN:O	1:F:424:TYR:N	2.37	0.56
1:A:218:LEU:HD22	1:A:252:LEU:CD1	2.36	0.56
1:A:422:ASN:C	1:A:424:TYR:H	2.14	0.56
1:B:173:ILE:HD13	1:B:192:THR:O	2.06	0.56
1:B:283:LEU:O	1:B:287:LYS:HB3	2.06	0.56
1:C:281:ILE:HG12	1:C:282:ASP:N	2.22	0.56
1:C:423:LYS:HD2	1:C:423:LYS:O	2.06	0.56
1:E:47:ILE:CD1	1:E:443:ILE:HD11	2.36	0.56
1:E:280:LEU:HD23	1:E:284:LYS:NZ	2.20	0.56
1:E:283:LEU:O	1:E:287:LYS:HB3	2.05	0.56
1:D:128:SER:C	1:D:130:PHE:H	2.13	0.55
1:B:-10:LYS:HA	1:B:-5:TYR:CE1	2.41	0.55
1:B:280:LEU:HD23	1:B:284:LYS:NZ	2.20	0.55
1:C:218:LEU:HD22	1:C:252:LEU:CD1	2.36	0.55
1:D:196:ASN:HD22	1:D:198:LYS:H	1.54	0.55
1:E:-10:LYS:HA	1:E:-5:TYR:CE1	2.41	0.55
1:E:287:LYS:O	1:E:287:LYS:HG2	2.01	0.55
1:F:347:ASN:O	1:F:348:MET:C	2.49	0.55
1:A:85:LEU:HD22	1:A:437:LYS:HG2	1.89	0.55
1:C:15:ASP:HB3	1:C:18:GLN:CG	2.35	0.55
1:E:278:GLU:CA	1:E:281:ILE:HG22	2.37	0.55
1:E:351:THR:HG22	1:E:354:ALA:N	2.19	0.55
1:D:-18:THR:CG2	1:D:-16:ARG:H	2.12	0.55
1:D:224:LEU:HD22	1:D:424:TYR:CZ	2.42	0.55
1:D:351:THR:HG22	1:D:354:ALA:CB	2.37	0.55
1:D:447:CYS:SG	1:F:63:CYS:HB3	2.46	0.55
1:E:204:LEU:HA	1:E:207:GLU:OE2	2.06	0.55
1:F:141:LEU:O	1:F:145:GLN:HG3	2.06	0.55
1:A:310:TRP:HH2	1:A:319:PRO:HA	1.72	0.55
1:B:351:THR:HG22	1:B:354:ALA:CB	2.37	0.55
1:C:350:SER:HB2	1:C:366:TYR:OH	2.05	0.55
1:E:41:LYS:O	1:E:46:PRO:HD2	2.07	0.55
1:F:-12:LEU:O	1:F:-11:ASP:CB	2.54	0.55
1:F:206:VAL:HG13	1:F:240:ASN:CG	2.31	0.55
1:F:265:TYR:CB	1:F:309:PRO:HG3	2.36	0.55
1:F:285:GLU:O	1:F:288:LYS:HG2	2.06	0.55
1:A:61:ARG:HD2	1:E:50:THR:HG23	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:LYS:HG2	1:A:303:TYR:CZ	2.41	0.55
1:A:302:LYS:HG3	1:A:304:PHE:HE1	1.72	0.55
1:B:219:GLU:OE2	1:B:407:ARG:NH1	2.39	0.55
1:C:285:GLU:O	1:C:288:LYS:HG2	2.06	0.55
1:D:278:GLU:CA	1:D:281:ILE:HG22	2.37	0.55
1:E:280:LEU:HD23	1:E:284:LYS:HZ1	1.71	0.55
1:F:265:TYR:CD1	1:F:309:PRO:HG3	2.42	0.55
1:A:347:ASN:O	1:A:348:MET:C	2.49	0.55
1:D:331:ALA:CB	1:D:357:LEU:HD23	2.37	0.55
1:E:351:THR:HG23	1:E:353:ASP:N	2.22	0.55
1:A:243:LEU:HD22	1:A:281:ILE:HB	1.89	0.55
1:B:328:LEU:HD22	1:B:332:LYS:HE3	1.89	0.55
1:C:390:PHE:HB2	1:F:388:PHE:CD1	2.37	0.55
1:D:99:ASN:HD21	1:D:102:ILE:H	1.54	0.55
1:D:268:GLU:OE2	1:D:300:THR:HG23	2.07	0.55
1:E:268:GLU:OE2	1:E:300:THR:HG23	2.07	0.55
1:A:344:GLU:CD	1:A:349:PRO:HD2	2.32	0.55
1:B:204:LEU:HD22	1:B:207:GLU:HB2	1.89	0.55
1:C:175:TYR:OH	1:F:-16:ARG:NH2	2.39	0.55
1:C:347:ASN:O	1:C:348:MET:C	2.49	0.55
1:D:-10:LYS:HA	1:D:-5:TYR:CE1	2.41	0.55
1:E:172:GLU:N	1:E:172:GLU:OE2	2.39	0.55
1:A:265:TYR:CB	1:A:309:PRO:HG3	2.36	0.55
1:B:268:GLU:OE2	1:B:300:THR:HG23	2.07	0.55
1:B:278:GLU:CA	1:B:281:ILE:HG22	2.36	0.55
1:C:422:ASN:C	1:C:424:TYR:H	2.14	0.55
1:A:-16:ARG:NH2	1:F:175:TYR:OH	2.40	0.54
1:A:9:GLU:OE2	1:A:9:GLU:HA	2.07	0.54
1:A:265:TYR:CD1	1:A:309:PRO:HG3	2.42	0.54
1:D:173:ILE:HD13	1:D:192:THR:O	2.06	0.54
1:F:218:LEU:HD22	1:F:252:LEU:CD1	2.36	0.54
1:B:207:GLU:HG3	1:B:244:TYR:CD2	2.43	0.54
1:B:224:LEU:HD22	1:B:424:TYR:CZ	2.42	0.54
1:C:216:PHE:O	1:C:220:VAL:HG23	2.07	0.54
1:C:265:TYR:CD1	1:C:309:PRO:HG3	2.41	0.54
1:D:35:LEU:HD11	1:D:436:LEU:HD21	1.90	0.54
1:D:50:THR:HG23	1:F:61:ARG:HD2	1.88	0.54
1:C:187:PHE:CD2	1:F:86:GLY:HA2	2.42	0.54
1:C:302:LYS:HG3	1:C:304:PHE:HE1	1.72	0.54
1:E:207:GLU:HG3	1:E:244:TYR:CD2	2.42	0.54
1:F:85:LEU:HD22	1:F:437:LYS:HG2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:GLU:O	1:A:288:LYS:HG2	2.08	0.54
1:A:328:LEU:HD23	1:A:357:LEU:HD22	1.90	0.54
1:A:368:PRO:HG2	1:A:426:LEU:C	2.33	0.54
1:D:211:TYR:CE1	1:D:248:LYS:HD3	2.43	0.54
1:E:351:THR:HG22	1:E:354:ALA:CB	2.37	0.54
1:A:-12:LEU:O	1:A:-11:ASP:HB3	2.08	0.54
1:F:317:ALA:O	1:F:319:PRO:HD3	2.08	0.54
1:F:350:SER:CB	1:F:366:TYR:OH	2.56	0.54
1:F:411:ILE:O	1:F:415:GLU:HG3	2.07	0.54
1:A:390:PHE:HB2	1:C:388:PHE:CD1	2.38	0.54
1:A:411:ILE:O	1:A:415:GLU:HG3	2.08	0.54
1:C:328:LEU:HD23	1:C:357:LEU:HD22	1.90	0.54
1:D:-13:VAL:HG12	1:D:-12:LEU:N	2.23	0.54
1:E:-13:VAL:HG12	1:E:-12:LEU:N	2.22	0.54
1:E:99:ASN:HD21	1:E:102:ILE:H	1.55	0.54
1:B:99:ASN:HD21	1:B:102:ILE:H	1.55	0.54
1:D:388:PHE:HB3	1:E:388:PHE:O	2.07	0.54
1:E:224:LEU:HD22	1:E:424:TYR:CZ	2.42	0.54
1:F:89:LYS:HD3	1:F:384:MET:HE2	1.90	0.54
1:F:311:GLY:O	1:F:312:VAL:C	2.49	0.54
1:B:172:GLU:OE2	1:B:172:GLU:N	2.41	0.54
1:B:284:LYS:CE	1:B:291:ILE:HA	2.38	0.54
1:B:287:LYS:NZ	1:B:293:GLU:OE1	2.34	0.54
1:D:204:LEU:HA	1:D:207:GLU:OE2	2.07	0.54
1:D:328:LEU:HD22	1:D:332:LYS:HE3	1.88	0.54
1:A:148:MET:HE2	1:A:176:LEU:CD2	2.38	0.54
1:B:128:SER:C	1:B:130:PHE:H	2.13	0.54
1:B:331:ALA:CB	1:B:357:LEU:HD23	2.38	0.54
1:C:198:LYS:HE3	1:F:440:GLU:HB2	1.90	0.54
1:D:41:LYS:O	1:D:46:PRO:HD2	2.07	0.54
1:F:328:LEU:HD23	1:F:357:LEU:HD22	1.90	0.54
1:F:344:GLU:CD	1:F:349:PRO:HD2	2.33	0.54
1:A:194:LYS:HB3	1:A:199:TRP:CZ3	2.42	0.54
1:A:224:LEU:HB3	1:A:226:ILE:HG13	1.90	0.54
1:B:41:LYS:O	1:B:46:PRO:HD2	2.07	0.54
1:C:99:ASN:ND2	1:C:99:ASN:C	2.60	0.54
1:C:148:MET:HE2	1:C:176:LEU:CD2	2.36	0.54
1:C:310:TRP:HH2	1:C:319:PRO:HA	1.73	0.54
1:F:148:MET:HE2	1:F:176:LEU:CD2	2.35	0.54
1:F:292:LYS:HG2	1:F:303:TYR:CZ	2.43	0.54
1:B:207:GLU:CD	1:B:395:ARG:HH12	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:-12:LEU:O	1:C:-11:ASP:HB3	2.08	0.53
1:C:9:GLU:OE2	1:C:9:GLU:HA	2.08	0.53
1:D:204:LEU:HD22	1:D:207:GLU:HB2	1.90	0.53
1:F:15:ASP:HB3	1:F:18:GLN:CG	2.37	0.53
1:F:196:ASN:ND2	1:F:198:LYS:HZ1	2.06	0.53
1:A:141:LEU:O	1:A:145:GLN:HG3	2.08	0.53
1:B:35:LEU:HD11	1:B:436:LEU:HD21	1.90	0.53
1:D:290:ARG:HD3	1:D:292:LYS:HZ1	1.74	0.53
1:F:280:LEU:HD23	1:F:284:LYS:HE2	1.91	0.53
1:A:355:ILE:HG12	1:A:366:TYR:CZ	2.43	0.53
1:C:89:LYS:HD3	1:C:161:VAL:HB	1.90	0.53
1:F:194:LYS:HB3	1:F:199:TRP:CZ3	2.43	0.53
1:A:227:PRO:O	1:A:231:GLN:NE2	2.28	0.53
1:C:194:LYS:HB3	1:C:199:TRP:CZ3	2.44	0.53
1:E:211:TYR:CE1	1:E:248:LYS:HD3	2.44	0.53
1:F:243:LEU:HD22	1:F:281:ILE:HB	1.90	0.53
1:F:422:ASN:C	1:F:424:TYR:H	2.15	0.53
1:A:89:LYS:HD3	1:A:161:VAL:HB	1.91	0.53
1:C:292:LYS:HG2	1:C:303:TYR:CZ	2.43	0.53
1:C:317:ALA:O	1:C:319:PRO:HD3	2.08	0.53
1:E:204:LEU:HD22	1:E:207:GLU:HB2	1.89	0.53
1:F:216:PHE:O	1:F:220:VAL:HG23	2.07	0.53
1:F:355:ILE:HG12	1:F:366:TYR:CZ	2.44	0.53
1:F:439:ALA:O	1:F:443:ILE:HG13	2.08	0.53
1:A:281:ILE:HG12	1:A:282:ASP:N	2.23	0.53
1:E:331:ALA:CB	1:E:357:LEU:HD23	2.38	0.53
1:F:310:TRP:HH2	1:F:319:PRO:HA	1.72	0.53
1:A:198:LYS:HE3	1:C:440:GLU:HB2	1.91	0.53
1:B:179:GLN:NE2	1:B:179:GLN:HA	2.24	0.53
1:B:196:ASN:HD22	1:B:198:LYS:H	1.56	0.53
1:D:207:GLU:HG3	1:D:244:TYR:CD2	2.44	0.53
1:E:207:GLU:CD	1:E:395:ARG:HH12	2.16	0.53
1:F:-12:LEU:O	1:F:-11:ASP:HB3	2.09	0.53
1:A:280:LEU:HA	1:A:284:LYS:HZ1	1.71	0.53
1:A:388:PHE:CD1	1:F:390:PHE:HB2	2.40	0.53
1:E:344:GLU:CD	1:E:349:PRO:HD2	2.34	0.53
1:F:270:ASN:HD22	1:F:270:ASN:C	2.16	0.53
1:A:328:LEU:HD21	1:A:357:LEU:HD13	1.91	0.53
1:C:350:SER:CB	1:C:366:TYR:OH	2.57	0.53
1:D:279:PHE:CE1	1:D:297:HIS:HB3	2.44	0.53
1:F:359:LYS:NZ	1:F:427:GLN:HB3	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:PHE:CE1	1:B:297:HIS:HB3	2.44	0.53
1:C:224:LEU:HB3	1:C:226:ILE:HG13	1.91	0.53
1:D:211:TYR:CD1	1:D:248:LYS:HD3	2.44	0.53
1:E:196:ASN:HD22	1:E:198:LYS:H	1.55	0.53
1:F:9:GLU:OE2	1:F:9:GLU:HA	2.07	0.53
1:F:328:LEU:HD21	1:F:357:LEU:HD13	1.89	0.53
1:A:317:ALA:O	1:A:319:PRO:HD3	2.09	0.52
1:B:211:TYR:CE1	1:B:248:LYS:HD3	2.44	0.52
1:C:7:VAL:O	1:C:11:VAL:HG23	2.09	0.52
1:C:232:THR:HG23	1:C:255:LYS:HE3	1.91	0.52
1:C:328:LEU:HD21	1:C:357:LEU:HD13	1.90	0.52
1:A:92:LEU:O	1:A:165:ASP:CB	2.56	0.52
1:A:216:PHE:O	1:A:220:VAL:HG23	2.07	0.52
1:D:273:THR:HG22	1:D:274:HIS:N	2.24	0.52
1:E:261:ASP:HB2	1:E:291:ILE:HG22	1.91	0.52
1:E:284:LYS:CE	1:E:291:ILE:HA	2.40	0.52
1:F:281:ILE:HG12	1:F:282:ASP:N	2.23	0.52
1:A:350:SER:CB	1:A:366:TYR:OH	2.57	0.52
1:A:359:LYS:NZ	1:A:427:GLN:HB3	2.24	0.52
1:B:-13:VAL:HG12	1:B:-12:LEU:N	2.24	0.52
1:D:56:ARG:HD3	1:F:150:GLU:OE1	2.09	0.52
1:D:351:THR:HG23	1:D:353:ASP:N	2.23	0.52
1:B:50:THR:HG23	1:C:61:ARG:HD2	1.90	0.52
1:B:187:PHE:CG	1:E:86:GLY:HA2	2.45	0.52
1:F:161:VAL:HA	1:F:190:THR:O	2.09	0.52
1:D:261:ASP:HB2	1:D:291:ILE:HG22	1.92	0.52
1:E:179:GLN:HA	1:E:179:GLN:NE2	2.25	0.52
1:F:85:LEU:CD2	1:F:437:LYS:HG2	2.40	0.52
1:F:89:LYS:HD3	1:F:161:VAL:HB	1.92	0.52
1:F:224:LEU:HB3	1:F:226:ILE:HG13	1.90	0.52
1:C:264:GLY:HA3	1:C:303:TYR:CE2	2.45	0.52
1:E:279:PHE:CE1	1:E:297:HIS:HB3	2.45	0.52
1:F:113:LYS:HE2	1:F:377:VAL:CG2	2.39	0.52
1:F:302:LYS:HG3	1:F:304:PHE:HE1	1.73	0.52
1:C:113:LYS:HE2	1:C:377:VAL:CG2	2.39	0.52
1:C:243:LEU:HD22	1:C:281:ILE:HB	1.90	0.52
1:C:280:LEU:HD23	1:C:284:LYS:HE2	1.91	0.52
1:C:284:LYS:NZ	1:C:284:LYS:CB	2.72	0.52
1:F:7:VAL:O	1:F:11:VAL:HG23	2.10	0.52
1:A:264:GLY:HA3	1:A:303:TYR:CE2	2.45	0.52
1:C:85:LEU:CD2	1:C:437:LYS:HG2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:355:ILE:HG12	1:C:366:TYR:CZ	2.44	0.52
1:D:284:LYS:CE	1:D:291:ILE:HA	2.39	0.52
1:D:344:GLU:CD	1:D:349:PRO:HD2	2.33	0.52
1:F:368:PRO:HG2	1:F:426:LEU:C	2.35	0.52
1:F:393:TRP:CZ3	1:F:401:LYS:HD2	2.45	0.52
1:A:280:LEU:HD23	1:A:284:LYS:HE2	1.91	0.52
1:B:211:TYR:CD1	1:B:248:LYS:HD3	2.45	0.52
1:F:395:ARG:HG3	1:F:395:ARG:HH11	1.75	0.52
1:B:273:THR:HG22	1:B:274:HIS:N	2.25	0.52
1:B:351:THR:HG23	1:B:353:ASP:N	2.23	0.52
1:C:368:PRO:HG2	1:C:426:LEU:C	2.35	0.52
1:E:321:ALA:HB3	1:E:325:ASP:OD1	2.10	0.52
1:A:85:LEU:CD2	1:A:437:LYS:HG2	2.40	0.51
1:C:215:TYR:CE1	1:C:403:LYS:HG2	2.45	0.51
1:C:395:ARG:HG3	1:C:395:ARG:HH11	1.75	0.51
1:E:308:LYS:HD2	1:E:330:GLN:OE1	2.09	0.51
1:A:89:LYS:HD3	1:A:384:MET:HE2	1.92	0.51
1:A:393:TRP:CZ3	1:A:401:LYS:HD2	2.45	0.51
1:A:439:ALA:O	1:A:443:ILE:HG13	2.09	0.51
1:D:172:GLU:OE2	1:D:172:GLU:N	2.40	0.51
1:A:33:LYS:N	1:A:34:PRO:CD	2.74	0.51
1:B:160:ASP:O	1:B:162:PRO:HD3	2.10	0.51
1:B:344:GLU:CD	1:B:349:PRO:HD2	2.35	0.51
1:D:65:LEU:HD21	1:F:-16:ARG:HD3	1.92	0.51
1:D:280:LEU:HD23	1:D:284:LYS:HZ1	1.75	0.51
1:D:321:ALA:HB3	1:D:325:ASP:OD1	2.11	0.51
1:A:7:VAL:O	1:A:11:VAL:HG23	2.09	0.51
1:D:96:PRO:HG3	1:D:131:ASP:HB2	1.92	0.51
1:D:308:LYS:HD2	1:D:330:GLN:OE1	2.10	0.51
1:E:35:LEU:HD11	1:E:436:LEU:HD21	1.92	0.51
1:F:232:THR:HG21	1:F:257:LEU:HD11	1.92	0.51
1:A:161:VAL:HA	1:A:190:THR:O	2.10	0.51
1:A:382:LEU:O	1:A:386:GLN:HG3	2.10	0.51
1:C:277:LEU:O	1:C:277:LEU:HD22	2.11	0.51
1:F:232:THR:HG23	1:F:255:LYS:HE3	1.92	0.51
1:C:393:TRP:CZ3	1:C:401:LYS:HD2	2.46	0.51
1:D:179:GLN:NE2	1:D:179:GLN:HA	2.26	0.51
1:B:447:CYS:SG	1:C:63:CYS:HB3	2.50	0.51
1:C:232:THR:HG21	1:C:257:LEU:HD11	1.93	0.51
1:D:99:ASN:ND2	1:D:99:ASN:C	2.69	0.51
1:D:350:SER:HB2	1:D:366:TYR:OH	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:LEU:HD22	1:B:254:VAL:HG11	1.93	0.51
1:B:280:LEU:HD23	1:B:284:LYS:HZ1	1.76	0.51
1:C:382:LEU:O	1:C:386:GLN:HG3	2.10	0.51
1:D:58:ILE:HD13	1:D:154:HIS:CD2	2.46	0.51
1:D:207:GLU:CD	1:D:395:ARG:HH12	2.18	0.51
1:E:219:GLU:HG2	1:E:407:ARG:HA	1.93	0.51
1:B:351:THR:HG22	1:B:354:ALA:N	2.20	0.51
1:E:211:TYR:CD1	1:E:248:LYS:HD3	2.46	0.51
1:E:224:LEU:HB3	1:E:226:ILE:HG13	1.93	0.51
1:B:65:LEU:HD21	1:C:-16:ARG:HD3	1.93	0.51
1:B:217:VAL:O	1:B:221:LEU:HG	2.11	0.51
1:C:280:LEU:HA	1:C:284:LYS:HZ1	1.75	0.51
1:C:439:ALA:O	1:C:443:ILE:HG13	2.11	0.50
1:E:273:THR:HG22	1:E:274:HIS:N	2.24	0.50
1:A:336:LYS:HG3	1:A:337:ASN:OD1	2.11	0.50
1:B:198:LYS:HE3	1:E:440:GLU:CB	2.41	0.50
1:C:292:LYS:O	1:C:294:TYR:N	2.44	0.50
1:C:411:ILE:O	1:C:415:GLU:HG3	2.11	0.50
1:F:280:LEU:HA	1:F:284:LYS:HZ1	1.76	0.50
1:A:277:LEU:O	1:A:277:LEU:HD22	2.11	0.50
1:B:58:ILE:HD13	1:B:154:HIS:CD2	2.46	0.50
1:B:308:LYS:HD2	1:B:330:GLN:OE1	2.10	0.50
1:C:161:VAL:HA	1:C:190:THR:O	2.10	0.50
1:F:422:ASN:C	1:F:422:ASN:HD22	2.19	0.50
1:A:422:ASN:C	1:A:422:ASN:HD22	2.20	0.50
1:C:-22:LEU:HD23	1:C:-22:LEU:O	2.12	0.50
1:C:33:LYS:N	1:C:34:PRO:CD	2.75	0.50
1:C:284:LYS:N	1:C:284:LYS:HZ2	2.10	0.50
1:D:89:LYS:HE2	1:D:380:SER:OG	2.11	0.50
1:D:219:GLU:HG2	1:D:407:ARG:HA	1.94	0.50
1:F:-22:LEU:HD23	1:F:-22:LEU:O	2.12	0.50
1:F:92:LEU:O	1:F:165:ASP:CB	2.60	0.50
1:F:215:TYR:CE1	1:F:403:LYS:HG2	2.47	0.50
1:A:215:TYR:CE1	1:A:403:LYS:HG2	2.45	0.50
1:B:96:PRO:HG3	1:B:131:ASP:HB2	1.94	0.50
1:B:261:ASP:HB2	1:B:291:ILE:HG22	1.92	0.50
1:B:321:ALA:HB3	1:B:325:ASP:OD1	2.11	0.50
1:C:121:MET:CE	1:C:377:VAL:HG12	2.41	0.50
1:C:368:PRO:HG2	1:C:426:LEU:O	2.12	0.50
1:D:298:SER:OG	1:D:300:THR:HG22	2.12	0.50
1:E:89:LYS:HE2	1:E:380:SER:OG	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:334:LEU:O	1:F:339:CYS:HB2	2.12	0.50
1:C:89:LYS:HD3	1:C:384:MET:HE2	1.93	0.50
1:D:160:ASP:O	1:D:162:PRO:HD3	2.12	0.50
1:D:217:VAL:O	1:D:221:LEU:HG	2.12	0.50
1:E:350:SER:HB2	1:E:366:TYR:OH	2.12	0.50
1:A:175:TYR:OH	1:C:-16:ARG:NH2	2.44	0.50
1:E:298:SER:OG	1:E:300:THR:HG22	2.12	0.50
1:F:382:LEU:O	1:F:386:GLN:HG3	2.11	0.50
1:A:15:ASP:HB3	1:A:18:GLN:CG	2.37	0.50
1:A:56:ARG:HH22	1:F:185:ASN:CG	2.19	0.50
1:A:395:ARG:HG3	1:A:395:ARG:HH11	1.77	0.50
1:B:89:LYS:HE2	1:B:380:SER:OG	2.12	0.50
1:B:290:ARG:HD3	1:B:292:LYS:HZ1	1.75	0.50
1:D:351:THR:HG22	1:D:354:ALA:N	2.20	0.50
1:B:187:PHE:CD2	1:E:86:GLY:HA2	2.47	0.49
1:B:198:LYS:HE3	1:E:440:GLU:HB2	1.94	0.49
1:C:273:THR:HB	1:C:276:ASN:OD1	2.12	0.49
1:E:96:PRO:HG3	1:E:131:ASP:HB2	1.94	0.49
1:A:-16:ARG:HD3	1:E:65:LEU:HD21	1.93	0.49
1:A:113:LYS:HE2	1:A:377:VAL:CG2	2.42	0.49
1:A:310:TRP:CH2	1:A:319:PRO:HA	2.47	0.49
1:E:249:LEU:HD22	1:E:254:VAL:HG11	1.94	0.49
1:F:277:LEU:O	1:F:277:LEU:HD22	2.12	0.49
1:F:336:LYS:HG3	1:F:337:ASN:OD1	2.12	0.49
1:A:322:THR:O	1:A:325:ASP:HB2	2.12	0.49
1:E:160:ASP:O	1:E:162:PRO:HD3	2.12	0.49
1:F:284:LYS:N	1:F:284:LYS:HZ2	2.10	0.49
1:A:284:LYS:NZ	1:A:284:LYS:CB	2.75	0.49
1:B:298:SER:OG	1:B:300:THR:HG22	2.11	0.49
1:C:328:LEU:HG	1:C:353:ASP:CB	2.39	0.49
1:E:58:ILE:HD13	1:E:154:HIS:CD2	2.48	0.49
1:A:80:GLN:HB3	1:A:88:TYR:CD1	2.48	0.49
1:B:224:LEU:HB3	1:B:226:ILE:HG13	1.93	0.49
1:C:273:THR:H	1:C:276:ASN:CB	2.24	0.49
1:C:336:LYS:HG3	1:C:337:ASN:OD1	2.13	0.49
1:D:197:VAL:HG13	1:D:392:HIS:CE1	2.48	0.49
1:D:331:ALA:HB3	1:D:357:LEU:HD23	1.95	0.49
1:D:422:ASN:O	1:D:423:LYS:CB	2.60	0.49
1:E:272:PHE:HE2	1:E:280:LEU:HD11	1.77	0.49
1:F:121:MET:CE	1:F:377:VAL:HG12	2.42	0.49
1:F:273:THR:HB	1:F:276:ASN:OD1	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:CYS:HB3	1:E:447:CYS:SG	2.52	0.49
1:A:194:LYS:HE2	1:A:200:GLY:HA3	1.95	0.49
1:C:310:TRP:CH2	1:C:319:PRO:HA	2.48	0.49
1:F:284:LYS:NZ	1:F:284:LYS:CB	2.75	0.49
1:A:-22:LEU:HD23	1:A:-22:LEU:O	2.12	0.49
1:A:232:THR:HG21	1:A:257:LEU:HD11	1.95	0.49
1:B:234:VAL:CG2	1:B:314:CYS:HB3	2.42	0.49
1:B:277:LEU:O	1:B:281:ILE:CG2	2.61	0.49
1:F:33:LYS:N	1:F:34:PRO:CD	2.75	0.49
1:C:131:ASP:O	1:C:135:LYS:HD3	2.13	0.49
1:E:138:ASN:O	1:E:142:LYS:HG3	2.12	0.49
1:A:232:THR:HG23	1:A:255:LYS:HE3	1.94	0.49
1:A:350:SER:OG	1:A:366:TYR:OH	2.31	0.49
1:E:-18:THR:CG2	1:E:-16:ARG:H	2.15	0.49
1:E:74:ASN:ND2	1:E:130:PHE:CA	2.75	0.49
1:F:89:LYS:CG	1:F:384:MET:HE1	2.43	0.49
1:F:227:PRO:O	1:F:231:GLN:NE2	2.28	0.49
1:F:292:LYS:O	1:F:294:TYR:N	2.46	0.49
1:A:196:ASN:ND2	1:A:198:LYS:HZ1	2.11	0.48
1:B:197:VAL:HG13	1:B:392:HIS:CE1	2.48	0.48
1:F:194:LYS:HE2	1:F:200:GLY:HA3	1.95	0.48
1:A:121:MET:CE	1:A:377:VAL:HG12	2.41	0.48
1:A:368:PRO:HG2	1:A:426:LEU:O	2.12	0.48
1:B:4:MET:HE1	1:B:30:TYR:HA	1.96	0.48
1:B:219:GLU:HG2	1:B:407:ARG:HA	1.94	0.48
1:C:270:ASN:C	1:C:270:ASN:HD22	2.20	0.48
1:B:138:ASN:O	1:B:142:LYS:HG3	2.14	0.48
1:D:224:LEU:HB3	1:D:226:ILE:HG13	1.94	0.48
1:E:379:ILE:CD1	1:E:398:VAL:CG1	2.91	0.48
1:F:273:THR:H	1:F:276:ASN:CB	2.25	0.48
1:D:138:ASN:O	1:D:142:LYS:HG3	2.13	0.48
1:D:227:PRO:O	1:D:231:GLN:NE2	2.46	0.48
1:D:440:GLU:HB2	1:E:198:LYS:HE3	1.96	0.48
1:F:309:PRO:O	1:F:311:GLY:N	2.46	0.48
1:B:326:VAL:HA	1:B:330:GLN:HE21	1.78	0.48
1:C:105:PHE:HE1	1:C:109:GLU:OE2	1.96	0.48
1:D:341:LEU:C	1:D:341:LEU:HD23	2.39	0.48
1:C:80:GLN:HB3	1:C:88:TYR:CD1	2.48	0.48
1:E:227:PRO:O	1:E:231:GLN:NE2	2.47	0.48
1:F:284:LYS:O	1:F:288:LYS:CA	2.61	0.48
1:B:331:ALA:HB3	1:B:357:LEU:HD23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:LEU:C	1:B:341:LEU:HD23	2.38	0.48
1:C:14:LEU:C	1:C:16:PRO:HD3	2.39	0.48
1:C:322:THR:O	1:C:325:ASP:HB2	2.13	0.48
1:D:272:PHE:HE2	1:D:280:LEU:HD11	1.79	0.48
1:E:197:VAL:HG13	1:E:392:HIS:CE1	2.48	0.48
1:F:264:GLY:HA3	1:F:303:TYR:CE2	2.49	0.48
1:F:379:ILE:CD1	1:F:398:VAL:CG1	2.90	0.48
1:A:294:TYR:C	1:A:296:ASN:H	2.22	0.48
1:B:388:PHE:O	1:E:388:PHE:HB3	2.13	0.48
1:D:277:LEU:O	1:D:281:ILE:CG2	2.59	0.48
1:D:326:VAL:HA	1:D:330:GLN:HE21	1.78	0.48
1:B:261:ASP:HB2	1:B:291:ILE:CG2	2.44	0.48
1:C:197:VAL:HG13	1:C:392:HIS:CE1	2.49	0.48
1:D:141:LEU:O	1:D:145:GLN:HG3	2.13	0.48
1:C:294:TYR:C	1:C:296:ASN:H	2.22	0.48
1:C:309:PRO:O	1:C:311:GLY:N	2.47	0.48
1:E:341:LEU:C	1:E:341:LEU:HD23	2.39	0.48
1:E:422:ASN:O	1:E:423:LYS:CB	2.58	0.48
1:A:273:THR:HB	1:A:276:ASN:OD1	2.13	0.47
1:C:92:LEU:O	1:C:165:ASP:CB	2.60	0.47
1:D:4:MET:HE1	1:D:30:TYR:HA	1.96	0.47
1:E:217:VAL:O	1:E:221:LEU:HG	2.14	0.47
1:F:294:TYR:C	1:F:296:ASN:H	2.22	0.47
1:A:292:LYS:O	1:A:294:TYR:N	2.48	0.47
1:C:284:LYS:O	1:C:288:LYS:CA	2.62	0.47
1:F:310:TRP:CH2	1:F:319:PRO:HA	2.48	0.47
1:A:14:LEU:C	1:A:16:PRO:HD3	2.38	0.47
1:A:270:ASN:HD22	1:A:270:ASN:C	2.19	0.47
1:A:334:LEU:O	1:A:339:CYS:HB2	2.14	0.47
1:B:74:ASN:ND2	1:B:130:PHE:CA	2.77	0.47
1:C:334:LEU:O	1:C:339:CYS:HB2	2.14	0.47
1:D:-12:LEU:O	1:D:-11:ASP:C	2.57	0.47
1:D:379:ILE:CD1	1:D:398:VAL:CG1	2.93	0.47
1:F:131:ASP:O	1:F:135:LYS:HD3	2.15	0.47
1:D:-22:LEU:O	1:D:-14:VAL:HA	2.14	0.47
1:D:249:LEU:HD22	1:D:254:VAL:HG11	1.95	0.47
1:D:261:ASP:HB2	1:D:291:ILE:CG2	2.45	0.47
1:D:341:LEU:HD23	1:D:342:VAL:N	2.29	0.47
1:A:110:GLN:NE2	1:A:114:ASN:ND2	2.62	0.47
1:B:227:PRO:O	1:B:231:GLN:NE2	2.47	0.47
1:C:-18:THR:HG22	1:C:-16:ARG:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:SER:C	1:C:130:PHE:H	2.23	0.47
1:E:261:ASP:HB2	1:E:291:ILE:CG2	2.44	0.47
1:F:80:GLN:HB3	1:F:88:TYR:CD1	2.50	0.47
1:A:207:GLU:HG3	1:A:244:TYR:CD2	2.49	0.47
1:A:328:LEU:CD2	1:A:357:LEU:HD22	2.45	0.47
1:D:86:GLY:HA2	1:E:187:PHE:CD2	2.48	0.47
1:E:4:MET:HE1	1:E:30:TYR:HA	1.96	0.47
1:A:128:SER:C	1:A:130:PHE:H	2.21	0.47
1:A:131:ASP:O	1:A:135:LYS:HD3	2.14	0.47
1:A:197:VAL:HG13	1:A:392:HIS:CE1	2.50	0.47
1:B:350:SER:HB2	1:B:366:TYR:OH	2.14	0.47
1:C:194:LYS:HE2	1:C:200:GLY:HA3	1.95	0.47
1:D:174:GLY:HA2	1:D:199:TRP:CH2	2.50	0.47
1:F:14:LEU:C	1:F:16:PRO:HD3	2.40	0.47
1:F:197:VAL:HG13	1:F:392:HIS:CE1	2.50	0.47
1:F:207:GLU:HG3	1:F:244:TYR:CD2	2.50	0.47
1:F:322:THR:O	1:F:325:ASP:HB2	2.15	0.47
1:A:107:GLY:HA2	1:A:125:LYS:HB2	1.97	0.47
1:A:379:ILE:CD1	1:A:398:VAL:CG1	2.90	0.47
1:B:-12:LEU:O	1:B:-11:ASP:C	2.58	0.47
1:B:106:LEU:HD13	1:B:125:LYS:HE2	1.96	0.47
1:B:388:PHE:HB3	1:D:388:PHE:O	2.14	0.47
1:E:-22:LEU:O	1:E:-14:VAL:HA	2.15	0.47
1:A:328:LEU:HG	1:A:353:ASP:CB	2.41	0.47
1:B:440:GLU:CB	1:D:198:LYS:HE3	2.45	0.47
1:C:292:LYS:C	1:C:294:TYR:N	2.73	0.47
1:F:-21:LYS:HB3	1:F:-17:GLY:HA2	1.96	0.47
1:F:128:SER:C	1:F:130:PHE:H	2.23	0.47
1:A:45:LEU:N	1:A:46:PRO:CD	2.78	0.47
1:A:284:LYS:O	1:A:288:LYS:CA	2.63	0.47
1:A:445:GLN:O	1:F:178:GLY:HA3	2.15	0.47
1:B:272:PHE:HE2	1:B:280:LEU:HD11	1.80	0.47
1:B:379:ILE:CD1	1:B:398:VAL:CG1	2.92	0.47
1:C:207:GLU:O	1:C:211:TYR:HB2	2.14	0.47
1:E:331:ALA:HB3	1:E:357:LEU:HD23	1.96	0.47
1:A:273:THR:H	1:A:276:ASN:CB	2.25	0.46
1:D:440:GLU:CB	1:E:198:LYS:HE3	2.44	0.46
1:F:45:LEU:N	1:F:46:PRO:CD	2.78	0.46
1:E:-12:LEU:O	1:E:-11:ASP:C	2.58	0.46
1:E:141:LEU:O	1:E:145:GLN:HG3	2.15	0.46
1:F:280:LEU:CA	1:F:284:LYS:NZ	2.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:-22:LEU:O	1:B:-14:VAL:HA	2.15	0.46
1:C:-21:LYS:HB3	1:C:-17:GLY:HA2	1.96	0.46
1:D:12:MET:HA	1:D:22:LEU:CD2	2.46	0.46
1:D:234:VAL:CG2	1:D:314:CYS:HB3	2.45	0.46
1:A:284:LYS:N	1:A:284:LYS:HZ2	2.14	0.46
1:A:335:GLN:C	1:A:335:GLN:CD	2.83	0.46
1:A:379:ILE:CD1	1:A:398:VAL:HG13	2.43	0.46
1:F:-18:THR:HG22	1:F:-16:ARG:CB	2.45	0.46
1:F:290:ARG:HD3	1:F:292:LYS:NZ	2.30	0.46
1:A:290:ARG:HD3	1:A:292:LYS:NZ	2.30	0.46
1:C:266:VAL:CG2	1:C:267:TYR:H	2.27	0.46
1:D:86:GLY:HA2	1:E:187:PHE:CG	2.51	0.46
1:F:99:ASN:ND2	1:F:99:ASN:C	2.60	0.46
1:F:207:GLU:O	1:F:211:TYR:HB2	2.15	0.46
1:F:335:GLN:C	1:F:335:GLN:CD	2.83	0.46
1:B:86:GLY:HA2	1:D:187:PHE:CG	2.50	0.46
1:B:141:LEU:O	1:B:145:GLN:HG3	2.16	0.46
1:E:106:LEU:HD13	1:E:125:LYS:HE2	1.98	0.46
1:E:341:LEU:HD23	1:E:342:VAL:N	2.31	0.46
1:A:-21:LYS:HB3	1:A:-17:GLY:HA2	1.97	0.46
1:A:-18:THR:HG22	1:A:-16:ARG:CB	2.45	0.46
1:A:-5:TYR:OH	1:A:40:PRO:HG3	2.15	0.46
1:A:309:PRO:O	1:A:311:GLY:N	2.49	0.46
1:C:266:VAL:CG2	1:C:267:TYR:N	2.78	0.46
1:C:379:ILE:CD1	1:C:398:VAL:CG1	2.90	0.46
1:E:174:GLY:HA2	1:E:199:TRP:CH2	2.51	0.46
1:F:213:LEU:HA	1:F:372:ALA:O	2.16	0.46
1:A:89:LYS:CG	1:A:384:MET:HE1	2.46	0.46
1:A:311:GLY:HA2	1:A:333:LEU:HD13	1.98	0.46
1:C:207:GLU:HG3	1:C:244:TYR:CD2	2.51	0.46
1:C:328:LEU:CD2	1:C:357:LEU:HD22	2.45	0.46
1:E:-18:THR:HG23	1:E:-16:ARG:N	2.16	0.46
1:E:12:MET:HA	1:E:22:LEU:CD2	2.46	0.46
1:F:-5:TYR:OH	1:F:40:PRO:HG3	2.15	0.46
1:F:89:LYS:HD3	1:F:384:MET:CE	2.45	0.46
1:F:105:PHE:HE1	1:F:109:GLU:OE2	1.99	0.46
1:F:266:VAL:CG2	1:F:267:TYR:N	2.78	0.46
1:F:379:ILE:CD1	1:F:398:VAL:HG13	2.45	0.46
1:A:80:GLN:HB3	1:A:88:TYR:CE1	2.51	0.46
1:A:215:TYR:OH	1:A:403:LYS:HE2	2.16	0.46
1:A:266:VAL:CG2	1:A:267:TYR:H	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:VAL:CG2	1:A:267:TYR:N	2.79	0.46
1:B:86:GLY:HA2	1:D:187:PHE:CD2	2.51	0.46
1:D:106:LEU:HD13	1:D:125:LYS:HE2	1.98	0.46
1:E:292:LYS:HG2	1:E:303:TYR:CE1	2.51	0.46
1:F:277:LEU:O	1:F:280:LEU:HB2	2.16	0.46
1:B:278:GLU:C	1:B:281:ILE:HG22	2.41	0.45
1:B:341:LEU:HD23	1:B:342:VAL:N	2.31	0.45
1:D:364:ILE:O	1:D:364:ILE:HG22	2.16	0.45
1:E:325:ASP:N	1:E:349:PRO:O	2.50	0.45
1:F:279:PHE:CD1	1:F:297:HIS:CG	3.04	0.45
1:A:273:THR:CG2	1:A:274:HIS:N	2.80	0.45
1:C:110:GLN:NE2	1:C:114:ASN:ND2	2.64	0.45
1:E:3:GLU:OE2	1:E:3:GLU:HA	2.16	0.45
1:E:439:ALA:O	1:E:440:GLU:C	2.59	0.45
1:F:379:ILE:CD1	1:F:382:LEU:HD12	2.40	0.45
1:A:105:PHE:HE1	1:A:109:GLU:OE2	1.98	0.45
1:A:207:GLU:O	1:A:211:TYR:HB2	2.16	0.45
1:B:174:GLY:HA2	1:B:199:TRP:CH2	2.51	0.45
1:C:368:PRO:HG3	1:C:427:GLN:CA	2.47	0.45
1:D:367:CYS:HA	1:D:368:PRO:HD3	1.67	0.45
1:C:80:GLN:HB3	1:C:88:TYR:CE1	2.51	0.45
1:D:319:PRO:HD2	1:D:343:GLY:O	2.17	0.45
1:F:334:LEU:HB3	1:F:339:CYS:SG	2.57	0.45
1:B:292:LYS:HG2	1:B:303:TYR:CE1	2.51	0.45
1:C:89:LYS:CG	1:C:384:MET:HE1	2.45	0.45
1:F:99:ASN:O	1:F:103:VAL:HG23	2.17	0.45
1:F:306:ASN:O	1:F:307:GLU:HG3	2.16	0.45
1:F:328:LEU:CD2	1:F:357:LEU:HD22	2.45	0.45
1:B:99:ASN:ND2	1:B:99:ASN:C	2.71	0.45
1:C:78:ARG:NH1	1:C:92:LEU:HD23	2.32	0.45
1:C:311:GLY:HA2	1:C:333:LEU:HD13	1.98	0.45
1:C:335:GLN:CD	1:C:335:GLN:C	2.84	0.45
1:C:379:ILE:CD1	1:C:398:VAL:HG13	2.45	0.45
1:E:278:GLU:C	1:E:281:ILE:HG22	2.41	0.45
1:F:80:GLN:HB3	1:F:88:TYR:CE1	2.51	0.45
1:F:395:ARG:HG3	1:F:395:ARG:NH1	2.32	0.45
1:E:-13:VAL:HG12	1:E:-12:LEU:H	1.81	0.45
1:E:326:VAL:HA	1:E:330:GLN:HE21	1.78	0.45
1:A:147:PHE:CE2	1:A:151:LEU:HD22	2.51	0.45
1:B:-18:THR:HG23	1:B:-16:ARG:N	2.15	0.45
1:B:12:MET:HA	1:B:22:LEU:CD2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:LYS:HA	1:C:248:LYS:HD2	1.80	0.45
1:D:74:ASN:ND2	1:D:130:PHE:CA	2.79	0.45
1:F:292:LYS:C	1:F:294:TYR:N	2.74	0.45
1:F:305:PRO:O	1:F:306:ASN:C	2.60	0.45
1:F:396:GLU:OE2	1:F:396:GLU:N	2.45	0.45
1:A:305:PRO:O	1:A:306:ASN:C	2.59	0.45
1:A:306:ASN:O	1:A:307:GLU:HG3	2.16	0.45
1:A:347:ASN:HD22	1:A:347:ASN:HA	1.58	0.45
1:C:284:LYS:HZ3	1:C:284:LYS:HB2	1.82	0.45
1:D:106:LEU:HB3	1:D:125:LYS:HE2	1.99	0.45
1:E:92:LEU:O	1:E:165:ASP:HB3	2.17	0.45
1:E:277:LEU:O	1:E:281:ILE:CG2	2.61	0.45
1:F:311:GLY:HA2	1:F:333:LEU:HD13	1.99	0.45
1:F:368:PRO:HG2	1:F:426:LEU:O	2.16	0.45
1:A:86:GLY:HA2	1:F:187:PHE:CE2	2.52	0.45
1:A:292:LYS:C	1:A:294:TYR:N	2.75	0.45
1:B:351:THR:HG22	1:B:354:ALA:HB2	1.98	0.45
1:C:273:THR:CG2	1:C:274:HIS:N	2.79	0.45
1:D:-13:VAL:HG12	1:D:-12:LEU:H	1.81	0.45
1:D:92:LEU:HA	1:D:126:GLY:O	2.16	0.45
1:D:325:ASP:N	1:D:349:PRO:O	2.49	0.45
1:E:78:ARG:HD2	1:E:78:ARG:HA	1.80	0.45
1:E:92:LEU:HA	1:E:126:GLY:O	2.17	0.45
1:E:351:THR:HG22	1:E:354:ALA:HB2	1.98	0.45
1:F:107:GLY:HA2	1:F:125:LYS:HB2	1.98	0.45
1:A:378:ALA:O	1:A:382:LEU:HG	2.18	0.44
1:B:106:LEU:HB3	1:B:125:LYS:HE2	1.99	0.44
1:C:178:GLY:HA3	1:F:445:GLN:O	2.17	0.44
1:C:334:LEU:HB3	1:C:339:CYS:SG	2.57	0.44
1:F:273:THR:CG2	1:F:274:HIS:N	2.80	0.44
1:A:78:ARG:HA	1:A:78:ARG:HD2	1.64	0.44
1:B:-20:ASP:OD1	1:B:-18:THR:HG22	2.17	0.44
1:C:279:PHE:CD1	1:C:297:HIS:CG	3.05	0.44
1:C:280:LEU:CA	1:C:284:LYS:NZ	2.75	0.44
1:C:395:ARG:HG3	1:C:395:ARG:NH1	2.32	0.44
1:D:278:GLU:C	1:D:281:ILE:HG22	2.41	0.44
1:D:292:LYS:HG2	1:D:303:TYR:CE1	2.52	0.44
1:F:328:LEU:HG	1:F:353:ASP:CB	2.39	0.44
1:A:94:PHE:CE1	1:A:143:PHE:HE2	2.36	0.44
1:A:416:ASN:ND2	1:A:433:ALA:HB2	2.33	0.44
1:B:325:ASP:N	1:B:349:PRO:O	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:LEU:N	1:C:46:PRO:CD	2.79	0.44
1:C:58:ILE:HD13	1:C:154:HIS:CG	2.52	0.44
1:C:89:LYS:HD2	1:C:89:LYS:HA	1.77	0.44
1:C:206:VAL:O	1:C:240:ASN:HB3	2.17	0.44
1:F:60:PHE:CE1	1:F:76:CYS:HB2	2.53	0.44
1:F:147:PHE:CE2	1:F:151:LEU:HD22	2.52	0.44
1:F:206:VAL:O	1:F:240:ASN:HB3	2.17	0.44
1:F:308:LYS:HB3	1:F:310:TRP:CD1	2.52	0.44
1:B:3:GLU:OE2	1:B:3:GLU:HA	2.18	0.44
1:B:147:PHE:CE2	1:B:151:LEU:HD22	2.52	0.44
1:C:107:GLY:HA2	1:C:125:LYS:HB2	1.98	0.44
1:C:185:ASN:CG	1:F:56:ARG:HH22	2.25	0.44
1:D:149:ASN:ND2	1:D:183:ILE:CD1	2.80	0.44
1:F:204:LEU:HD11	1:F:399:ASP:HB2	1.99	0.44
1:F:232:THR:H	1:F:315:THR:HG1	1.66	0.44
1:A:60:PHE:CE1	1:A:76:CYS:HB2	2.53	0.44
1:A:89:LYS:HD3	1:A:384:MET:CE	2.48	0.44
1:A:187:PHE:HB3	1:C:87:PRO:HG3	1.99	0.44
1:B:147:PHE:HE2	1:B:151:LEU:HD22	1.82	0.44
1:C:233:ALA:HA	1:C:316:LEU:O	2.18	0.44
1:E:15:ASP:HB3	1:E:18:GLN:HG3	1.99	0.44
1:E:147:PHE:HE2	1:E:151:LEU:HD22	1.83	0.44
1:E:276:ASN:HB3	1:E:294:TYR:OH	2.18	0.44
1:F:94:PHE:CE1	1:F:143:PHE:HE2	2.35	0.44
1:A:78:ARG:NH1	1:A:92:LEU:HD23	2.33	0.44
1:A:99:ASN:O	1:A:103:VAL:HG23	2.18	0.44
1:A:280:LEU:CA	1:A:284:LYS:NZ	2.74	0.44
1:B:364:ILE:O	1:B:364:ILE:HG22	2.17	0.44
1:D:224:LEU:O	1:D:225:ASN:HB3	2.18	0.44
1:E:147:PHE:CE2	1:E:151:LEU:HD22	2.53	0.44
1:F:204:LEU:HD12	1:F:398:VAL:HG12	2.00	0.44
1:F:284:LYS:O	1:F:288:LYS:HA	2.17	0.44
1:A:284:LYS:O	1:A:288:LYS:HA	2.18	0.44
1:A:284:LYS:O	1:A:289:GLY:N	2.49	0.44
1:B:440:GLU:HB2	1:D:198:LYS:HE3	1.99	0.44
1:E:234:VAL:CG2	1:E:314:CYS:HB3	2.43	0.44
1:F:110:GLN:NE2	1:F:114:ASN:ND2	2.64	0.44
1:F:279:PHE:CD1	1:F:297:HIS:HB3	2.53	0.44
1:F:350:SER:OG	1:F:366:TYR:OH	2.30	0.44
1:A:56:ARG:HH22	1:F:185:ASN:ND2	2.15	0.44
1:A:185:ASN:CG	1:C:56:ARG:HH22	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:PHE:CD1	1:A:297:HIS:CG	3.05	0.44
1:B:276:ASN:HB3	1:B:294:TYR:OH	2.17	0.44
1:C:89:LYS:HD3	1:C:384:MET:CE	2.48	0.44
1:D:196:ASN:ND2	1:D:198:LYS:NZ	2.66	0.44
1:D:351:THR:HG22	1:D:354:ALA:HB2	1.98	0.44
1:E:106:LEU:HB3	1:E:125:LYS:HE2	1.98	0.44
1:F:105:PHE:O	1:F:109:GLU:HG3	2.18	0.44
1:A:206:VAL:HG12	1:A:244:TYR:CE1	2.52	0.44
1:A:233:ALA:HA	1:A:316:LEU:O	2.18	0.44
1:A:308:LYS:HB3	1:A:310:TRP:CD1	2.53	0.44
1:B:-13:VAL:HG12	1:B:-12:LEU:H	1.82	0.44
1:C:284:LYS:O	1:C:288:LYS:HA	2.17	0.44
1:D:28:ILE:HD11	1:D:370:LYS:NZ	2.33	0.44
1:E:149:ASN:ND2	1:E:183:ILE:CD1	2.80	0.44
1:F:281:ILE:HG23	1:F:282:ASP:H	1.83	0.44
1:F:328:LEU:HD22	1:F:332:LYS:HE3	2.00	0.44
1:A:328:LEU:HD22	1:A:332:LYS:HE3	2.00	0.43
1:B:196:ASN:ND2	1:B:198:LYS:NZ	2.65	0.43
1:C:-5:TYR:OH	1:C:40:PRO:HG3	2.17	0.43
1:C:94:PHE:CE1	1:C:143:PHE:HE2	2.35	0.43
1:C:147:PHE:CE2	1:C:151:LEU:HD22	2.53	0.43
1:C:203:ASN:O	1:C:204:LEU:HB2	2.18	0.43
1:D:92:LEU:O	1:D:165:ASP:HB3	2.17	0.43
1:E:319:PRO:HD2	1:E:343:GLY:O	2.18	0.43
1:F:284:LYS:O	1:F:288:LYS:N	2.51	0.43
1:A:206:VAL:O	1:A:240:ASN:HB3	2.18	0.43
1:A:252:LEU:O	1:A:253:ASN:HB2	2.18	0.43
1:A:279:PHE:CD1	1:A:297:HIS:HB3	2.53	0.43
1:C:78:ARG:HD2	1:C:78:ARG:HA	1.64	0.43
1:C:232:THR:O	1:C:314:CYS:HB2	2.18	0.43
1:C:273:THR:N	1:C:276:ASN:HB2	2.28	0.43
1:D:246:VAL:O	1:D:250:LEU:HG	2.18	0.43
1:D:439:ALA:O	1:D:440:GLU:C	2.61	0.43
1:B:92:LEU:HA	1:B:126:GLY:O	2.18	0.43
1:D:406:MET:HE3	1:D:406:MET:HA	2.01	0.43
1:F:203:ASN:O	1:F:204:LEU:HB2	2.18	0.43
1:A:-5:TYR:HA	1:A:-2:LEU:HD12	2.00	0.43
1:A:203:ASN:O	1:A:204:LEU:HB2	2.18	0.43
1:B:246:VAL:O	1:B:250:LEU:HG	2.18	0.43
1:C:378:ALA:O	1:C:382:LEU:HG	2.18	0.43
1:D:3:GLU:OE2	1:D:3:GLU:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:ASP:HB3	1:D:18:GLN:HG3	1.99	0.43
1:D:147:PHE:CE2	1:D:151:LEU:HD22	2.53	0.43
1:F:-18:THR:HG22	1:F:-16:ARG:N	2.33	0.43
1:F:273:THR:N	1:F:276:ASN:HB2	2.29	0.43
1:F:310:TRP:CE2	1:F:326:VAL:HG22	2.54	0.43
1:B:78:ARG:HD2	1:B:78:ARG:HA	1.80	0.43
1:B:92:LEU:O	1:B:165:ASP:HB3	2.19	0.43
1:B:149:ASN:HD22	1:B:183:ILE:CD1	2.31	0.43
1:B:224:LEU:O	1:B:225:ASN:HB3	2.18	0.43
1:C:-18:THR:HG22	1:C:-16:ARG:N	2.33	0.43
1:C:-18:THR:HG21	1:C:-16:ARG:CZ	2.49	0.43
1:C:174:GLY:HA2	1:C:199:TRP:CH2	2.53	0.43
1:C:308:LYS:HB3	1:C:310:TRP:CD1	2.53	0.43
1:C:310:TRP:CE2	1:C:326:VAL:HG22	2.54	0.43
1:D:14:LEU:HD22	1:F:75:ARG:CZ	2.48	0.43
1:D:28:ILE:HD11	1:D:370:LYS:HZ1	1.83	0.43
1:E:-20:ASP:OD1	1:E:-18:THR:HG22	2.18	0.43
1:F:232:THR:O	1:F:314:CYS:HB2	2.19	0.43
1:F:356:ASN:O	1:F:360:SER:N	2.52	0.43
1:A:58:ILE:HD13	1:A:154:HIS:CG	2.53	0.43
1:C:279:PHE:CD1	1:C:297:HIS:HB3	2.53	0.43
1:C:290:ARG:HD3	1:C:292:LYS:NZ	2.33	0.43
1:C:414:SER:O	1:C:415:GLU:C	2.61	0.43
1:D:273:THR:CG2	1:D:274:HIS:N	2.82	0.43
1:E:99:ASN:ND2	1:E:99:ASN:C	2.70	0.43
1:F:233:ALA:HA	1:F:316:LEU:O	2.18	0.43
1:B:290:ARG:C	1:B:292:LYS:N	2.77	0.43
1:B:369:SER:O	1:B:373:ASN:OD1	2.37	0.43
1:B:406:MET:HE3	1:B:406:MET:HA	2.00	0.43
1:C:26:HIS:CD2	1:C:26:HIS:C	2.97	0.43
1:C:313:PRO:CB	1:C:337:ASN:HD22	2.32	0.43
1:C:327:ASP:OD1	1:C:328:LEU:N	2.52	0.43
1:C:422:ASN:C	1:C:422:ASN:HD22	2.21	0.43
1:E:196:ASN:ND2	1:E:198:LYS:NZ	2.64	0.43
1:E:246:VAL:O	1:E:250:LEU:HG	2.19	0.43
1:F:78:ARG:NH1	1:F:92:LEU:HD23	2.34	0.43
1:F:206:VAL:HG12	1:F:244:TYR:CE1	2.54	0.43
1:F:266:VAL:CG2	1:F:267:TYR:H	2.28	0.43
1:B:206:VAL:HG12	1:B:244:TYR:CE1	2.54	0.43
1:C:60:PHE:CE1	1:C:76:CYS:HB2	2.53	0.43
1:C:164:GLY:N	1:C:173:ILE:HD11	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:LEU:HA	1:C:372:ALA:O	2.18	0.43
1:C:252:LEU:O	1:C:253:ASN:HB2	2.19	0.43
1:C:356:ASN:O	1:C:360:SER:N	2.52	0.43
1:E:4:MET:HE1	1:E:33:LYS:HB2	2.01	0.43
1:F:164:GLY:N	1:F:173:ILE:HD11	2.33	0.43
1:A:187:PHE:CE2	1:C:86:GLY:HA2	2.53	0.43
1:A:440:GLU:CB	1:F:198:LYS:HE3	2.49	0.43
1:B:15:ASP:HB3	1:B:18:GLN:HG3	2.00	0.43
1:B:78:ARG:HG2	1:B:151:LEU:HD11	1.99	0.43
1:D:147:PHE:HE2	1:D:151:LEU:HD22	1.83	0.43
1:E:3:GLU:O	1:E:7:VAL:HG23	2.19	0.43
1:F:113:LYS:HE2	1:F:377:VAL:HG23	2.00	0.43
1:A:334:LEU:HB3	1:A:339:CYS:SG	2.58	0.43
1:A:368:PRO:O	1:A:369:SER:C	2.62	0.43
1:C:232:THR:H	1:C:315:THR:HG1	1.67	0.43
1:D:149:ASN:HD22	1:D:183:ILE:CD1	2.32	0.43
1:E:37:MET:HE3	1:E:37:MET:HB3	1.76	0.43
1:E:385:SER:O	1:E:389:GLN:HG3	2.18	0.43
1:F:58:ILE:HD13	1:F:154:HIS:CG	2.54	0.43
1:F:313:PRO:CB	1:F:337:ASN:HD22	2.32	0.43
1:B:85:LEU:HD21	1:B:437:LYS:HG2	2.00	0.42
1:B:290:ARG:O	1:B:292:LYS:N	2.52	0.42
1:B:439:ALA:O	1:B:440:GLU:C	2.58	0.42
1:C:174:GLY:HA2	1:C:199:TRP:HH2	1.84	0.42
1:C:206:VAL:HG12	1:C:244:TYR:CE1	2.54	0.42
1:C:350:SER:OG	1:C:366:TYR:OH	2.27	0.42
1:D:78:ARG:HD2	1:D:78:ARG:HA	1.79	0.42
1:F:174:GLY:HA2	1:F:199:TRP:CH2	2.53	0.42
1:A:232:THR:O	1:A:314:CYS:HB2	2.18	0.42
1:B:3:GLU:O	1:B:7:VAL:HG23	2.19	0.42
1:B:319:PRO:HD2	1:B:343:GLY:O	2.19	0.42
1:C:113:LYS:HE2	1:C:377:VAL:HG23	2.00	0.42
1:D:-20:ASP:OD1	1:D:-18:THR:HG22	2.18	0.42
1:D:344:GLU:OE1	1:D:366:TYR:OH	2.33	0.42
1:F:393:TRP:CD1	1:F:393:TRP:N	2.87	0.42
1:A:327:ASP:OD1	1:A:328:LEU:N	2.53	0.42
1:A:368:PRO:HG3	1:A:427:GLN:CA	2.48	0.42
1:C:105:PHE:O	1:C:109:GLU:HG3	2.18	0.42
1:C:284:LYS:O	1:C:288:LYS:N	2.52	0.42
1:C:284:LYS:O	1:C:289:GLY:N	2.50	0.42
1:D:242:ALA:HB2	1:D:320:CYS:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3:GLU:CG	1:E:45:LEU:HD13	2.49	0.42
1:F:416:ASN:ND2	1:F:433:ALA:HB2	2.34	0.42
1:A:92:LEU:HB2	1:A:168:VAL:HG21	2.02	0.42
1:A:116:LEU:O	1:A:409:ILE:HG12	2.19	0.42
1:A:178:GLY:HA3	1:C:445:GLN:O	2.19	0.42
1:A:310:TRP:CE2	1:A:326:VAL:HG22	2.54	0.42
1:B:149:ASN:ND2	1:B:183:ILE:CD1	2.79	0.42
1:C:187:PHE:CE2	1:F:86:GLY:HA2	2.54	0.42
1:C:215:TYR:OH	1:C:403:LYS:HE2	2.19	0.42
1:C:422:ASN:C	1:C:424:TYR:N	2.77	0.42
1:E:290:ARG:O	1:E:292:LYS:N	2.53	0.42
1:F:-18:THR:HG22	1:F:-16:ARG:H	1.84	0.42
1:F:-4:GLU:OE2	1:F:37:MET:HE1	2.19	0.42
1:F:174:GLY:HA2	1:F:199:TRP:HH2	1.84	0.42
1:F:308:LYS:CD	1:F:330:GLN:OE1	2.60	0.42
1:F:378:ALA:O	1:F:382:LEU:HG	2.19	0.42
1:A:174:GLY:HA2	1:A:199:TRP:CH2	2.54	0.42
1:A:356:ASN:O	1:A:360:SER:N	2.52	0.42
1:A:407:ARG:O	1:A:411:ILE:HG13	2.20	0.42
1:B:385:SER:O	1:B:389:GLN:HG3	2.18	0.42
1:C:416:ASN:ND2	1:C:433:ALA:HB2	2.34	0.42
1:D:229:GLU:CD	1:D:229:GLU:H	2.28	0.42
1:E:28:ILE:HD11	1:E:370:LYS:HZ1	1.83	0.42
1:E:28:ILE:HD11	1:E:370:LYS:NZ	2.34	0.42
1:F:252:LEU:O	1:F:253:ASN:HB2	2.20	0.42
1:A:-18:THR:HG22	1:A:-16:ARG:N	2.35	0.42
1:A:105:PHE:O	1:A:109:GLU:HG3	2.19	0.42
1:A:395:ARG:HG3	1:A:395:ARG:NH1	2.34	0.42
1:C:-4:GLU:OE2	1:C:37:MET:HE1	2.19	0.42
1:C:224:LEU:HD12	1:C:224:LEU:HA	1.80	0.42
1:D:-18:THR:CG2	1:D:-16:ARG:HB2	2.50	0.42
1:D:4:MET:HE1	1:D:33:LYS:HB2	2.01	0.42
1:F:284:LYS:O	1:F:289:GLY:N	2.48	0.42
1:B:14:LEU:HD22	1:C:75:ARG:CZ	2.50	0.42
1:D:85:LEU:HD21	1:D:437:LYS:HG2	2.02	0.42
1:D:385:SER:O	1:D:389:GLN:HG3	2.20	0.42
1:E:149:ASN:HD22	1:E:183:ILE:CD1	2.32	0.42
1:F:-5:TYR:HA	1:F:-2:LEU:HD12	2.00	0.42
1:F:327:ASP:OD1	1:F:328:LEU:N	2.52	0.42
1:F:422:ASN:C	1:F:424:TYR:N	2.78	0.42
1:A:277:LEU:O	1:A:280:LEU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417(A):LEU:CD1	1:A:423:LYS:HB2	2.39	0.42
1:A:419:TYR:CD1	1:A:432:ILE:HG21	2.54	0.42
1:C:393:TRP:CD1	1:C:393:TRP:N	2.87	0.42
1:D:78:ARG:HG2	1:D:151:LEU:HD11	2.01	0.42
1:D:276:ASN:HB3	1:D:294:TYR:OH	2.20	0.42
1:E:215:TYR:HH	1:E:248:LYS:HE2	1.83	0.42
1:A:107:GLY:CA	1:A:125:LYS:HB2	2.49	0.42
1:A:213:LEU:HA	1:A:372:ALA:O	2.19	0.42
1:A:313:PRO:CB	1:A:337:ASN:HD22	2.33	0.42
1:B:3:GLU:CG	1:B:45:LEU:HD13	2.50	0.42
1:B:273:THR:CG2	1:B:274:HIS:N	2.83	0.42
1:C:-6:ASN:ND2	1:C:-2:LEU:HD11	2.35	0.42
1:C:306:ASN:O	1:C:307:GLU:HG3	2.20	0.42
1:D:206:VAL:HG12	1:D:244:TYR:CE1	2.54	0.42
1:F:215:TYR:OH	1:F:403:LYS:HE2	2.20	0.42
1:A:204:LEU:HD11	1:A:399:ASP:HB2	2.02	0.42
1:B:242:ALA:HB2	1:B:320:CYS:HB2	2.02	0.42
1:C:150:GLU:OE1	1:C:154:HIS:HE1	2.03	0.42
1:C:204:LEU:HD11	1:C:399:ASP:HB2	2.02	0.42
1:C:366:TYR:O	1:C:368:PRO:HD3	2.20	0.42
1:C:419:TYR:CD1	1:C:432:ILE:HG21	2.55	0.42
1:D:-12:LEU:O	1:D:-5:TYR:HE1	2.02	0.42
1:D:290:ARG:O	1:D:292:LYS:N	2.53	0.42
1:D:359:LYS:NZ	1:D:427:GLN:HB3	2.35	0.42
1:D:422:ASN:C	1:D:422:ASN:ND2	2.77	0.42
1:E:85:LEU:HD21	1:E:437:LYS:HG2	2.01	0.42
1:A:96:PRO:HG3	1:A:131:ASP:CB	2.44	0.41
1:A:172:GLU:OE2	1:A:172:GLU:N	2.50	0.41
1:A:174:GLY:HA2	1:A:199:TRP:HH2	1.85	0.41
1:A:204:LEU:HD12	1:A:398:VAL:HG12	2.00	0.41
1:A:351:THR:HG22	1:A:352:VAL:N	2.34	0.41
1:B:359:LYS:NZ	1:B:427:GLN:HB3	2.35	0.41
1:C:107:GLY:CA	1:C:125:LYS:HB2	2.50	0.41
1:C:212:GLY:HA2	1:C:215:TYR:HB2	2.01	0.41
1:C:328:LEU:HD22	1:C:332:LYS:HE3	2.01	0.41
1:C:346:ALA:HB3	1:C:349:PRO:HG3	2.02	0.41
1:D:45:LEU:HB2	1:D:46:PRO:HD3	2.02	0.41
1:F:-6:ASN:ND2	1:F:-2:LEU:HD11	2.35	0.41
1:F:96:PRO:HG3	1:F:131:ASP:CB	2.43	0.41
1:F:116:LEU:O	1:F:409:ILE:HG12	2.20	0.41
1:A:-6:ASN:ND2	1:A:-2:LEU:HD11	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ARG:NH2	1:F:185:ASN:OD1	2.53	0.41
1:A:284:LYS:O	1:A:288:LYS:N	2.52	0.41
1:B:28:ILE:HD11	1:B:370:LYS:NZ	2.35	0.41
1:B:229:GLU:H	1:B:229:GLU:CD	2.28	0.41
1:C:99:ASN:O	1:C:103:VAL:HG23	2.19	0.41
1:C:268:GLU:OE1	1:C:298:SER:OG	2.29	0.41
1:C:268:GLU:OE2	1:C:300:THR:HG23	2.19	0.41
1:C:305:PRO:O	1:C:306:ASN:C	2.62	0.41
1:C:368:PRO:O	1:C:369:SER:C	2.62	0.41
1:E:206:VAL:HG12	1:E:244:TYR:CE1	2.55	0.41
1:E:290:ARG:HD3	1:E:292:LYS:HZ1	1.85	0.41
1:F:419:TYR:CD1	1:F:432:ILE:HG21	2.55	0.41
1:A:164:GLY:N	1:A:173:ILE:HD11	2.35	0.41
1:A:346:ALA:HB3	1:A:349:PRO:HG3	2.02	0.41
1:A:358:PHE:HD2	1:A:364:ILE:HD12	1.85	0.41
1:C:-18:THR:HG22	1:C:-16:ARG:H	1.84	0.41
1:C:-5:TYR:HA	1:C:-2:LEU:HD12	2.01	0.41
1:C:227:PRO:O	1:C:231:GLN:NE2	2.28	0.41
1:E:224:LEU:O	1:E:225:ASN:HB3	2.19	0.41
1:E:273:THR:CG2	1:E:274:HIS:N	2.83	0.41
1:F:358:PHE:HD2	1:F:364:ILE:HD12	1.85	0.41
1:A:-18:THR:HG22	1:A:-16:ARG:H	1.86	0.41
1:C:187:PHE:HB3	1:F:87:PRO:HG3	2.02	0.41
1:C:277:LEU:O	1:C:280:LEU:HB2	2.20	0.41
1:C:379:ILE:CD1	1:C:382:LEU:HD12	2.42	0.41
1:D:-12:LEU:O	1:D:-5:TYR:CE1	2.73	0.41
1:E:364:ILE:O	1:E:364:ILE:HG22	2.20	0.41
1:F:26:HIS:CD2	1:F:26:HIS:C	2.98	0.41
1:F:54:PRO:HG3	1:F:81:TYR:CZ	2.56	0.41
1:F:100:LEU:O	1:F:104:LYS:HG3	2.20	0.41
1:F:237:GLY:C	1:F:238:SER:HG	2.29	0.41
1:F:417(A):LEU:CD1	1:F:423:LYS:HB2	2.39	0.41
1:A:-18:THR:HG21	1:A:-16:ARG:CZ	2.49	0.41
1:A:273:THR:N	1:A:276:ASN:HB2	2.29	0.41
1:A:351:THR:CG2	1:A:352:VAL:N	2.84	0.41
1:A:414:SER:O	1:A:415:GLU:C	2.63	0.41
1:B:344:GLU:OE1	1:B:366:TYR:OH	2.29	0.41
1:C:92:LEU:HB2	1:C:168:VAL:HG21	2.01	0.41
1:C:436:LEU:HD23	1:C:436:LEU:HA	1.80	0.41
1:E:149:ASN:HD22	1:E:149:ASN:HA	1.58	0.41
1:F:215:TYR:CZ	1:F:248:LYS:HE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:298:SER:C	1:F:300:THR:N	2.77	0.41
1:A:281:ILE:HG23	1:A:282:ASP:H	1.85	0.41
1:A:298:SER:C	1:A:300:THR:N	2.78	0.41
1:B:4:MET:CE	1:B:30:TYR:HA	2.50	0.41
1:B:96:PRO:HG3	1:B:131:ASP:CG	2.46	0.41
1:B:99:ASN:O	1:B:103:VAL:HG23	2.21	0.41
1:B:185:ASN:OD1	1:E:56:ARG:NH2	2.53	0.41
1:B:290:ARG:C	1:B:292:LYS:H	2.28	0.41
1:C:204:LEU:HD12	1:C:398:VAL:HG12	2.01	0.41
1:E:4:MET:CE	1:E:30:TYR:HA	2.50	0.41
1:E:45:LEU:HB2	1:E:46:PRO:HD3	2.02	0.41
1:E:229:GLU:H	1:E:229:GLU:CD	2.28	0.41
1:E:290:ARG:C	1:E:292:LYS:H	2.28	0.41
1:E:290:ARG:C	1:E:292:LYS:N	2.77	0.41
1:F:89:LYS:HG3	1:F:384:MET:HE1	2.03	0.41
1:F:346:ALA:HB3	1:F:349:PRO:HG3	2.03	0.41
1:A:75:ARG:CZ	1:E:14:LEU:HD22	2.50	0.41
1:A:284:LYS:HZ3	1:A:284:LYS:HB2	1.82	0.41
1:B:4:MET:HE1	1:B:33:LYS:HB2	2.02	0.41
1:B:268:GLU:OE2	1:B:300:THR:CG2	2.69	0.41
1:C:351:THR:HG22	1:C:352:VAL:N	2.36	0.41
1:D:174:GLY:HA2	1:D:199:TRP:HH2	1.86	0.41
1:D:290:ARG:C	1:D:292:LYS:N	2.77	0.41
1:E:78:ARG:HG2	1:E:151:LEU:HD11	2.02	0.41
1:E:278:GLU:HA	1:E:281:ILE:HG21	2.02	0.41
1:E:436:LEU:HD23	1:E:436:LEU:HA	1.89	0.41
1:F:63:CYS:HA	1:F:72:ARG:O	2.20	0.41
1:F:212:GLY:HA2	1:F:215:TYR:HB2	2.02	0.41
1:A:53:GLU:HA	1:A:54:PRO:HD3	1.91	0.41
1:C:172:GLU:OE2	1:C:172:GLU:N	2.50	0.41
1:C:215:TYR:CZ	1:C:248:LYS:HE2	2.55	0.41
1:C:367:CYS:HA	1:C:368:PRO:HD3	1.72	0.41
1:C:377:VAL:O	1:C:380:SER:HB3	2.21	0.41
1:D:382:LEU:O	1:D:386:GLN:HG3	2.20	0.41
1:E:-18:THR:CG2	1:E:-16:ARG:HB2	2.51	0.41
1:A:54:PRO:HG3	1:A:81:TYR:CZ	2.56	0.41
1:A:87:PRO:HG3	1:F:187:PHE:HB3	2.02	0.41
1:A:93:ARG:NH2	1:A:166:ILE:HD12	2.36	0.41
1:A:100:LEU:O	1:A:104:LYS:HG3	2.20	0.41
1:A:161:VAL:HG13	1:A:190:THR:C	2.46	0.41
1:A:248:LYS:HD2	1:A:248:LYS:HA	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:VAL:O	1:A:380:SER:HB3	2.21	0.41
1:A:393:TRP:CD1	1:A:393:TRP:N	2.85	0.41
1:B:179:GLN:HA	1:B:179:GLN:HE21	1.86	0.41
1:B:252:LEU:O	1:B:253:ASN:HB2	2.20	0.41
1:C:-6:ASN:O	1:C:-5:TYR:C	2.64	0.41
1:C:100:LEU:O	1:C:104:LYS:HG3	2.21	0.41
1:C:273:THR:O	1:C:274:HIS:C	2.64	0.41
1:C:281:ILE:HG23	1:C:282:ASP:H	1.86	0.41
1:C:298:SER:C	1:C:300:THR:N	2.79	0.41
1:C:323:GLN:O	1:C:324:ASN:HB2	2.21	0.41
1:D:278:GLU:HA	1:D:281:ILE:HG21	2.01	0.41
1:D:290:ARG:C	1:D:292:LYS:H	2.29	0.41
1:D:359:LYS:HZ3	1:D:427:GLN:HB3	1.86	0.41
1:E:359:LYS:NZ	1:E:427:GLN:HB3	2.36	0.41
1:F:331:ALA:C	1:F:357:LEU:HD23	2.46	0.41
1:F:368:PRO:HG3	1:F:427:GLN:CA	2.48	0.41
1:A:75:ARG:NH2	1:E:14:LEU:HB3	2.36	0.41
1:A:212:GLY:HA2	1:A:215:TYR:HB2	2.01	0.41
1:A:331:ALA:C	1:A:357:LEU:HD23	2.46	0.41
1:A:379:ILE:CD1	1:A:382:LEU:HD12	2.39	0.41
1:D:1:ASP:OD1	1:D:33:LYS:HE3	2.21	0.41
1:D:3:GLU:O	1:D:7:VAL:HG23	2.21	0.41
1:D:268:GLU:OE2	1:D:300:THR:CG2	2.68	0.41
1:E:130:PHE:O	1:E:132:PRO:HD3	2.21	0.41
1:F:147:PHE:HE2	1:F:151:LEU:HD22	1.86	0.41
1:F:246:VAL:CG2	1:F:259:LEU:HD21	2.32	0.41
1:B:96:PRO:HG3	1:B:131:ASP:CB	2.51	0.40
1:B:282:ASP:O	1:B:283:LEU:CG	2.65	0.40
1:D:96:PRO:HG3	1:D:131:ASP:CB	2.51	0.40
1:E:63:CYS:HA	1:E:72:ARG:O	2.22	0.40
1:E:99:ASN:O	1:E:103:VAL:HG23	2.21	0.40
1:E:382:LEU:O	1:E:386:GLN:HG3	2.21	0.40
1:F:-18:THR:HG21	1:F:-16:ARG:CZ	2.51	0.40
1:F:66:ASP:OD2	1:F:66:ASP:C	2.64	0.40
1:F:347:ASN:HD22	1:F:347:ASN:HA	1.58	0.40
1:A:150:GLU:OE1	1:A:154:HIS:HE1	2.04	0.40
1:A:224:LEU:HD12	1:A:224:LEU:HA	1.79	0.40
1:B:32:LEU:HD12	1:B:48:ILE:HD12	2.04	0.40
1:B:359:LYS:HZ3	1:B:427:GLN:HB3	1.86	0.40
1:B:382:LEU:O	1:B:386:GLN:HG3	2.22	0.40
1:C:218:LEU:HD12	1:C:218:LEU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:ALA:O	1:D:335:GLN:HB2	2.20	0.40
1:D:369:SER:O	1:D:373:ASN:OD1	2.40	0.40
1:E:282:ASP:O	1:E:283:LEU:CG	2.65	0.40
1:E:406:MET:HE3	1:E:406:MET:HA	2.03	0.40
1:F:113:LYS:HE2	1:F:377:VAL:HG21	2.02	0.40
1:F:351:THR:CG2	1:F:352:VAL:N	2.84	0.40
1:F:368:PRO:O	1:F:369:SER:C	2.64	0.40
1:A:-22:LEU:O	1:A:-21:LYS:HG3	2.22	0.40
1:B:54:PRO:HG3	1:B:81:TYR:CZ	2.57	0.40
1:B:331:ALA:O	1:B:335:GLN:HB2	2.21	0.40
1:D:224:LEU:HD13	1:D:224:LEU:HA	1.86	0.40
1:E:268:GLU:OE2	1:E:300:THR:CG2	2.69	0.40
1:A:-4:GLU:OE2	1:A:37:MET:HE1	2.21	0.40
1:A:366:TYR:O	1:A:368:PRO:HD3	2.22	0.40
1:B:-12:LEU:O	1:B:-5:TYR:HE1	2.03	0.40
1:B:-12:LEU:O	1:B:-5:TYR:CE1	2.74	0.40
1:B:45:LEU:HB2	1:B:46:PRO:HD3	2.03	0.40
1:B:367:CYS:HA	1:B:368:PRO:HD3	1.67	0.40
1:D:32:LEU:HD12	1:D:48:ILE:HD12	2.03	0.40
1:D:282:ASP:O	1:D:283:LEU:CG	2.64	0.40
1:E:221:LEU:HD23	1:E:221:LEU:HA	1.90	0.40
1:E:224:LEU:HD13	1:E:224:LEU:HA	1.87	0.40
1:E:344:GLU:OE1	1:E:366:TYR:OH	2.33	0.40
1:F:150:GLU:OE1	1:F:154:HIS:HE1	2.03	0.40
1:A:228:VAL:HG13	1:A:229:GLU:N	2.37	0.40
1:B:55:GLU:HG3	1:B:81:TYR:O	2.22	0.40
1:B:156:GLY:HA2	1:B:190:THR:OG1	2.22	0.40
1:C:197:VAL:HA	1:C:201:GLY:HA3	2.04	0.40
1:D:3:GLU:CG	1:D:45:LEU:HD13	2.50	0.40
1:D:96:PRO:HG3	1:D:131:ASP:CG	2.47	0.40
1:D:261:ASP:C	1:D:263:ASN:N	2.80	0.40
1:E:242:ALA:HB2	1:E:320:CYS:HB2	2.02	0.40
1:E:367:CYS:HA	1:E:368:PRO:HD3	1.67	0.40
1:F:107:GLY:CA	1:F:125:LYS:HB2	2.51	0.40
1:F:197:VAL:HA	1:F:201:GLY:HA3	2.03	0.40
1:F:268:GLU:OE2	1:F:300:THR:HG23	2.22	0.40
1:F:323:GLN:O	1:F:324:ASN:HB2	2.21	0.40
1:F:351:THR:HG22	1:F:352:VAL:N	2.35	0.40

There are no symmetry-related clashes.

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	465/470 (99%)	408 (88%)	40 (9%)	17 (4%)	2	6
1	B	465/470 (99%)	428 (92%)	31 (7%)	6 (1%)	9	25
1	C	465/470 (99%)	408 (88%)	41 (9%)	16 (3%)	3	7
1	D	465/470 (99%)	430 (92%)	29 (6%)	6 (1%)	9	25
1	E	465/470 (99%)	429 (92%)	29 (6%)	7 (2%)	8	22
1	F	465/470 (99%)	407 (88%)	41 (9%)	17 (4%)	2	6
All	All	2790/2820 (99%)	2510 (90%)	211 (8%)	69 (2%)	4	11

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	-5	TYR
1	B	-11	ASP
1	B	285	GLU
1	C	-5	TYR
1	C	305	PRO
1	D	-11	ASP
1	D	285	GLU
1	E	-11	ASP
1	E	285	GLU
1	F	-5	TYR
1	F	305	PRO
1	A	-11	ASP
1	A	111	ILE
1	A	281	ILE
1	A	293	GLU
1	A	301	ALA
1	A	305	PRO
1	A	306	ASN
1	A	310	TRP
1	C	-11	ASP

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Mol	Chain	Res	Type
1	C	111	ILE
1	C	281	ILE
1	C	293	GLU
1	C	301	ALA
1	C	306	ASN
1	C	310	TRP
1	F	-11	ASP
1	F	111	ILE
1	F	293	GLU
1	F	301	ALA
1	F	306	ASN
1	F	310	TRP
1	A	238	SER
1	A	280	LEU
1	A	423	LYS
1	B	283	LEU
1	B	423	LYS
1	C	238	SER
1	C	280	LEU
1	C	423	LYS
1	D	283	LEU
1	D	423	LYS
1	E	283	LEU
1	E	423	LYS
1	F	238	SER
1	F	280	LEU
1	F	281	ILE
1	F	423	LYS
1	A	282	ASP
1	B	281	ILE
1	C	282	ASP
1	D	281	ILE
1	A	165	ASP
1	C	165	ASP
1	C	295	LEU
1	D	78	ARG
1	E	78	ARG
1	E	281	ILE
1	F	165	ASP
1	F	282	ASP
1	F	295	LEU
1	A	295	LEU

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Mol	Chain	Res	Type
1	A	348	MET
1	B	291	ILE
1	C	348	MET
1	F	348	MET
1	A	227	PRO
1	E	291	ILE
1	F	227	PRO

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	401/403 (100%)	375 (94%)	26 (6%)	15	37
1	B	401/403 (100%)	382 (95%)	19 (5%)	23	51
1	C	401/403 (100%)	374 (93%)	27 (7%)	15	36
1	D	401/403 (100%)	382 (95%)	19 (5%)	23	51
1	E	401/403 (100%)	381 (95%)	20 (5%)	22	48
1	F	401/403 (100%)	374 (93%)	27 (7%)	15	36
All	All	2406/2418 (100%)	2268 (94%)	138 (6%)	18	43

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-19	LYS
1	A	-18	THR
1	A	-12	LEU
1	A	-6	ASN
1	A	72	ARG
1	A	81	TYR
1	A	95	HIS
1	A	99	ASN
1	A	105	PHE
1	A	110	GLN
1	A	213	LEU

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Mol	Chain	Res	Type
1	A	224	LEU
1	A	273	THR
1	A	277	LEU
1	A	281	ILE
1	A	284	LYS
1	A	305	PRO
1	A	315	THR
1	A	320	CYS
1	A	328	LEU
1	A	347	ASN
1	A	350	SER
1	A	352	VAL
1	A	363	ASN
1	A	397	THR
1	A	404	GLU
1	B	-22	LEU
1	B	-18	THR
1	B	-4	GLU
1	B	81	TYR
1	B	99	ASN
1	B	109	GLU
1	B	190	THR
1	B	204	LEU
1	B	213	LEU
1	B	224	LEU
1	B	231	GLN
1	B	261	ASP
1	B	277	LEU
1	B	300	THR
1	B	328	LEU
1	B	351	THR
1	B	363	ASN
1	B	364	ILE
1	B	422	ASN
1	C	-19	LYS
1	C	-18	THR
1	C	-12	LEU
1	C	-6	ASN
1	C	72	ARG
1	C	81	TYR
1	C	95	HIS
1	C	99	ASN

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Mol	Chain	Res	Type
1	C	105	PHE
1	C	110	GLN
1	C	213	LEU
1	C	224	LEU
1	C	273	THR
1	C	277	LEU
1	C	281	ILE
1	C	284	LYS
1	C	305	PRO
1	C	315	THR
1	C	320	CYS
1	C	328	LEU
1	C	347	ASN
1	C	350	SER
1	C	352	VAL
1	C	363	ASN
1	C	397	THR
1	C	402	LEU
1	C	404	GLU
1	D	-22	LEU
1	D	-18	THR
1	D	-4	GLU
1	D	81	TYR
1	D	99	ASN
1	D	109	GLU
1	D	190	THR
1	D	204	LEU
1	D	213	LEU
1	D	224	LEU
1	D	231	GLN
1	D	261	ASP
1	D	277	LEU
1	D	300	THR
1	D	328	LEU
1	D	351	THR
1	D	363	ASN
1	D	364	ILE
1	D	422	ASN
1	E	-22	LEU
1	E	-18	THR
1	E	-4	GLU
1	E	81	TYR

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Mol	Chain	Res	Type
1	E	99	ASN
1	E	109	GLU
1	E	190	THR
1	E	204	LEU
1	E	213	LEU
1	E	224	LEU
1	E	231	GLN
1	E	261	ASP
1	E	277	LEU
1	E	300	THR
1	E	328	LEU
1	E	342	VAL
1	E	351	THR
1	E	363	ASN
1	E	364	ILE
1	E	422	ASN
1	F	-19	LYS
1	F	-18	THR
1	F	-12	LEU
1	F	-6	ASN
1	F	72	ARG
1	F	81	TYR
1	F	95	HIS
1	F	99	ASN
1	F	105	PHE
1	F	110	GLN
1	F	213	LEU
1	F	224	LEU
1	F	273	THR
1	F	277	LEU
1	F	281	ILE
1	F	284	LYS
1	F	305	PRO
1	F	315	THR
1	F	320	CYS
1	F	328	LEU
1	F	347	ASN
1	F	350	SER
1	F	352	VAL
1	F	363	ASN
1	F	397	THR
1	F	402	LEU

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Mol	Chain	Res	Type
1	F	404	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (125) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-9	ASN
1	A	6	ASN
1	A	26	HIS
1	A	68	ASN
1	A	95	HIS
1	A	99	ASN
1	A	110	GLN
1	A	114	ASN
1	A	149	ASN
1	A	154	HIS
1	A	179	GLN
1	A	185	ASN
1	A	196	ASN
1	A	270	ASN
1	A	347	ASN
1	A	363	ASN
1	A	389	GLN
1	A	392	HIS
1	A	416	ASN
1	B	5	ASN
1	B	6	ASN
1	B	17	ASN
1	B	68	ASN
1	B	95	HIS
1	B	99	ASN
1	B	110	GLN
1	B	114	ASN
1	B	149	ASN
1	B	154	HIS
1	B	179	GLN
1	B	196	ASN
1	B	240	ASN
1	B	270	ASN
1	B	276	ASN
1	B	297	HIS
1	B	324	ASN
1	B	363	ASN

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Mol	Chain	Res	Type
1	B	392	HIS
1	B	416	ASN
1	B	422	ASN
1	C	-9	ASN
1	C	6	ASN
1	C	26	HIS
1	C	68	ASN
1	C	95	HIS
1	C	99	ASN
1	C	110	GLN
1	C	114	ASN
1	C	149	ASN
1	C	154	HIS
1	C	179	GLN
1	C	185	ASN
1	C	196	ASN
1	C	270	ASN
1	C	323	GLN
1	C	347	ASN
1	C	363	ASN
1	C	389	GLN
1	C	392	HIS
1	C	416	ASN
1	D	5	ASN
1	D	6	ASN
1	D	17	ASN
1	D	68	ASN
1	D	95	HIS
1	D	99	ASN
1	D	110	GLN
1	D	114	ASN
1	D	149	ASN
1	D	154	HIS
1	D	179	GLN
1	D	188	ASN
1	D	196	ASN
1	D	240	ASN
1	D	270	ASN
1	D	276	ASN
1	D	297	HIS
1	D	324	ASN
1	D	363	ASN

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Mol	Chain	Res	Type
1	D	392	HIS
1	D	416	ASN
1	D	422	ASN
1	E	5	ASN
1	E	6	ASN
1	E	17	ASN
1	E	68	ASN
1	E	95	HIS
1	E	99	ASN
1	E	110	GLN
1	E	114	ASN
1	E	149	ASN
1	E	154	HIS
1	E	179	GLN
1	E	196	ASN
1	E	231	GLN
1	E	240	ASN
1	E	270	ASN
1	E	276	ASN
1	E	297	HIS
1	E	324	ASN
1	E	363	ASN
1	E	392	HIS
1	E	416	ASN
1	E	422	ASN
1	E	427	GLN
1	F	-9	ASN
1	F	6	ASN
1	F	26	HIS
1	F	68	ASN
1	F	95	HIS
1	F	99	ASN
1	F	110	GLN
1	F	114	ASN
1	F	149	ASN
1	F	154	HIS
1	F	179	GLN
1	F	185	ASN
1	F	196	ASN
1	F	203	ASN
1	F	270	ASN
1	F	347	ASN

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Mol	Chain	Res	Type
1	F	363	ASN
1	F	389	GLN
1	F	392	HIS
1	F	416	ASN

5.3.3 RNA [i](#)

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](#)

There are no ligands in this entry.

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	467/470 (99%)	0.56	24 (5%) 33 29	21, 46, 66, 77	0
1	B	467/470 (99%)	-0.04	6 (1%) 75 73	12, 26, 44, 65	0
1	C	467/470 (99%)	0.55	20 (4%) 40 36	20, 46, 66, 76	0
1	D	467/470 (99%)	0.02	6 (1%) 75 73	14, 26, 45, 65	0
1	E	467/470 (99%)	0.03	4 (0%) 81 80	12, 26, 44, 65	0
1	F	467/470 (99%)	0.56	21 (4%) 38 34	21, 46, 67, 77	0
All	All	2802/2820 (99%)	0.28	81 (2%) 53 50	12, 35, 63, 77	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	301	ALA	4.7
1	F	279	PHE	3.9
1	E	282	ASP	3.7
1	A	373	ASN	3.7
1	C	283	LEU	3.6
1	A	289	GLY	3.4
1	F	-8	ALA	3.3
1	F	270	ASN	3.3
1	E	283	LEU	3.3
1	D	283	LEU	3.2
1	C	284	LYS	3.2
1	F	284	LYS	3.2
1	D	284	LYS	3.1
1	F	325	ASP	3.1
1	F	283	LEU	3.0
1	C	270	ASN	2.9
1	A	-12	LEU	2.9
1	B	285	GLU	2.9
1	B	282	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	297	HIS	2.9
1	A	297	HIS	2.7
1	F	301	ALA	2.7
1	C	251	HIS	2.7
1	F	217	VAL	2.7
1	F	321	ALA	2.7
1	C	226	ILE	2.6
1	C	336	LYS	2.6
1	A	-13	VAL	2.6
1	D	282	ASP	2.6
1	B	284	LYS	2.6
1	C	210	GLY	2.6
1	F	373	ASN	2.5
1	F	377	VAL	2.5
1	B	283	LEU	2.5
1	A	285	GLU	2.5
1	A	254	VAL	2.5
1	A	364	ILE	2.5
1	F	285	GLU	2.5
1	C	348	MET	2.5
1	A	279	PHE	2.5
1	D	281	ILE	2.4
1	A	325	ASP	2.4
1	F	303	TYR	2.4
1	F	255	LYS	2.4
1	A	338	GLY	2.4
1	C	279	PHE	2.3
1	A	283	LEU	2.3
1	F	295	LEU	2.3
1	A	348	MET	2.3
1	F	269	PRO	2.3
1	E	284	LYS	2.3
1	E	297	HIS	2.2
1	C	255	LYS	2.2
1	C	-8	ALA	2.2
1	A	240	ASN	2.2
1	C	262	SER	2.2
1	A	270	ASN	2.2
1	C	306	ASN	2.2
1	A	284	LYS	2.2
1	F	282	ASP	2.2
1	C	326	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	279	PHE	2.2
1	A	333	LEU	2.2
1	A	273	THR	2.1
1	A	326	VAL	2.1
1	A	380	SER	2.1
1	F	208	ALA	2.1
1	C	285	GLU	2.1
1	C	138	ASN	2.1
1	A	376	GLY	2.1
1	A	258	THR	2.1
1	B	373	ASN	2.1
1	F	347	ASN	2.1
1	F	348	MET	2.0
1	D	297	HIS	2.0
1	C	307	GLU	2.0
1	F	349	PRO	2.0
1	A	47	ILE	2.0
1	C	291	ILE	2.0
1	C	256	VAL	2.0
1	C	267	TYR	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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.