



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:54 AM UTC

PDB ID : 7EOZ / pdb_00007eoz
Title : The structure of rice Defective Pollen Wall (DPW) in the complex with its cofactor NADP
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Deposited on : 2021-04-24
Resolution : 3.40 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

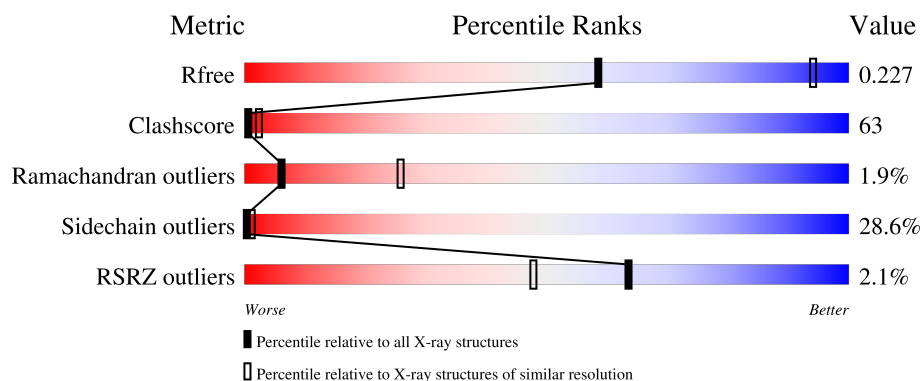
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

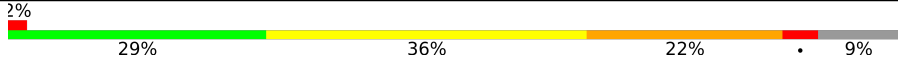
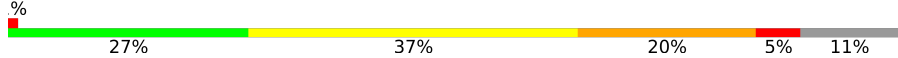
The reported resolution of this entry is 3.40 Å.

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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	532	
1	B	532	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7616 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 Fatty acyl-CoA reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	0
			3753	2387	654	694	18			
1	B	473	Total	C	N	O	S	0	0	0
			3682	2344	639	681	18			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

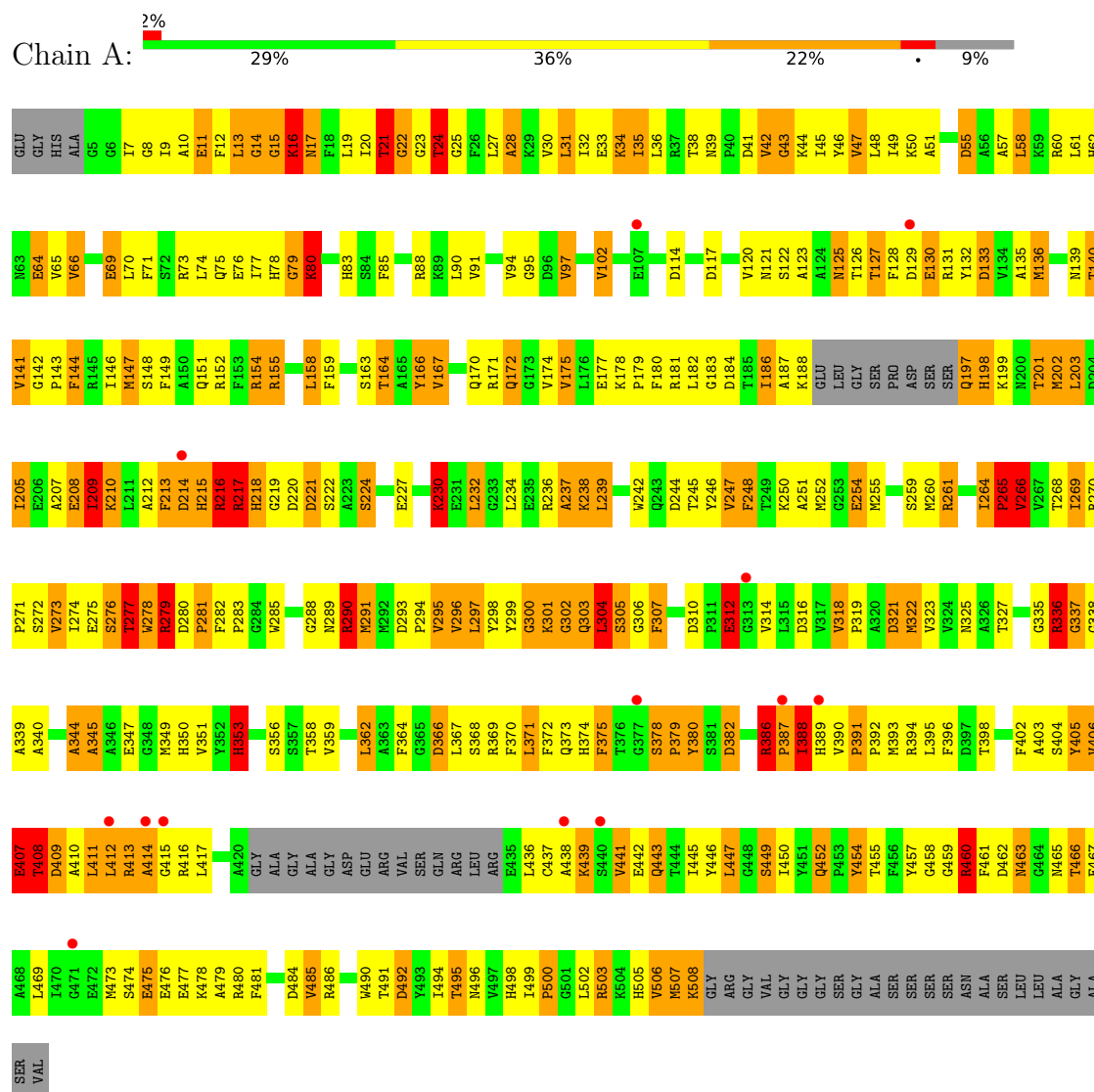
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	45	Total 45	O 45	0	0
3	B	40	Total 40	O 40	0	0

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: Fatty acyl-CoA reductase



SER	G459	D397	A832	I269	L203	H136	V66	GLU
ASN	R460	T398	K333	R270	D204	M139	D67	GLY
ALA	N463	M399	E400	S271	I205	T140	T68	HIS
SER	N464	E401	R336	S272	E208	V141	B69	ALA
LEU	N465	F402	G337	V273	L209	G142	L70	G5
ALA	N466	A403	G338	L274	K210	P143	R73	G6
GLY	E467	S404	A839	E275	L211	F144	L74	I7
ALA	A468	Y405	A340	S276	A212	R145	Q75	G8
SER	L469	V406	A341	T277	F213	I146	L75	I9
VAL	I470	E407	A342	W278	D214	M147	E76	
	G471	I468	A343	R279	H215	S148	I77	L13
	E472	D409	A344	D280	H216		H78	G14
	M473	A410	A345	F281	R217	A152	G79	G15
	S474	L411	A346	F282	H218	F153	K80	K16
	E475	L412	E347	P283	G219	R154	D81	N17
	E476	R413	G348	G284	H219	R154	Y82	F18
	E477	M414	M285	M349	D220	R155	H83	L19
	K478	A415	H350	M286	D221	L156	I20	I20
	A479	G416	V851	E287	S223	K157	S84	T21
	R480	R416	Y352		A223	L158	R88	G22
	F481	L417	H353	R290	S224	F159	R89	G23
	H482	A418	V354	M291	F225	L160	L90	T24
	F483	GLY		M292	S226		G95	G25
	D484	ALA	V359	D293	E227	S163	D96	F26
	V485	GLY	N360	P294	E228	T164	L27	L27
	R486	ALA	P361	V295	M229	A165	A28	A28
		GLY	A363	V296	K230	V167	R29	R29
		ALA	L362	L297	E231		V30	V30
		GLY	F364	Y298	L232		M101	I31
		ASP	G365	Y299			V102	I32
		GLU	D366	G300			A105	E33
		ARG	L367	K301	E235		P106	K34
		VAL	S368	G302	R236		E107	I35
		SER	R369	Q303	A237		L108	L36
		GLN	F370	L304	K238		A109	R37
		ARG	L371	S305	L239		G110	T38
		LEU	F372	G306			V111	N39
		GLU	Q373	F307	W242		I112	P40
		LEU	T376	L308	Q243		A113	D41
		VAL	G377	A309	D244		D114	V42
		A438	S378	D310	Y246		E115	G43
		K439	P379	P311	V247		V116	K44
		S440	Y380	E312	F248		D117	I45
		V441	S381	L315	T249		I118	Y46
			D382		K250		I119	V47
		I445	A383	V318	A251		N120	L48
		Y446	A384	P319	M252		N121	I49
		L447	G385	A320	G253		S122	K50
		G448	R386	D321	E254		A123	A51
		S449	P387	M322	M255		A124	
		I450	I388	V323	N258		R125	D85
		Y451	H389	V324	S259		T126	A56
		Q452	V390	N325	M260		T127	A57
		P453	P391	A326	R261		E130	L58
		Y454	P392	G262	G262		R131	L61
		T455	M393	L328	D263		Y132	H62
		F456	R394	I264	L264		D133	N63
		Y457	L395	S330	P265		T201	E64
		G458	F396	M331			A135	V65

4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	222.81Å 222.81Å 114.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.45 – 3.40 48.45 – 3.40	Depositor EDS
% Data completeness (in resolution range)	97.7 (48.45-3.40) 97.7 (48.45-3.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.21 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.191 , 0.240 0.216 , 0.227	Depositor DCC
R_{free} test set	2223 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	96.1	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 174.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.478 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	7616	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.15	7/3833 (0.2%)	2.19	116/5180 (2.2%)
1	B	1.21	13/3761 (0.3%)	2.26	140/5085 (2.8%)
All	All	1.18	20/7594 (0.3%)	2.22	256/10265 (2.5%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	391	PRO	N-CD	15.57	1.69	1.47
1	B	392	PRO	N-CD	10.07	1.61	1.47
1	A	339	ALA	CA-C	-9.81	1.40	1.52
1	B	22	GLY	C-O	8.73	1.35	1.23
1	B	483	PHE	CA-C	8.62	1.64	1.53
1	B	378	SER	N-CA	-7.54	1.38	1.46
1	B	482	HIS	CA-C	6.91	1.60	1.52
1	A	340	ALA	N-CA	6.82	1.55	1.46
1	A	23	GLY	C-O	6.73	1.33	1.23
1	B	65	VAL	CA-C	-6.58	1.44	1.52
1	B	95	GLY	C-O	6.43	1.30	1.23
1	B	354	VAL	C-O	6.18	1.31	1.24
1	A	503	ARG	C-O	6.12	1.31	1.24
1	B	377	GLY	CA-C	6.08	1.58	1.52
1	B	483	PHE	N-CA	-6.02	1.39	1.46
1	A	22	GLY	C-O	5.70	1.31	1.23
1	B	79	GLY	C-O	5.49	1.31	1.23
1	A	79	GLY	C-O	5.46	1.31	1.23
1	A	21	THR	C-O	5.38	1.31	1.24
1	B	497	VAL	C-O	5.08	1.28	1.23

All (256) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	PHE	N-CA-C	32.90	153.26	112.47
1	B	66	VAL	N-CA-C	-25.29	74.56	109.46
1	B	382	ASP	N-CA-C	-24.88	73.56	110.14
1	B	392	PRO	N-CA-C	-24.38	74.80	111.13
1	B	391	PRO	N-CA-C	-24.33	81.02	110.70
1	B	301	LYS	CB-CA-C	-23.55	75.05	110.62
1	A	278	TRP	CB-CA-C	-23.45	75.45	112.03
1	B	96	ASP	CB-CA-C	22.61	151.64	110.95
1	A	388	ILE	N-CA-C	22.54	135.68	110.21
1	B	217	ARG	CB-CA-C	-22.52	77.82	112.05
1	A	265	PRO	CB-CA-C	-19.93	78.67	111.56
1	A	44	LYS	N-CA-C	19.21	136.48	110.35
1	A	303	GLN	N-CA-C	19.05	135.67	113.38
1	A	336	ARG	CB-CA-C	-18.53	80.73	111.68
1	A	387	PRO	CB-CA-C	-18.03	81.81	111.56
1	A	304	LEU	N-CA-CB	-17.62	78.49	110.90
1	A	13	LEU	N-CA-C	-16.90	84.81	109.15
1	A	406	VAL	CB-CA-C	-16.89	83.58	111.29
1	B	96	ASP	N-CA-C	-16.79	82.63	108.14
1	A	277	THR	CB-CA-C	-16.59	89.40	109.80
1	B	393	MET	N-CA-CB	-16.41	86.44	110.24
1	B	304	LEU	N-CA-C	16.34	134.28	110.59
1	B	65	VAL	CB-CA-C	-16.26	93.06	110.62
1	A	213	PHE	CB-CA-C	-16.17	85.78	111.48
1	B	392	PRO	CB-CA-C	15.76	134.07	110.75
1	B	213	PHE	N-CA-C	15.47	132.53	113.50
1	A	507	MET	N-CA-C	-15.16	87.51	110.10
1	B	275	GLU	CB-CA-C	15.14	140.55	110.42
1	B	65	VAL	N-CA-C	14.99	128.62	113.47
1	B	80	LYS	N-CA-C	-14.62	93.20	114.39
1	A	460	ARG	N-CA-C	-14.54	86.50	108.46
1	A	15	GLY	N-CA-C	-14.40	79.05	113.18
1	B	172	GLN	N-CA-C	13.92	132.09	112.04
1	A	507	MET	CB-CA-C	13.78	131.40	109.90
1	A	303	GLN	CB-CA-C	-13.69	88.92	111.23
1	A	44	LYS	N-CA-CB	-13.53	90.15	110.04
1	A	508	LYS	N-CA-CB	13.51	133.46	110.50
1	A	345	ALA	N-CA-C	13.32	127.89	110.43
1	B	348	GLY	N-CA-C	13.25	132.79	112.51
1	B	364	PHE	N-CA-C	-13.06	95.02	112.26
1	B	366	ASP	N-CA-C	-13.02	97.30	113.97
1	A	279	ARG	N-CA-C	13.02	139.32	113.29
1	B	65	VAL	N-CA-CB	-12.87	97.01	112.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	VAL	N-CA-CB	-12.68	86.81	111.15
1	B	97	VAL	N-CA-C	-11.94	101.83	113.53
1	A	414	ALA	CB-CA-C	-11.88	86.78	110.42
1	A	43	GLY	N-CA-C	-11.86	96.46	112.82
1	B	482	HIS	N-CA-CB	-11.82	92.20	110.77
1	A	340	ALA	N-CA-C	-11.52	99.24	113.18
1	A	336	ARG	N-CA-C	-11.52	85.23	107.57
1	B	213	PHE	CB-CA-C	-11.22	88.87	109.29
1	A	386	ARG	CA-C-N	11.17	133.80	119.84
1	A	386	ARG	C-N-CA	11.17	133.80	119.84
1	B	276	SER	N-CA-CB	-11.12	91.70	110.49
1	B	382	ASP	CB-CA-C	11.11	130.13	110.36
1	B	409	ASP	N-CA-C	-10.94	98.88	111.03
1	B	291	MET	N-CA-CB	-10.86	91.26	109.72
1	A	460	ARG	CB-CA-C	10.84	127.17	109.72
1	A	80	LYS	N-CA-C	-10.76	96.89	113.89
1	B	347	GLU	CB-CA-C	-10.71	88.22	109.33
1	B	304	LEU	N-CA-CB	-10.70	94.16	110.42
1	B	218	HIS	N-CA-CB	-10.48	92.73	110.33
1	B	391	PRO	CB-CA-C	10.33	123.53	110.92
1	B	178	LYS	CB-CA-C	10.14	124.16	109.45
1	B	336	ARG	N-CA-C	-10.14	94.54	109.15
1	B	79	GLY	N-CA-C	9.94	136.73	113.18
1	A	378	SER	CA-C-N	9.92	129.73	120.21
1	A	378	SER	C-N-CA	9.92	129.73	120.21
1	B	21	THR	CB-CA-C	9.89	126.88	110.17
1	A	463	ASN	CB-CA-C	9.86	126.90	111.02
1	B	381	SER	CB-CA-C	9.83	127.35	109.37
1	B	481	PHE	CB-CA-C	-9.78	96.10	111.17
1	B	481	PHE	N-CA-C	-9.71	87.40	107.70
1	A	409	ASP	CB-CA-C	9.69	129.70	110.42
1	A	345	ALA	N-CA-CB	-9.67	96.44	110.26
1	B	383	ALA	CB-CA-C	9.66	129.65	110.42
1	A	407	GLU	N-CA-C	-9.65	101.53	113.20
1	A	273	VAL	N-CA-C	9.57	129.25	109.34
1	B	263	ASP	N-CA-C	-9.57	101.61	113.38
1	B	276	SER	N-CA-C	9.55	131.14	110.80
1	B	383	ALA	N-CA-CB	-9.55	94.36	110.49
1	B	174	VAL	N-CA-C	9.53	129.16	109.34
1	B	221	ASP	N-CA-CB	-9.45	96.60	110.49
1	A	47	VAL	N-CA-C	9.41	128.92	109.34
1	A	216	ARG	N-CA-C	9.38	124.11	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	97	VAL	N-CA-CB	-9.38	99.45	112.12
1	A	215	HIS	CB-CA-C	9.31	127.36	110.88
1	A	410	ALA	N-CA-CB	-9.31	95.76	110.19
1	A	344	ALA	CB-CA-C	-9.31	94.34	110.45
1	A	388	ILE	N-CA-CB	-9.27	93.36	111.15
1	A	55	ASP	CB-CA-C	9.15	128.05	109.67
1	A	141	VAL	CB-CA-C	-8.91	99.09	111.65
1	A	338	GLY	N-CA-C	-8.83	96.52	111.27
1	A	414	ALA	N-CA-C	8.81	129.57	110.80
1	B	221	ASP	N-CA-C	8.81	124.18	108.24
1	A	239	LEU	N-CA-CB	-8.68	97.01	109.94
1	B	55	ASP	CB-CA-C	8.50	126.17	110.11
1	A	322	MET	N-CA-C	-8.49	102.85	113.55
1	B	287	GLU	N-CA-C	8.49	124.57	114.04
1	A	265	PRO	N-CA-C	8.44	129.85	112.47
1	B	220	ASP	CB-CA-C	-8.39	97.67	111.68
1	B	364	PHE	CB-CA-C	-8.23	97.87	111.13
1	B	13	LEU	N-CA-C	-8.09	94.49	108.56
1	B	290	ARG	CB-CA-C	7.96	129.21	113.45
1	A	24	THR	N-CA-C	-7.93	103.33	113.16
1	A	408	THR	CB-CA-C	7.90	125.02	110.56
1	B	381	SER	N-CA-CB	-7.89	98.22	110.85
1	B	66	VAL	CB-CA-C	7.84	124.19	112.03
1	B	291	MET	N-CA-C	7.79	124.15	111.37
1	B	391	PRO	CA-N-CD	-7.76	101.14	112.00
1	A	344	ALA	N-CA-C	-7.75	98.99	110.46
1	B	380	TYR	N-CA-C	-7.62	101.04	110.41
1	B	376	THR	N-CA-C	-7.54	102.19	111.40
1	B	139	ASN	N-CA-C	-7.54	102.20	111.40
1	B	96	ASP	CA-C-N	7.52	130.73	121.71
1	B	96	ASP	C-N-CA	7.52	130.73	121.71
1	B	507	MET	CB-CA-C	7.51	120.97	110.16
1	A	214	ASP	N-CA-CB	-7.46	97.88	110.49
1	B	214	ASP	N-CA-C	-7.44	95.62	108.56
1	A	415	GLY	N-CA-C	-7.42	106.11	115.31
1	A	14	GLY	N-CA-C	-7.42	95.60	113.18
1	B	24	THR	N-CA-C	-7.36	102.56	112.94
1	A	183	GLY	CA-C-N	7.36	131.27	120.90
1	A	183	GLY	C-N-CA	7.36	131.27	120.90
1	B	385	GLY	N-CA-C	7.33	130.55	113.18
1	B	281	PRO	N-CA-C	-7.27	103.66	113.40
1	B	140	THR	N-CA-CB	-7.22	99.37	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	449	SER	CB-CA-C	-7.19	98.70	110.79
1	A	79	GLY	N-CA-C	7.17	130.17	113.18
1	A	379	PRO	CB-CA-C	-7.08	100.53	111.22
1	A	55	ASP	N-CA-C	-6.99	103.75	112.90
1	B	140	THR	CB-CA-C	6.97	121.05	109.56
1	A	9	ILE	N-CA-C	6.96	123.82	109.34
1	B	384	ALA	N-CA-CB	-6.85	98.91	110.49
1	A	289	ASN	N-CA-C	6.84	120.30	112.57
1	B	507	MET	N-CA-C	-6.82	99.80	109.96
1	B	463	ASN	CB-CA-C	6.76	121.94	110.85
1	A	300	GLY	N-CA-C	-6.73	104.16	112.77
1	B	381	SER	N-CA-C	-6.67	99.34	109.95
1	B	497	VAL	N-CA-C	6.62	117.26	111.90
1	B	408	THR	N-CA-CB	-6.62	100.92	110.65
1	A	276	SER	N-CA-C	6.58	120.18	110.30
1	A	492	ASP	N-CA-C	6.53	119.37	111.40
1	A	238	LYS	CB-CA-C	-6.49	96.63	109.67
1	A	461	PHE	N-CA-CB	6.48	121.38	110.69
1	B	450	ILE	N-CA-CB	-6.46	100.57	111.23
1	B	275	GLU	N-CA-C	-6.46	97.05	110.80
1	A	304	LEU	CB-CA-C	-6.45	102.87	112.09
1	A	179	PRO	CB-CA-C	-6.43	102.52	110.95
1	B	336	ARG	CB-CA-C	6.35	120.33	110.67
1	B	312	GLU	CA-C-N	6.28	127.28	120.44
1	B	312	GLU	C-N-CA	6.28	127.28	120.44
1	A	350	HIS	CB-CA-C	6.26	120.80	110.78
1	B	272	SER	CA-C-O	-6.25	114.82	121.88
1	B	272	SER	N-CA-C	-6.25	101.73	110.35
1	B	392	PRO	CA-N-CD	-6.24	103.26	112.00
1	B	83	HIS	CA-C-O	-6.23	113.90	120.63
1	B	33	GLU	CB-CG-CD	6.19	123.12	112.60
1	A	28	ALA	CA-C-N	6.12	128.80	120.54
1	A	28	ALA	C-N-CA	6.12	128.80	120.54
1	B	78	HIS	CB-CA-C	6.10	119.79	109.84
1	B	218	HIS	N-CA-C	-6.04	104.65	112.68
1	B	15	GLY	N-CA-C	-6.03	98.88	113.18
1	B	172	GLN	CB-CA-C	-6.01	99.56	110.56
1	A	58	LEU	N-CA-C	-6.00	104.74	111.28
1	A	16	LYS	N-CA-C	-5.97	100.00	109.07
1	B	287	GLU	CA-C-N	-5.95	118.08	122.18
1	B	287	GLU	C-N-CA	-5.95	118.08	122.18
1	B	58	LEU	N-CA-C	-5.94	104.88	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	VAL	CA-C-N	5.93	130.55	122.07
1	B	66	VAL	C-N-CA	5.93	130.55	122.07
1	A	140	THR	CB-CA-C	5.91	119.58	109.65
1	A	21	THR	CB-CA-C	5.86	119.40	109.55
1	A	303	GLN	CA-C-O	-5.86	113.51	119.78
1	B	390	VAL	C-N-CD	-5.83	101.10	125.00
1	B	238	LYS	CB-CA-C	-5.80	98.54	110.38
1	A	290	ARG	N-CA-CB	-5.77	100.74	110.49
1	B	9	ILE	N-CA-CB	5.76	120.74	111.23
1	A	281	PRO	N-CA-C	-5.75	100.62	112.47
1	A	30	VAL	O-C-N	5.74	127.52	121.89
1	B	350	HIS	CB-CA-C	5.73	119.69	110.29
1	A	312	GLU	CA-C-N	5.71	126.98	120.53
1	A	312	GLU	C-N-CA	5.71	126.98	120.53
1	A	217	ARG	N-CA-C	-5.71	103.12	111.17
1	B	452	GLN	CA-C-N	5.70	126.97	119.84
1	B	452	GLN	C-N-CA	5.70	126.97	119.84
1	B	183	GLY	CA-C-N	5.70	129.80	121.31
1	B	183	GLY	C-N-CA	5.70	129.80	121.31
1	A	149	PHE	CA-CB-CG	5.69	119.49	113.80
1	B	213	PHE	CA-C-N	5.69	130.69	122.16
1	B	213	PHE	C-N-CA	5.69	130.69	122.16
1	B	277	THR	CB-CA-C	-5.69	101.97	110.16
1	A	382	ASP	CB-CA-C	-5.68	99.64	113.15
1	A	151	GLN	N-CA-C	-5.67	105.09	112.23
1	B	139	ASN	CB-CA-C	5.65	120.28	110.79
1	B	55	ASP	N-CA-C	-5.64	104.61	112.45
1	B	166	TYR	N-CA-C	-5.60	106.40	113.18
1	B	125	ASN	CB-CA-C	5.60	118.99	109.75
1	B	361	PRO	CB-CA-C	-5.57	102.83	111.40
1	A	148	SER	CA-C-N	5.57	128.01	120.38
1	A	148	SER	C-N-CA	5.57	128.01	120.38
1	A	406	VAL	N-CA-C	-5.57	97.76	109.34
1	B	391	PRO	N-CA-CB	5.55	108.47	103.08
1	A	463	ASN	N-CA-C	-5.52	105.85	112.59
1	A	302	GLY	N-CA-C	5.51	126.23	113.18
1	B	167	VAL	CA-C-O	-5.50	115.33	121.05
1	A	303	GLN	N-CA-CB	5.50	121.19	112.78
1	A	78	HIS	CB-CA-C	5.48	118.78	109.84
1	A	184	ASP	CA-CB-CG	5.46	118.06	112.60
1	B	220	ASP	N-CA-C	5.46	118.17	107.57
1	A	264	ILE	CB-CA-C	-5.45	101.45	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	466	THR	CB-CA-C	5.44	120.70	110.63
1	A	353	HIS	N-CA-C	-5.43	100.32	108.96
1	B	345	ALA	N-CA-C	5.43	117.31	110.24
1	A	230	LYS	O-C-N	5.42	128.33	122.15
1	B	459	GLY	CA-C-O	-5.40	116.72	121.58
1	A	439	LYS	N-CA-C	-5.39	106.67	113.20
1	A	127	THR	CA-C-N	5.38	127.75	120.65
1	A	127	THR	C-N-CA	5.38	127.75	120.65
1	B	279	ARG	CB-CA-C	-5.37	103.82	112.09
1	B	325	ASN	CB-CA-C	5.37	120.25	110.11
1	B	498	HIS	N-CA-CB	5.36	118.65	110.39
1	B	175	VAL	N-CA-C	5.36	120.48	109.34
1	B	83	HIS	CB-CA-C	5.35	119.77	110.68
1	B	303	GLN	CB-CA-C	-5.33	110.41	116.54
1	B	55	ASP	CA-CB-CG	5.33	117.93	112.60
1	B	390	VAL	CA-C-N	-5.32	114.90	120.38
1	B	390	VAL	C-N-CA	-5.32	114.90	120.38
1	B	439	LYS	N-CA-C	-5.32	106.64	113.02
1	B	239	LEU	N-CA-CB	-5.30	101.77	110.14
1	B	215	HIS	CA-CB-CG	-5.29	108.51	113.80
1	B	490	TRP	O-C-N	5.29	127.59	122.09
1	B	238	LYS	CA-C-N	5.26	128.06	120.38
1	B	238	LYS	C-N-CA	5.26	128.06	120.38
1	A	454	TYR	CB-CA-C	5.25	118.43	109.24
1	A	407	GLU	CB-CA-C	5.24	120.07	110.11
1	A	69	GLU	N-CA-C	-5.22	106.41	112.89
1	A	503	ARG	O-C-N	5.22	127.65	122.12
1	A	209	ILE	CA-C-O	-5.20	115.64	121.05
1	B	148	SER	CA-C-N	5.19	127.23	120.28
1	B	148	SER	C-N-CA	5.19	127.23	120.28
1	A	337	GLY	N-CA-C	-5.19	100.89	113.18
1	B	380	TYR	CB-CA-C	-5.18	98.90	110.19
1	A	166	TYR	N-CA-C	-5.16	106.81	113.01
1	B	210	LYS	N-CA-C	-5.14	106.52	112.89
1	B	32	ILE	CA-C-O	-5.13	116.07	121.41
1	A	495	THR	CA-CB-OG1	-5.12	101.91	109.60
1	A	83	HIS	CA-C-O	-5.12	115.10	120.63
1	B	508	LYS	N-CA-CB	5.10	119.17	110.50
1	B	495	THR	CA-CB-OG1	-5.06	102.00	109.60
1	A	500	PRO	CA-C-N	5.04	126.44	120.14
1	A	500	PRO	C-N-CA	5.04	126.44	120.14
1	B	111	VAL	O-C-N	5.03	126.75	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	GLY	N-CA-C	5.03	125.10	113.18
1	A	380	TYR	N-CA-C	5.01	116.44	108.67
1	A	201	THR	CB-CA-C	5.01	117.14	109.03

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	3753	0	3712	509	2
1	B	3682	0	3639	465	2
2	A	48	0	25	10	0
2	B	48	0	25	3	0
3	A	45	0	0	38	0
3	B	40	0	0	30	0
All	All	7616	0	7401	948	2

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 63.

All (948) 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:A:215:HIS:CD2	1:B:216:ARG:HG2	1.26	1.69
1:B:306:GLY:HA2	1:B:393:MET:CE	1.26	1.59
1:B:446:TYR:CE1	1:B:450:ILE:HD11	1.43	1.51
1:B:446:TYR:HE1	1:B:450:ILE:CD1	1.25	1.50
1:A:215:HIS:CD2	1:B:216:ARG:CG	1.94	1.47
1:A:294:PRO:O	1:A:298:TYR:CD2	1.69	1.45
1:A:299:TYR:HA	1:A:304:LEU:CD2	1.48	1.42
1:A:306:GLY:HA2	1:A:393:MET:CE	1.46	1.42
1:A:409:ASP:OD2	1:A:438:ALA:CB	1.67	1.41
1:B:372:PHE:CD1	1:B:390:VAL:CG1	2.01	1.41
1:B:372:PHE:CD1	1:B:390:VAL:HG12	1.57	1.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:GLY:O	1:A:80:LYS:CE	1.72	1.37
1:B:306:GLY:CA	1:B:393:MET:CE	2.03	1.34
1:B:391:PRO:N	1:B:391:PRO:CD	1.69	1.32
1:A:187:ALA:HB2	3:A:739:HOH:O	1.18	1.32
1:A:79:GLY:O	1:A:80:LYS:HE3	1.28	1.31
1:A:215:HIS:NE2	1:B:216:ARG:NE	1.72	1.31
1:A:299:TYR:CA	1:A:304:LEU:HD22	1.61	1.30
1:A:175:VAL:HG23	1:A:460:ARG:O	1.32	1.30
1:B:446:TYR:CE1	1:B:450:ILE:CD1	2.08	1.30
1:A:65:VAL:O	1:A:71:PHE:CD2	1.86	1.29
1:B:276:SER:OG	1:B:286:MET:HG3	1.31	1.26
1:A:409:ASP:OD2	1:A:438:ALA:HB2	1.13	1.25
1:A:215:HIS:NE2	1:B:216:ARG:CD	1.99	1.25
1:B:451:TYR:O	1:B:455:THR:CG2	1.84	1.25
1:A:306:GLY:CA	1:A:393:MET:CE	2.14	1.24
1:A:298:TYR:O	1:A:304:LEU:CD2	1.87	1.23
1:A:394:ARG:HD2	1:A:405:TYR:OH	1.39	1.21
1:B:64:GLU:O	1:B:68:THR:HG21	1.40	1.21
1:B:380:TYR:O	1:B:387:PRO:HD2	1.05	1.21
1:B:271:PRO:HA	3:B:705:HOH:O	1.40	1.20
1:B:62:HIS:HA	1:B:66:VAL:CG2	1.73	1.18
1:B:380:TYR:O	1:B:387:PRO:CD	1.93	1.16
1:B:451:TYR:O	1:B:455:THR:HG23	1.02	1.16
1:B:306:GLY:HA2	1:B:393:MET:HE3	1.25	1.15
1:B:275:GLU:OE2	1:B:293:ASP:CG	1.87	1.15
1:B:275:GLU:OE2	1:B:293:ASP:OD2	1.62	1.15
1:B:365:GLY:O	1:B:369:ARG:NH2	1.79	1.15
1:B:372:PHE:CE1	1:B:390:VAL:CG1	2.31	1.14
1:A:215:HIS:CD2	1:B:216:ARG:HE	1.66	1.14
1:A:47:VAL:HG12	1:A:47:VAL:O	1.47	1.12
1:A:299:TYR:N	1:A:304:LEU:HD22	1.64	1.12
1:B:306:GLY:HA2	1:B:393:MET:HE2	1.31	1.12
1:B:306:GLY:CA	1:B:393:MET:HE1	1.66	1.11
1:A:146:ILE:HG23	3:A:743:HOH:O	1.51	1.11
1:B:372:PHE:O	1:B:376:THR:HG23	1.48	1.11
1:B:290:ARG:O	1:B:294:PRO:CD	1.99	1.11
1:A:306:GLY:CA	1:A:393:MET:HE2	1.77	1.09
1:A:62:HIS:HA	1:A:66:VAL:CG2	1.80	1.09
1:A:344:ALA:O	1:B:345:ALA:HB2	1.51	1.09
1:A:321:ASP:O	1:A:325:ASN:ND2	1.84	1.08
1:B:279:ARG:O	1:B:279:ARG:CG	2.00	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:TYR:CD1	1:A:304:LEU:HD13	1.88	1.08
1:A:300:GLY:HA2	1:A:375:PHE:CE2	1.88	1.08
1:B:372:PHE:CE1	1:B:390:VAL:HG12	1.88	1.08
1:A:215:HIS:CD2	1:B:216:ARG:NE	2.20	1.07
1:A:345:ALA:HA	1:B:345:ALA:HA	1.36	1.07
1:B:275:GLU:OE2	1:B:293:ASP:OD1	1.72	1.07
1:A:299:TYR:HA	1:A:304:LEU:HD22	1.14	1.07
1:B:279:ARG:O	1:B:279:ARG:HG3	1.32	1.07
1:A:391:PRO:HB2	1:A:392:PRO:HD2	1.29	1.06
1:A:294:PRO:HB2	3:A:726:HOH:O	1.53	1.06
1:A:353:HIS:O	1:A:466:THR:HG21	1.53	1.06
1:A:304:LEU:HD12	1:A:304:LEU:O	1.55	1.05
1:B:34:LYS:O	1:B:38:THR:HG22	1.52	1.05
1:B:304:LEU:O	3:B:701:HOH:O	1.72	1.05
1:A:306:GLY:N	1:A:393:MET:HE1	1.69	1.05
1:A:298:TYR:C	1:A:304:LEU:HD22	1.81	1.05
1:B:62:HIS:HA	1:B:66:VAL:HG23	1.08	1.05
1:B:290:ARG:O	1:B:294:PRO:HD3	1.57	1.05
1:A:24:THR:HG22	2:A:601:NAP:O1X	1.56	1.04
1:B:280:ASP:HB3	1:B:281:PRO:CD	1.86	1.04
1:A:65:VAL:O	1:A:71:PHE:CE2	2.09	1.04
1:A:300:GLY:CA	1:A:375:PHE:CE2	2.40	1.03
1:B:172:GLN:HE21	1:B:458:GLY:HA3	1.20	1.03
1:A:79:GLY:O	1:A:80:LYS:HE2	1.55	1.02
1:B:277:THR:HG21	1:B:281:PRO:HD2	1.41	1.02
1:A:214:ASP:O	1:B:214:ASP:OD1	1.75	1.02
1:A:270:ARG:NH1	1:A:351:VAL:HG11	1.75	1.02
1:B:290:ARG:N	3:B:703:HOH:O	1.93	1.01
1:A:274:ILE:CD1	1:A:323:VAL:HG21	1.90	1.01
1:B:372:PHE:CE1	1:B:390:VAL:HG11	1.96	1.00
1:B:452:GLN:HB3	1:B:453:PRO:HD3	1.41	1.00
1:A:322:MET:HE1	1:A:485:VAL:HA	1.43	1.00
1:A:306:GLY:HA2	1:A:393:MET:HE2	1.00	1.00
1:B:390:VAL:C	1:B:391:PRO:CD	2.35	0.99
1:B:64:GLU:O	1:B:68:THR:CG2	2.09	0.99
1:A:302:GLY:O	1:A:304:LEU:HD23	1.61	0.99
1:B:330:SER:HA	3:B:727:HOH:O	1.61	0.99
1:A:507:MET:O	1:A:508:LYS:HD2	1.60	0.99
1:B:354:VAL:H	1:B:466:THR:HG21	1.24	0.99
1:A:299:TYR:HD1	1:A:304:LEU:CD1	1.76	0.99
1:A:306:GLY:CA	1:A:393:MET:HE1	1.88	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:HIS:CA	1:B:66:VAL:HG23	1.93	0.99
1:A:146:ILE:CG2	3:A:743:HOH:O	2.09	0.99
1:A:215:HIS:CG	1:B:216:ARG:HG2	1.98	0.98
1:A:391:PRO:HB2	1:A:392:PRO:CD	1.93	0.98
1:B:299:TYR:OH	1:B:372:PHE:HA	1.64	0.98
1:B:393:MET:HE3	1:B:393:MET:HA	1.42	0.97
1:B:174:VAL:HG12	1:B:174:VAL:O	1.64	0.97
1:B:370:PHE:CE1	1:B:491:THR:HA	1.98	0.97
1:A:299:TYR:CB	1:A:304:LEU:HD13	1.94	0.97
1:B:406:VAL:HG13	1:B:441:VAL:HG11	1.46	0.97
1:B:220:ASP:O	1:B:220:ASP:CG	2.04	0.96
1:A:65:VAL:O	1:A:71:PHE:HD2	1.40	0.96
1:B:322:MET:HE1	1:B:485:VAL:HA	1.47	0.96
1:B:372:PHE:CD1	1:B:390:VAL:HG11	1.99	0.95
1:B:261:ARG:HH11	1:B:261:ARG:HG3	1.29	0.95
1:A:394:ARG:HD2	1:A:405:TYR:HH	1.23	0.94
1:A:201:THR:HG22	3:A:730:HOH:O	1.64	0.94
1:B:167:VAL:O	1:B:242:TRP:HZ3	1.49	0.94
1:B:499:ILE:O	1:B:503:ARG:HG3	1.68	0.94
1:A:205:ILE:HD12	1:A:205:ILE:N	1.83	0.94
1:A:215:HIS:HD2	1:B:216:ARG:CG	1.77	0.94
1:B:295:VAL:HA	1:B:298:TYR:HD2	1.32	0.94
1:B:221:ASP:OD1	1:B:221:ASP:N	1.99	0.93
1:B:365:GLY:O	1:B:369:ARG:CZ	2.16	0.93
1:B:372:PHE:HD1	1:B:390:VAL:CG1	1.58	0.93
1:B:61:LEU:O	1:B:66:VAL:HG22	1.68	0.93
1:B:290:ARG:CA	3:B:703:HOH:O	2.16	0.92
1:A:407:GLU:O	1:A:411:LEU:HB2	1.68	0.92
1:A:215:HIS:CD2	1:B:216:ARG:CD	2.44	0.92
1:A:394:ARG:CD	1:A:405:TYR:OH	2.17	0.92
1:A:215:HIS:NE2	1:B:216:ARG:HG2	1.85	0.92
1:B:143:PRO:HA	1:B:146:ILE:HD12	1.52	0.92
1:B:446:TYR:HE1	1:B:450:ILE:HD12	1.35	0.91
1:A:14:GLY:O	1:A:41:ASP:O	1.89	0.91
1:A:38:THR:HB	3:A:736:HOH:O	1.70	0.91
1:A:47:VAL:N	3:A:702:HOH:O	2.02	0.91
1:A:164:THR:O	1:A:270:ARG:HG2	1.71	0.91
1:A:294:PRO:O	1:A:298:TYR:HD2	1.30	0.90
1:A:299:TYR:CD1	1:A:304:LEU:CD1	2.52	0.90
1:B:368:SER:HB2	1:B:393:MET:HB3	1.54	0.90
1:A:186:ILE:HG13	1:A:242:TRP:CH2	2.07	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:ASP:HB3	1:B:281:PRO:HD3	1.54	0.90
1:A:205:ILE:HD12	1:A:205:ILE:H	1.37	0.89
1:A:62:HIS:HA	1:A:66:VAL:HG23	1.53	0.89
1:A:277:THR:HG21	1:A:281:PRO:HD2	1.53	0.89
1:A:344:ALA:C	1:B:345:ALA:HB2	1.95	0.89
1:B:205:ILE:N	1:B:205:ILE:HD12	1.87	0.89
1:A:298:TYR:C	1:A:304:LEU:CD2	2.42	0.88
1:A:300:GLY:HA2	1:A:375:PHE:CD2	2.08	0.88
1:B:408:THR:HG23	1:B:412:LEU:HD13	1.55	0.88
1:A:50:LYS:HA	3:A:710:HOH:O	1.74	0.88
1:B:306:GLY:N	1:B:393:MET:HE1	1.87	0.88
1:B:496:ASN:O	1:B:500:PRO:HG2	1.73	0.87
1:A:299:TYR:HA	1:A:304:LEU:HD21	1.56	0.87
1:B:167:VAL:O	1:B:242:TRP:CZ3	2.28	0.87
1:A:294:PRO:O	1:A:298:TYR:CE2	2.28	0.87
1:A:182:LEU:HD21	1:A:205:ILE:HG12	1.57	0.86
1:B:79:GLY:O	3:B:702:HOH:O	1.92	0.86
1:B:372:PHE:HD1	1:B:390:VAL:HG12	1.07	0.86
1:A:182:LEU:HD21	1:A:205:ILE:CG1	2.06	0.86
1:A:171:ARG:NH1	1:A:186:ILE:HD13	1.89	0.86
1:A:46:TYR:O	1:A:91:VAL:O	1.92	0.86
1:A:345:ALA:CA	1:B:345:ALA:HA	2.04	0.85
1:B:33:GLU:O	3:B:704:HOH:O	1.94	0.85
1:B:182:LEU:HD21	1:B:205:ILE:HG12	1.59	0.85
1:A:370:PHE:CE1	1:A:491:THR:HA	2.12	0.85
1:A:393:MET:HE3	1:A:394:ARG:H	1.41	0.85
1:B:304:LEU:O	1:B:304:LEU:HD23	1.76	0.85
1:B:276:SER:OG	1:B:286:MET:CG	2.23	0.85
1:A:65:VAL:HG13	1:A:71:PHE:CE2	2.11	0.84
1:A:406:VAL:HG12	1:A:406:VAL:O	1.74	0.84
1:B:62:HIS:O	1:B:66:VAL:O	1.95	0.84
1:B:403:ALA:O	1:B:406:VAL:HG22	1.76	0.84
1:B:446:TYR:CZ	1:B:450:ILE:HD11	2.11	0.84
1:A:409:ASP:OD2	1:A:438:ALA:CA	2.26	0.84
1:A:298:TYR:O	1:A:304:LEU:HD23	1.75	0.84
1:A:187:ALA:CB	3:A:739:HOH:O	1.89	0.84
1:A:7:ILE:HG23	1:A:477:GLU:OE1	1.78	0.84
1:A:299:TYR:CG	1:A:304:LEU:HD13	2.12	0.83
1:B:293:ASP:HB3	1:B:502:LEU:HD11	1.59	0.83
1:B:205:ILE:HD12	1:B:205:ILE:H	1.42	0.83
1:A:274:ILE:HD12	1:A:323:VAL:HG21	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:TYR:HA	1:A:304:LEU:CG	2.07	0.83
1:A:382:ASP:OD2	1:A:386:ARG:HG3	1.79	0.83
1:B:236:ARG:HH11	1:B:236:ARG:HG3	1.42	0.83
1:A:388:ILE:HG23	1:A:390:VAL:HG13	1.61	0.83
1:A:182:LEU:HD23	1:A:182:LEU:O	1.79	0.82
1:B:295:VAL:HA	1:B:298:TYR:CD2	2.13	0.82
1:A:463:ASN:O	1:A:466:THR:HG23	1.78	0.82
1:B:287:GLU:O	1:B:505:HIS:CE1	2.33	0.82
1:A:215:HIS:CD2	1:B:216:ARG:HG3	2.13	0.82
1:A:299:TYR:CA	1:A:304:LEU:CD2	2.30	0.81
1:A:375:PHE:HB3	1:A:390:VAL:HG21	1.59	0.81
1:B:404:SER:O	1:B:407:GLU:OE1	1.97	0.81
1:B:412:LEU:C	1:B:414:ALA:H	1.88	0.81
1:A:47:VAL:O	1:A:47:VAL:CG1	2.22	0.81
1:A:304:LEU:O	1:A:304:LEU:CD1	2.29	0.81
1:B:397:ASP:HB2	3:B:708:HOH:O	1.80	0.81
1:A:368:SER:HB2	1:A:393:MET:HB3	1.60	0.81
1:A:273:VAL:HG12	1:A:273:VAL:O	1.80	0.80
1:A:180:PHE:CE2	1:A:242:TRP:HH2	2.00	0.80
1:A:405:TYR:C	1:A:407:GLU:H	1.89	0.80
1:A:305:SER:C	1:A:393:MET:HE1	2.06	0.80
1:B:280:ASP:HB2	1:B:321:ASP:CB	2.11	0.80
1:A:302:GLY:O	1:A:304:LEU:CD2	2.30	0.80
1:A:261:ARG:HG3	1:A:261:ARG:HH11	1.45	0.80
1:B:203:LEU:CD1	1:B:255:MET:HE1	2.12	0.80
1:A:299:TYR:HA	1:A:304:LEU:CD1	2.12	0.79
1:A:270:ARG:HH11	1:A:351:VAL:HG11	1.47	0.79
1:A:393:MET:N	3:A:703:HOH:O	2.15	0.79
1:B:407:GLU:N	1:B:407:GLU:OE2	2.15	0.79
1:A:305:SER:O	1:A:393:MET:HE3	1.83	0.79
1:B:287:GLU:O	1:B:505:HIS:NE2	2.16	0.79
1:B:388:ILE:O	1:B:390:VAL:HG23	1.82	0.79
1:A:215:HIS:NE2	1:B:216:ARG:HD3	1.95	0.79
1:B:299:TYR:CE2	1:B:371:LEU:HB3	2.18	0.78
1:A:298:TYR:O	1:A:304:LEU:HD21	1.83	0.78
1:A:364:PHE:HB3	3:A:732:HOH:O	1.82	0.78
1:B:280:ASP:CB	1:B:281:PRO:CD	2.62	0.78
1:B:399:MET:O	1:B:399:MET:HG3	1.83	0.77
1:B:301:LYS:O	1:B:303:GLN:HG2	1.84	0.77
1:A:65:VAL:CG1	1:A:71:PHE:CE2	2.67	0.77
1:B:299:TYR:OH	1:B:372:PHE:CA	2.33	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:TYR:CE1	1:B:450:ILE:CG1	2.67	0.77
1:B:180:PHE:CE2	1:B:242:TRP:HH2	2.03	0.77
1:B:274:ILE:HD13	1:B:323:VAL:HG21	1.66	0.77
1:B:393:MET:HE3	1:B:393:MET:CA	2.13	0.76
1:B:310:ASP:N	1:B:456:PHE:CE1	2.53	0.76
1:A:172:GLN:HG3	1:A:458:GLY:HA3	1.66	0.76
1:A:299:TYR:HD1	1:A:304:LEU:HD13	1.33	0.76
1:B:496:ASN:C	1:B:500:PRO:HG2	2.11	0.76
1:B:177:GLU:OE1	1:B:465:ASN:N	2.18	0.75
1:B:306:GLY:C	1:B:393:MET:CE	2.58	0.75
1:B:132:TYR:OH	1:B:208:GLU:HG3	1.87	0.75
1:A:280:ASP:HB3	1:A:281:PRO:HD3	1.67	0.74
1:A:409:ASP:OD2	1:A:438:ALA:HB1	1.84	0.74
1:B:220:ASP:OD1	1:B:220:ASP:C	2.28	0.74
1:A:22:GLY:N	3:A:704:HOH:O	2.20	0.74
1:A:299:TYR:HB2	1:A:304:LEU:HD13	1.67	0.74
1:A:390:VAL:HG22	3:A:719:HOH:O	1.88	0.74
1:B:280:ASP:HB3	1:B:281:PRO:HD2	1.70	0.74
1:A:33:GLU:HG3	1:A:70:LEU:CD2	2.18	0.74
1:A:70:LEU:O	1:A:70:LEU:HD23	1.88	0.73
1:B:295:VAL:CA	1:B:298:TYR:HD2	2.01	0.73
1:B:354:VAL:HB	3:B:705:HOH:O	1.88	0.73
1:B:306:GLY:CA	1:B:393:MET:HE2	2.00	0.73
1:B:386:ARG:HD3	1:B:388:ILE:HD11	1.70	0.73
1:B:407:GLU:O	1:B:411:LEU:HB2	1.87	0.73
1:B:310:ASP:N	1:B:456:PHE:HE1	1.86	0.73
1:B:417:LEU:C	1:B:417:LEU:HD22	2.14	0.73
1:A:300:GLY:HA3	1:A:375:PHE:CE2	2.23	0.72
1:A:62:HIS:HA	1:A:66:VAL:HG21	1.70	0.72
1:B:405:TYR:HD1	1:B:405:TYR:O	1.71	0.72
1:A:301:LYS:O	1:A:304:LEU:HD21	1.88	0.72
1:B:280:ASP:HB2	1:B:321:ASP:HB2	1.69	0.72
1:A:475:GLU:N	1:A:475:GLU:CD	2.48	0.72
1:B:275:GLU:CG	1:B:498:HIS:CE1	2.73	0.72
1:B:274:ILE:HG13	2:B:601:NAP:O7N	1.88	0.71
1:A:158:LEU:HD23	1:A:265:PRO:O	1.89	0.71
1:A:65:VAL:HG13	1:A:71:PHE:HE2	1.55	0.71
1:B:275:GLU:HG2	1:B:498:HIS:CE1	2.25	0.71
1:A:203:LEU:HD13	1:A:255:MET:HE1	1.71	0.71
1:A:353:HIS:O	1:A:466:THR:CG2	2.35	0.71
1:A:130:GLU:OE1	1:A:131:ARG:N	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:ARG:O	1:B:294:PRO:HD2	1.89	0.71
1:A:133:ASP:OD1	1:A:133:ASP:N	2.22	0.71
1:B:304:LEU:HD23	1:B:304:LEU:C	2.15	0.71
1:A:405:TYR:O	1:A:408:THR:OG1	2.09	0.71
1:B:372:PHE:CD1	1:B:390:VAL:HG13	2.24	0.71
1:A:270:ARG:NH1	1:A:351:VAL:CG1	2.53	0.70
1:A:16:LYS:H	1:A:43:GLY:H	1.39	0.70
1:A:203:LEU:CD1	1:A:255:MET:HE1	2.21	0.70
1:A:215:HIS:NE2	1:B:216:ARG:CG	2.30	0.70
1:A:13:LEU:HD13	1:A:35:ILE:CG2	2.22	0.70
1:B:388:ILE:O	1:B:388:ILE:HG22	1.91	0.70
1:A:217:ARG:O	1:A:220:ASP:N	2.21	0.70
1:B:299:TYR:CD2	1:B:371:LEU:HB3	2.27	0.70
1:B:36:LEU:N	3:B:704:HOH:O	2.25	0.70
1:B:366:ASP:O	1:B:370:PHE:CD2	2.45	0.69
1:B:232:LEU:HD22	1:B:232:LEU:O	1.92	0.69
1:B:88:ARG:NH1	3:B:707:HOH:O	2.25	0.69
1:B:298:TYR:HA	1:B:303:GLN:HG3	1.73	0.69
1:A:171:ARG:CZ	1:A:186:ILE:CD1	2.70	0.69
1:A:380:TYR:HD2	3:A:728:HOH:O	1.75	0.69
1:A:48:LEU:HD11	1:A:95:GLY:HA3	1.73	0.69
1:B:22:GLY:HA3	1:B:28:ALA:HB3	1.74	0.69
1:A:114:ASP:OD1	1:A:154:ARG:NH1	2.26	0.69
1:A:290:ARG:N	3:A:706:HOH:O	2.25	0.69
1:A:8:GLY:O	1:A:11:GLU:HG2	1.92	0.69
1:A:214:ASP:O	1:B:214:ASP:CG	2.35	0.69
1:B:203:LEU:HD12	1:B:255:MET:HE1	1.73	0.69
1:A:171:ARG:NH1	1:A:186:ILE:CD1	2.56	0.68
1:A:215:HIS:HD2	1:B:216:ARG:HG3	1.52	0.68
1:A:236:ARG:O	1:A:237:ALA:C	2.36	0.68
1:B:306:GLY:C	1:B:393:MET:HE1	2.17	0.68
1:A:386:ARG:CZ	1:A:386:ARG:HB2	2.23	0.68
1:B:33:GLU:C	3:B:704:HOH:O	2.33	0.68
1:B:125:ASN:HD22	1:B:125:ASN:C	2.01	0.68
1:B:180:PHE:HE2	1:B:242:TRP:HH2	1.39	0.68
1:B:449:SER:OG	1:B:450:ILE:N	2.24	0.68
1:B:21:THR:HB	1:B:123:ALA:HB2	1.76	0.68
1:A:374:HIS:ND1	1:A:495:THR:O	2.24	0.68
1:A:392:PRO:CA	3:A:703:HOH:O	2.42	0.68
1:B:446:TYR:CD1	1:B:450:ILE:HG13	2.29	0.68
1:A:408:THR:O	1:A:412:LEU:N	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:VAL:HG12	1:B:441:VAL:HG21	1.75	0.67
1:A:142:GLY:O	1:A:146:ILE:HD12	1.94	0.67
1:A:382:ASP:OD2	1:A:386:ARG:CG	2.41	0.67
1:B:417:LEU:HD13	1:B:417:LEU:H	1.60	0.67
1:A:276:SER:HG	1:A:498:HIS:HD1	1.42	0.67
1:A:345:ALA:HA	1:B:345:ALA:CA	2.20	0.67
1:A:386:ARG:HG3	1:A:386:ARG:O	1.94	0.67
1:B:275:GLU:HG2	1:B:498:HIS:NE2	2.09	0.67
1:A:310:ASP:OD1	1:A:310:ASP:C	2.36	0.67
1:B:232:LEU:HD22	1:B:232:LEU:C	2.20	0.67
1:A:380:TYR:CD2	3:A:728:HOH:O	2.48	0.67
1:A:277:THR:OG1	1:A:285:TRP:HB3	1.95	0.67
1:B:261:ARG:HG3	1:B:261:ARG:NH1	2.02	0.67
1:A:16:LYS:O	1:A:43:GLY:CA	2.43	0.67
1:A:475:GLU:CD	1:A:475:GLU:H	2.03	0.67
1:B:321:ASP:O	1:B:325:ASN:ND2	2.27	0.67
1:B:393:MET:CE	1:B:393:MET:HA	2.24	0.67
1:A:294:PRO:CB	3:A:726:HOH:O	2.25	0.66
1:B:261:ARG:O	1:B:261:ARG:HG2	1.93	0.66
1:A:305:SER:O	1:A:393:MET:CE	2.42	0.66
1:B:141:VAL:O	1:B:144:PHE:HB3	1.95	0.66
1:B:236:ARG:HG3	1:B:236:ARG:NH1	2.08	0.66
1:B:396:PHE:CZ	1:B:405:TYR:HD2	2.13	0.66
1:B:306:GLY:C	1:B:393:MET:HE2	2.19	0.66
1:A:158:LEU:CD2	1:A:265:PRO:O	2.44	0.66
1:A:305:SER:C	1:A:393:MET:CE	2.69	0.66
1:B:174:VAL:O	1:B:174:VAL:CG1	2.37	0.66
1:B:494:ILE:O	1:B:499:ILE:HG13	1.96	0.66
1:A:164:THR:HG22	2:A:601:NAP:H5N	1.78	0.66
1:B:290:ARG:C	3:B:703:HOH:O	2.34	0.66
1:A:136:MET:HA	1:A:140:THR:HG22	1.77	0.66
1:A:216:ARG:H	1:A:216:ARG:HE	1.44	0.66
1:A:409:ASP:CG	1:A:438:ALA:HB2	2.13	0.65
1:A:48:LEU:CD1	1:A:95:GLY:HA3	2.26	0.65
1:B:13:LEU:HD13	1:B:35:ILE:CG2	2.26	0.65
1:B:223:ALA:O	1:B:227:GLU:N	2.26	0.65
1:A:31:LEU:HD22	1:A:35:ILE:HD11	1.77	0.65
1:A:303:GLN:OE1	1:A:303:GLN:O	2.14	0.65
1:B:330:SER:HB3	3:B:718:HOH:O	1.95	0.65
1:A:13:LEU:O	1:A:39:ASN:ND2	2.30	0.65
1:A:163:SER:O	1:A:270:ARG:HA	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:PHE:N	1:B:393:MET:HE2	2.11	0.65
1:A:28:ALA:O	1:A:31:LEU:HB3	1.97	0.65
1:B:139:ASN:O	1:B:143:PRO:HG3	1.97	0.64
1:B:172:GLN:O	1:B:458:GLY:O	2.15	0.64
1:B:408:THR:O	1:B:412:LEU:HB2	1.97	0.64
1:B:299:TYR:HE2	1:B:371:LEU:C	2.05	0.64
1:A:13:LEU:HD13	1:A:35:ILE:HG23	1.79	0.64
1:A:271:PRO:HB2	1:A:274:ILE:HD11	1.80	0.64
1:B:417:LEU:CD1	1:B:417:LEU:N	2.60	0.64
1:B:272:SER:OG	1:B:318:VAL:HG22	1.96	0.64
1:A:366:ASP:O	1:A:370:PHE:CD2	2.51	0.64
1:A:379:PRO:HB2	1:A:388:ILE:HG22	1.80	0.64
1:B:391:PRO:C	1:B:392:PRO:O	2.24	0.64
1:A:171:ARG:CZ	1:A:186:ILE:HD11	2.29	0.64
1:B:296:VAL:HG11	1:B:499:ILE:HD13	1.80	0.64
1:A:205:ILE:H	1:A:205:ILE:CD1	2.07	0.63
1:B:61:LEU:O	1:B:66:VAL:CG2	2.46	0.63
1:B:286:MET:C	1:B:286:MET:HE3	2.23	0.63
1:A:24:THR:CG2	2:A:601:NAP:O1X	2.42	0.63
1:B:220:ASP:O	1:B:220:ASP:OD1	2.16	0.63
1:B:280:ASP:CB	1:B:281:PRO:HD3	2.26	0.63
1:A:271:PRO:HG2	2:A:601:NAP:H6N	1.81	0.63
1:A:396:PHE:CZ	1:A:405:TYR:CE1	2.86	0.63
1:A:396:PHE:HZ	1:A:405:TYR:CE1	2.17	0.63
1:B:395:LEU:C	1:B:396:PHE:CD1	2.77	0.63
1:A:21:THR:C	3:A:704:HOH:O	2.42	0.63
1:B:309:ALA:O	1:B:311:PRO:HD3	1.99	0.63
1:A:147:MET:HE2	1:A:159:PHE:CD2	2.34	0.63
1:A:163:SER:O	1:A:271:PRO:HD2	1.99	0.63
1:A:345:ALA:HB2	1:B:344:ALA:C	2.24	0.63
1:A:17:ASN:N	1:A:17:ASN:HD22	1.96	0.63
1:A:270:ARG:HH11	1:A:351:VAL:CG1	2.10	0.63
1:B:73:ARG:HG3	1:B:73:ARG:HH11	1.63	0.63
1:A:254:GLU:HG2	3:A:727:HOH:O	1.99	0.63
1:B:368:SER:HB2	1:B:393:MET:CB	2.28	0.63
1:A:45:ILE:HG22	1:A:47:VAL:HG23	1.81	0.62
1:A:141:VAL:HG12	1:A:141:VAL:O	1.97	0.62
1:A:146:ILE:HG12	3:A:743:HOH:O	1.99	0.62
1:A:167:VAL:O	1:A:242:TRP:CZ3	2.52	0.62
1:A:164:THR:HG23	1:A:246:TYR:OH	1.98	0.62
1:B:446:TYR:CE1	1:B:450:ILE:HD12	2.19	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:THR:O	1:B:290:ARG:NH1	2.32	0.62
1:B:478:LYS:HG2	3:B:732:HOH:O	1.99	0.62
1:B:182:LEU:HD13	1:B:182:LEU:O	2.00	0.62
1:A:244:ASP:OD2	1:A:454:TYR:OH	2.16	0.62
1:A:306:GLY:C	1:A:393:MET:HE2	2.25	0.62
1:B:114:ASP:OD1	1:B:154:ARG:NH1	2.32	0.62
1:A:167:VAL:HG11	1:A:270:ARG:HE	1.63	0.62
1:A:177:GLU:HG2	1:A:353:HIS:CD2	2.34	0.62
1:A:140:THR:O	1:A:143:PRO:HG2	2.00	0.62
1:B:297:LEU:O	1:B:301:LYS:HG3	1.99	0.62
1:A:16:LYS:O	1:A:43:GLY:N	2.32	0.62
1:A:154:ARG:HG3	1:A:154:ARG:HH11	1.65	0.62
1:B:277:THR:CG2	1:B:321:ASP:HB3	2.29	0.62
1:A:164:THR:HG22	2:A:601:NAP:C5N	2.30	0.61
1:A:167:VAL:O	1:A:242:TRP:HZ3	1.83	0.61
1:A:88:ARG:NH1	3:A:708:HOH:O	2.33	0.61
1:A:50:LYS:HD2	2:A:601:NAP:C6A	2.31	0.61
1:A:269:ILE:CD1	1:A:327:THR:HA	2.31	0.61
1:B:24:THR:HG23	1:B:24:THR:O	2.00	0.61
1:A:216:ARG:HD2	1:A:216:ARG:N	2.16	0.61
1:A:298:TYR:O	1:A:302:GLY:O	2.18	0.61
1:A:299:TYR:CA	1:A:304:LEU:HD13	2.29	0.61
1:A:492:ASP:O	1:A:496:ASN:HB2	2.00	0.61
1:B:96:ASP:O	1:B:102:VAL:O	2.18	0.61
1:A:51:ALA:CB	1:A:57:ALA:HB2	2.30	0.61
1:B:395:LEU:C	1:B:396:PHE:HD1	2.08	0.61
1:A:177:GLU:OE1	1:A:465:ASN:N	2.27	0.61
1:A:232:LEU:HD12	1:A:232:LEU:C	2.25	0.61
1:B:409:ASP:OD2	1:B:437:CYS:O	2.19	0.61
1:B:394:ARG:HB3	1:B:396:PHE:HE1	1.66	0.60
1:A:80:LYS:HE2	1:A:80:LYS:HA	1.83	0.60
1:B:318:VAL:HG12	1:B:319:PRO:HD2	1.82	0.60
1:B:452:GLN:HB3	1:B:453:PRO:CD	2.23	0.60
1:A:449:SER:O	1:A:452:GLN:HB3	2.01	0.60
1:B:307:PHE:HA	1:B:402:PHE:HE1	1.67	0.60
1:B:372:PHE:O	1:B:376:THR:CG2	2.39	0.60
1:B:473:MET:HE1	1:B:481:PHE:O	2.02	0.60
1:B:376:THR:HG22	1:B:390:VAL:HG11	1.82	0.60
1:B:502:LEU:O	1:B:506:VAL:HG12	2.01	0.60
1:A:62:HIS:O	1:A:66:VAL:HG23	2.02	0.60
1:A:242:TRP:CD1	1:A:248:PHE:CD1	2.89	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ILE:HG22	1:A:473:MET:HA	1.84	0.60
1:A:370:PHE:CZ	1:A:491:THR:HA	2.37	0.60
1:B:40:PRO:HB3	3:B:721:HOH:O	2.02	0.60
1:B:274:ILE:CD1	1:B:323:VAL:HG21	2.31	0.60
1:B:406:VAL:N	1:B:407:GLU:OE2	2.35	0.60
1:B:208:GLU:OE2	1:B:208:GLU:HA	2.01	0.59
1:A:476:GLU:O	1:A:479:ALA:HB3	2.02	0.59
1:A:12:PHE:O	1:A:14:GLY:N	2.35	0.59
1:A:70:LEU:HD23	1:A:70:LEU:C	2.25	0.59
1:A:216:ARG:H	1:A:216:ARG:NE	1.99	0.59
1:A:405:TYR:C	1:A:407:GLU:N	2.58	0.59
1:B:403:ALA:O	1:B:406:VAL:CG2	2.50	0.59
1:A:131:ARG:HA	1:A:230:LYS:HA	1.85	0.59
1:A:499:ILE:N	1:A:500:PRO:CD	2.65	0.59
1:B:322:MET:CE	1:B:485:VAL:HA	2.25	0.59
1:B:417:LEU:H	1:B:417:LEU:CD1	2.16	0.59
1:A:62:HIS:CA	1:A:66:VAL:HG23	2.31	0.59
1:B:172:GLN:O	1:B:458:GLY:C	2.45	0.59
1:A:369:ARG:HG2	1:A:373:GLN:OE1	2.03	0.59
1:B:396:PHE:CZ	1:B:405:TYR:CD2	2.90	0.59
1:B:405:TYR:O	1:B:405:TYR:CD1	2.55	0.59
1:B:446:TYR:CE1	1:B:450:ILE:HG13	2.37	0.59
1:A:186:ILE:O	1:A:186:ILE:HG22	2.02	0.59
1:A:446:TYR:CE1	1:A:450:ILE:CD1	2.86	0.59
1:A:182:LEU:HD12	1:A:259:SER:OG	2.03	0.59
1:B:499:ILE:N	1:B:500:PRO:CD	2.66	0.59
1:A:65:VAL:HG13	1:A:71:PHE:CZ	2.37	0.59
1:B:274:ILE:HG13	2:B:601:NAP:C7N	2.33	0.59
1:A:34:LYS:NZ	1:A:325:ASN:OD1	2.35	0.58
1:A:216:ARG:N	1:A:216:ARG:CD	2.66	0.58
1:A:393:MET:HE3	1:A:394:ARG:N	2.16	0.58
1:B:406:VAL:CG1	1:B:441:VAL:HG11	2.28	0.58
1:B:446:TYR:HE1	1:B:450:ILE:HD11	0.79	0.58
1:A:271:PRO:HG2	2:A:601:NAP:C6N	2.33	0.58
1:A:438:ALA:HB1	1:A:441:VAL:HG23	1.85	0.58
1:B:73:ARG:HH11	1:B:73:ARG:CG	2.15	0.58
1:B:105:ALA:HB1	1:B:106:PRO:HD2	1.86	0.58
1:A:221:ASP:N	1:A:221:ASP:OD1	2.37	0.58
1:B:34:LYS:O	1:B:38:THR:CG2	2.40	0.58
1:A:164:THR:HB	1:A:166:TYR:H	1.68	0.57
1:A:207:ALA:HA	1:A:210:LYS:HD3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ARG:HB2	1:A:220:ASP:HB3	1.85	0.57
1:A:404:SER:O	1:A:407:GLU:OE1	2.22	0.57
1:B:254:GLU:OE1	1:B:270:ARG:NH2	2.32	0.57
1:A:349:MET:HE2	3:A:727:HOH:O	2.04	0.57
1:B:236:ARG:HH11	1:B:236:ARG:CG	2.17	0.57
1:A:299:TYR:CA	1:A:304:LEU:CD1	2.81	0.57
1:A:146:ILE:CG1	3:A:743:HOH:O	2.52	0.57
1:A:274:ILE:HB	2:A:601:NAP:O7N	2.05	0.57
1:B:164:THR:HG23	1:B:246:TYR:OH	2.05	0.57
1:B:205:ILE:H	1:B:205:ILE:CD1	2.07	0.57
1:A:232:LEU:HD12	1:A:232:LEU:O	2.05	0.57
1:B:285:TRP:CZ2	1:B:287:GLU:HG3	2.39	0.57
1:B:452:GLN:CB	1:B:453:PRO:HD3	2.20	0.57
1:A:62:HIS:CD2	1:A:66:VAL:HG21	2.39	0.56
1:B:164:THR:HB	1:B:166:TYR:H	1.69	0.56
1:B:295:VAL:O	1:B:298:TYR:N	2.38	0.56
1:A:79:GLY:C	1:A:80:LYS:CE	2.73	0.56
1:A:299:TYR:CE2	1:A:371:LEU:HB3	2.40	0.56
1:B:277:THR:HG23	1:B:321:ASP:HB3	1.86	0.56
1:A:216:ARG:NE	1:A:216:ARG:HA	2.20	0.56
1:A:300:GLY:HA3	1:A:375:PHE:CZ	2.40	0.56
1:A:364:PHE:CB	3:A:732:HOH:O	2.47	0.56
1:B:370:PHE:CZ	1:B:491:THR:HA	2.40	0.56
1:A:144:PHE:CD1	1:A:260:MET:CE	2.89	0.56
1:A:293:ASP:N	1:A:294:PRO:HD2	2.21	0.56
1:B:398:THR:HG23	3:B:708:HOH:O	2.06	0.56
1:A:141:VAL:O	1:A:141:VAL:CG1	2.53	0.56
1:A:252:MET:HA	1:A:255:MET:HE2	1.87	0.56
1:A:446:TYR:CE1	1:A:450:ILE:HD11	2.41	0.56
1:B:26:PHE:O	1:B:30:VAL:HG23	2.06	0.56
1:B:203:LEU:HD13	1:B:255:MET:HE1	1.84	0.56
1:B:463:ASN:ND2	1:B:467:GLU:OE1	2.39	0.56
1:A:306:GLY:N	1:A:393:MET:CE	2.46	0.56
1:B:136:MET:HA	1:B:140:THR:HG22	1.88	0.56
1:B:294:PRO:HB2	1:B:298:TYR:HE2	1.70	0.56
1:A:306:GLY:HA2	1:A:393:MET:HE3	1.73	0.56
1:B:217:ARG:HD3	1:B:225:PHE:CD1	2.41	0.56
1:B:263:ASP:OD1	1:B:263:ASP:N	2.39	0.56
1:B:279:ARG:HA	1:B:283:PRO:HG3	1.87	0.56
1:B:62:HIS:CA	1:B:66:VAL:CG2	2.64	0.56
1:B:22:GLY:HA3	1:B:28:ALA:CB	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:THR:O	1:B:201:THR:OG1	2.22	0.55
1:A:217:ARG:O	1:A:218:HIS:C	2.47	0.55
1:A:217:ARG:O	1:A:219:GLY:N	2.38	0.55
1:A:409:ASP:OD2	1:A:438:ALA:HA	2.04	0.55
1:B:296:VAL:CG1	1:B:499:ILE:HD13	2.37	0.55
1:A:278:TRP:H	1:A:321:ASP:HB2	1.72	0.55
1:A:390:VAL:HG23	1:A:390:VAL:O	2.05	0.55
1:A:159:PHE:O	1:A:266:VAL:HA	2.07	0.55
1:B:143:PRO:HA	1:B:146:ILE:CD1	2.33	0.55
1:A:65:VAL:HG12	1:A:71:PHE:CE2	2.42	0.55
1:B:13:LEU:HD13	1:B:35:ILE:HG23	1.87	0.55
1:B:48:LEU:HD21	1:B:96:ASP:O	2.07	0.55
1:A:496:ASN:C	1:A:500:PRO:HG2	2.32	0.55
1:A:131:ARG:HD3	1:A:133:ASP:OD1	2.07	0.55
1:A:17:ASN:N	1:A:17:ASN:ND2	2.54	0.55
1:A:125:ASN:C	1:A:125:ASN:HD22	2.14	0.55
1:A:144:PHE:CD1	1:A:260:MET:HE3	2.42	0.55
1:A:216:ARG:HE	1:A:216:ARG:HA	1.72	0.55
1:A:276:SER:HA	1:A:285:TRP:O	2.07	0.55
1:A:386:ARG:CZ	1:A:386:ARG:CB	2.85	0.55
1:A:496:ASN:O	1:A:500:PRO:HG2	2.06	0.55
1:B:291:MET:CE	1:B:291:MET:CA	2.85	0.55
1:B:282:PHE:CD1	1:B:282:PHE:C	2.85	0.54
1:B:365:GLY:O	1:B:369:ARG:NH1	2.40	0.54
1:B:475:GLU:OE2	1:B:476:GLU:N	2.40	0.54
1:A:125:ASN:C	1:A:125:ASN:ND2	2.65	0.54
1:B:305:SER:C	1:B:393:MET:HE1	2.32	0.54
1:B:17:ASN:N	1:B:17:ASN:ND2	2.55	0.54
1:B:13:LEU:HD13	1:B:35:ILE:HG22	1.88	0.54
1:B:242:TRP:CD1	1:B:248:PHE:CD1	2.96	0.54
1:B:338:GLY:HA3	1:B:341:ALA:HB3	1.89	0.54
1:B:180:PHE:HE2	1:B:242:TRP:CH2	2.24	0.54
1:B:307:PHE:HA	1:B:402:PHE:CE1	2.43	0.54
1:B:484:ASP:OD1	1:B:486:ARG:HB2	2.07	0.54
1:B:372:PHE:C	1:B:376:THR:HG23	2.27	0.54
1:B:452:GLN:N	1:B:453:PRO:CD	2.71	0.54
1:A:294:PRO:C	1:A:298:TYR:HD2	2.13	0.53
1:A:166:TYR:CE2	1:A:272:SER:HB2	2.43	0.53
1:A:244:ASP:OD1	1:A:247:VAL:HG22	2.08	0.53
1:B:65:VAL:HG12	1:B:65:VAL:O	2.07	0.53
1:A:79:GLY:C	1:A:80:LYS:HE2	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:MET:CE	1:A:394:ARG:H	2.17	0.53
1:A:413:ARG:O	1:A:413:ARG:HD3	2.09	0.53
1:B:277:THR:CG2	1:B:281:PRO:HD2	2.28	0.53
1:B:305:SER:O	1:B:393:MET:HE3	2.09	0.53
1:B:412:LEU:C	1:B:414:ALA:N	2.56	0.53
1:A:21:THR:HB	1:A:123:ALA:HB2	1.90	0.53
1:A:414:ALA:C	1:A:416:ARG:H	2.17	0.53
1:B:180:PHE:CE2	1:B:242:TRP:CH2	2.91	0.53
1:A:217:ARG:C	1:A:219:GLY:N	2.65	0.53
1:B:291:MET:HE2	1:B:291:MET:HA	1.89	0.53
1:B:449:SER:O	1:B:450:ILE:C	2.52	0.53
1:B:310:ASP:OD1	1:B:310:ASP:C	2.51	0.53
1:B:372:PHE:HD1	1:B:390:VAL:HG13	1.63	0.53
1:B:417:LEU:HD13	1:B:417:LEU:N	2.20	0.53
1:A:13:LEU:HD13	1:A:35:ILE:HG22	1.91	0.53
1:B:244:ASP:OD1	1:B:247:VAL:HG22	2.09	0.53
1:A:175:VAL:CG2	1:A:460:ARG:O	2.28	0.53
1:B:78:HIS:HB2	1:B:82:TYR:HB2	1.90	0.53
1:A:85:PHE:N	3:A:708:HOH:O	2.41	0.52
1:B:457:TYR:O	1:B:460:ARG:NH2	2.37	0.52
1:B:507:MET:O	1:B:508:LYS:HD2	2.09	0.52
1:A:391:PRO:CB	1:A:392:PRO:CD	2.70	0.52
1:A:392:PRO:HA	3:A:703:HOH:O	2.05	0.52
1:A:61:LEU:O	1:A:65:VAL:HB	2.10	0.52
1:A:345:ALA:N	1:B:345:ALA:N	2.57	0.52
1:B:291:MET:O	1:B:451:TYR:HE2	1.93	0.52
1:A:21:THR:OG1	1:A:121:ASN:HA	2.10	0.52
1:A:358:THR:HG21	1:A:462:ASP:HA	1.92	0.52
1:B:62:HIS:HA	1:B:66:VAL:HG21	1.81	0.52
1:B:404:SER:O	1:B:404:SER:OG	2.21	0.52
1:A:310:ASP:OD1	1:A:312:GLU:N	2.40	0.52
1:B:73:ARG:HG3	1:B:73:ARG:NH1	2.24	0.52
1:B:163:SER:O	1:B:271:PRO:HD2	2.09	0.52
1:A:21:THR:CA	3:A:704:HOH:O	2.57	0.52
1:A:506:VAL:O	1:A:506:VAL:CG2	2.57	0.52
1:B:182:LEU:HD11	1:B:205:ILE:HD11	1.91	0.52
1:A:254:GLU:OE1	1:A:270:ARG:NH2	2.42	0.52
1:A:484:ASP:OD1	1:A:486:ARG:HB2	2.09	0.52
1:B:17:ASN:HD22	1:B:17:ASN:H	1.58	0.52
1:A:49:ILE:HG22	1:A:50:LYS:O	2.10	0.51
1:A:406:VAL:O	1:A:406:VAL:CG1	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:ILE:O	3:B:704:HOH:O	2.18	0.51
1:B:304:LEU:HD22	1:B:304:LEU:H	1.75	0.51
1:B:16:LYS:O	1:B:43:GLY:N	2.43	0.51
1:B:26:PHE:CD1	1:B:26:PHE:C	2.85	0.51
1:A:318:VAL:HG12	1:A:319:PRO:HD2	1.92	0.51
1:A:506:VAL:O	1:A:506:VAL:HG22	2.11	0.51
1:B:275:GLU:HG2	1:B:498:HIS:CD2	2.45	0.51
1:B:17:ASN:N	1:B:17:ASN:HD22	2.08	0.51
1:A:386:ARG:CB	1:A:386:ARG:NH1	2.73	0.51
1:B:364:PHE:O	1:B:395:LEU:CD1	2.58	0.51
1:B:417:LEU:HD22	1:B:418:ALA:HB2	1.92	0.51
1:A:19:LEU:HA	3:A:702:HOH:O	2.11	0.51
1:A:51:ALA:N	3:A:710:HOH:O	2.43	0.51
1:A:158:LEU:HB2	1:A:335:GLY:HA3	1.93	0.51
1:A:299:TYR:HD1	1:A:304:LEU:HD12	1.70	0.51
1:B:295:VAL:C	1:B:297:LEU:N	2.69	0.51
1:B:390:VAL:N	1:B:391:PRO:HD3	2.25	0.51
1:A:141:VAL:O	1:A:144:PHE:HB3	2.11	0.51
1:B:82:TYR:CD2	1:B:83:HIS:HD2	2.28	0.51
1:B:139:ASN:O	1:B:143:PRO:CG	2.59	0.51
1:B:476:GLU:O	1:B:479:ALA:HB3	2.11	0.51
1:A:227:GLU:O	1:A:230:LYS:N	2.44	0.50
1:A:498:HIS:C	1:A:500:PRO:HD2	2.36	0.50
1:B:125:ASN:HD21	1:B:130:GLU:HG2	1.76	0.50
1:A:364:PHE:CZ	1:A:455:THR:HA	2.46	0.50
1:B:275:GLU:HG3	1:B:498:HIS:CE1	2.44	0.50
1:A:499:ILE:N	1:A:500:PRO:HD2	2.27	0.50
1:B:463:ASN:O	1:B:466:THR:HG23	2.12	0.50
1:A:143:PRO:HA	1:A:146:ILE:HD13	1.94	0.50
1:B:340:ALA:HB2	3:B:738:HOH:O	2.10	0.50
1:B:452:GLN:N	1:B:453:PRO:HD2	2.25	0.50
1:B:369:ARG:HG2	1:B:373:GLN:HE21	1.75	0.50
1:B:396:PHE:CD1	1:B:396:PHE:N	2.79	0.50
1:A:135:ALA:O	1:A:139:ASN:HB2	2.12	0.50
1:A:402:PHE:O	1:A:405:TYR:HB2	2.11	0.50
1:A:36:LEU:HD11	1:A:90:LEU:HD21	1.94	0.50
1:A:386:ARG:NH1	1:A:386:ARG:HB3	2.26	0.50
1:A:97:VAL:HA	1:A:102:VAL:HG12	1.94	0.50
1:A:307:PHE:HA	1:A:402:PHE:HE1	1.77	0.50
1:A:215:HIS:O	1:A:218:HIS:ND1	2.45	0.49
1:A:274:ILE:CB	2:A:601:NAP:O7N	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:GLU:OE1	1:B:131:ARG:N	2.42	0.49
1:A:70:LEU:CD2	1:A:70:LEU:C	2.85	0.49
1:A:273:VAL:HB	1:A:316:ASP:O	2.11	0.49
1:A:499:ILE:O	1:A:503:ARG:HG3	2.12	0.49
1:A:394:ARG:NH1	1:A:405:TYR:OH	2.43	0.49
1:A:502:LEU:O	1:A:506:VAL:HG12	2.12	0.49
1:B:34:LYS:C	1:B:38:THR:HG22	2.35	0.49
1:B:125:ASN:C	1:B:125:ASN:ND2	2.67	0.49
1:B:164:THR:CG2	1:B:246:TYR:OH	2.60	0.49
1:B:217:ARG:HH12	1:B:228:GLU:CD	2.20	0.49
1:A:272:SER:O	1:A:272:SER:OG	2.31	0.49
1:A:294:PRO:C	1:A:298:TYR:CD2	2.75	0.49
1:A:378:SER:O	1:A:378:SER:OG	2.20	0.49
1:A:374:HIS:CD2	1:A:374:HIS:C	2.90	0.49
1:B:45:ILE:HG22	1:B:47:VAL:HG22	1.94	0.49
1:A:293:ASP:HB3	1:A:502:LEU:HD11	1.94	0.49
1:A:12:PHE:HD2	1:A:13:LEU:HD23	1.78	0.49
1:B:21:THR:C	3:B:719:HOH:O	2.55	0.49
1:A:65:VAL:CG1	1:A:71:PHE:HE2	2.17	0.48
1:A:396:PHE:CE2	1:A:405:TYR:CD1	3.01	0.48
1:B:293:ASP:N	1:B:294:PRO:HD2	2.27	0.48
1:A:216:ARG:H	1:A:216:ARG:CD	2.26	0.48
1:B:205:ILE:N	1:B:205:ILE:CD1	2.60	0.48
1:B:235:GLU:O	1:B:239:LEU:HB2	2.12	0.48
1:B:399:MET:O	1:B:399:MET:CG	2.59	0.48
1:A:32:ILE:O	1:A:33:GLU:C	2.56	0.48
1:A:102:VAL:CG1	1:A:146:ILE:HG13	2.43	0.48
1:B:362:LEU:HD12	1:B:490:TRP:HB3	1.95	0.48
1:A:142:GLY:N	1:A:143:PRO:HD2	2.28	0.48
1:B:295:VAL:C	1:B:297:LEU:H	2.20	0.48
1:A:102:VAL:HG11	1:A:146:ILE:HG13	1.95	0.48
1:A:316:ASP:HA	3:A:716:HOH:O	2.14	0.48
1:B:261:ARG:HH22	1:B:348:GLY:HA2	1.78	0.48
1:A:182:LEU:CD2	1:A:205:ILE:HD11	2.44	0.48
1:A:268:THR:OG1	1:A:349:MET:HE3	2.13	0.48
1:A:494:ILE:O	1:A:499:ILE:HG13	2.14	0.48
1:A:505:HIS:O	1:A:507:MET:O	2.32	0.48
1:B:51:ALA:CB	1:B:57:ALA:HB2	2.43	0.48
1:B:304:LEU:N	1:B:304:LEU:CD2	2.77	0.48
1:B:31:LEU:HD22	1:B:35:ILE:HD11	1.96	0.48
1:B:265:PRO:CG	3:B:731:HOH:O	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:ASP:O	1:A:413:ARG:HB2	2.14	0.48
1:B:35:ILE:HA	1:B:38:THR:HG23	1.95	0.48
1:B:280:ASP:CB	1:B:321:ASP:CB	2.89	0.48
1:B:446:TYR:CD1	1:B:446:TYR:C	2.92	0.48
1:A:344:ALA:C	1:B:345:ALA:CB	2.79	0.48
1:B:290:ARG:O	1:B:294:PRO:CG	2.59	0.48
1:A:16:LYS:O	1:A:43:GLY:HA3	2.14	0.47
1:A:155:ARG:O	1:A:155:ARG:HG2	2.13	0.47
1:A:261:ARG:HH11	1:A:261:ARG:CG	2.22	0.47
1:A:388:ILE:CG2	1:A:390:VAL:HG13	2.40	0.47
1:B:269:ILE:CD1	1:B:327:THR:HA	2.44	0.47
1:B:298:TYR:HB3	1:B:303:GLN:HB2	1.96	0.47
1:A:144:PHE:CE1	1:A:260:MET:CE	2.96	0.47
1:B:393:MET:CE	1:B:393:MET:CA	2.85	0.47
1:A:28:ALA:O	1:A:31:LEU:CB	2.62	0.47
1:A:126:THR:HB	1:A:290:ARG:NH1	2.30	0.47
1:A:182:LEU:HD21	1:A:205:ILE:CD1	2.45	0.47
1:A:278:TRP:CE3	1:A:279:ARG:HG2	2.48	0.47
1:A:382:ASP:OD1	1:A:382:ASP:C	2.57	0.47
1:B:236:ARG:O	1:B:237:ALA:C	2.56	0.47
1:B:417:LEU:C	1:B:417:LEU:CD2	2.85	0.47
1:A:396:PHE:HZ	1:A:405:TYR:HE1	1.58	0.47
1:B:131:ARG:HD2	1:B:134:VAL:HG23	1.95	0.47
1:B:133:ASP:N	1:B:133:ASP:OD1	2.47	0.47
1:B:136:MET:HE2	1:B:209:ILE:HG13	1.95	0.47
1:B:390:VAL:C	1:B:391:PRO:HD3	2.33	0.47
1:B:301:LYS:NZ	1:B:380:TYR:CZ	2.83	0.47
1:A:197:GLN:CA	1:A:197:GLN:HE21	2.28	0.47
1:A:261:ARG:O	1:A:261:ARG:HG2	2.14	0.47
1:A:507:MET:HE3	3:A:718:HOH:O	2.13	0.47
1:B:18:PHE:HA	1:B:118:ILE:O	2.14	0.47
1:B:293:ASP:OD2	1:B:502:LEU:HD12	2.15	0.47
1:A:65:VAL:C	1:A:71:PHE:CE2	2.89	0.47
1:B:227:GLU:O	1:B:228:GLU:C	2.57	0.47
1:A:213:PHE:CD1	1:A:213:PHE:C	2.93	0.47
1:A:386:ARG:HA	1:A:387:PRO:HD2	1.54	0.47
1:B:252:MET:O	1:B:255:MET:HB2	2.14	0.47
1:B:380:TYR:CD2	1:B:381:SER:O	2.68	0.47
1:A:31:LEU:O	1:A:35:ILE:HG13	2.15	0.47
1:B:136:MET:O	1:B:140:THR:HG22	2.15	0.47
1:A:126:THR:O	1:A:290:ARG:NH1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:ASP:C	1:A:492:ASP:OD1	2.58	0.47
1:B:21:THR:OG1	1:B:121:ASN:HA	2.16	0.47
1:B:280:ASP:CB	1:B:321:ASP:HB2	2.40	0.47
1:B:389:HIS:N	1:B:389:HIS:ND1	2.62	0.47
1:A:136:MET:O	1:A:140:THR:HG22	2.15	0.46
1:A:215:HIS:NE2	1:B:216:ARG:CZ	2.68	0.46
1:A:378:SER:HA	1:A:379:PRO:HD2	1.78	0.46
1:B:272:SER:OG	1:B:318:VAL:CG2	2.63	0.46
1:B:354:VAL:O	3:B:705:HOH:O	2.20	0.46
1:B:380:TYR:O	1:B:387:PRO:CG	2.62	0.46
1:A:269:ILE:HD13	1:A:327:THR:HA	1.97	0.46
1:A:304:LEU:H	1:A:304:LEU:HG	0.79	0.46
1:B:232:LEU:C	1:B:232:LEU:CD2	2.88	0.46
1:A:345:ALA:CA	1:B:345:ALA:CA	2.84	0.46
1:A:414:ALA:C	1:A:416:ARG:N	2.71	0.46
1:B:291:MET:O	1:B:451:TYR:CE2	2.68	0.46
1:A:368:SER:CB	1:A:393:MET:HB3	2.37	0.46
1:A:375:PHE:HD1	1:A:375:PHE:HA	1.62	0.46
1:A:392:PRO:C	3:A:703:HOH:O	2.49	0.46
1:B:158:LEU:HD22	1:B:159:PHE:N	2.29	0.46
1:B:406:VAL:CG1	1:B:441:VAL:HG21	2.43	0.46
1:A:24:THR:O	1:A:25:GLY:C	2.59	0.46
1:A:380:TYR:HD1	1:A:380:TYR:O	1.98	0.46
1:B:261:ARG:NH1	1:B:261:ARG:CG	2.73	0.46
1:B:45:ILE:HG22	1:B:47:VAL:CG2	2.46	0.46
1:B:65:VAL:C	1:B:66:VAL:O	2.40	0.46
1:B:142:GLY:N	1:B:143:PRO:HD2	2.30	0.46
1:A:336:ARG:C	1:A:337:GLY:O	2.54	0.46
1:A:344:ALA:O	1:B:345:ALA:CB	2.43	0.46
1:B:291:MET:CE	1:B:291:MET:HA	2.45	0.46
1:B:296:VAL:HG13	1:B:371:LEU:HD22	1.98	0.46
1:A:34:LYS:CD	1:A:38:THR:HG23	2.46	0.46
1:B:101:ASN:OD1	1:B:152:ARG:NH2	2.49	0.46
1:B:399:MET:HE1	1:B:445:ILE:HG23	1.98	0.46
1:B:386:ARG:HH11	1:B:388:ILE:HD11	1.80	0.46
1:A:199:LYS:HG2	3:A:739:HOH:O	2.15	0.45
1:A:443:GLN:O	1:A:447:LEU:HB2	2.15	0.45
1:B:106:PRO:HA	1:B:109:ALA:HB3	1.98	0.45
1:A:216:ARG:HE	1:A:216:ARG:N	2.10	0.45
1:B:172:GLN:HE21	1:B:458:GLY:CA	2.09	0.45
1:B:277:THR:OG1	1:B:285:TRP:HB3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:ASP:HB2	1:B:321:ASP:CG	2.40	0.45
1:A:132:TYR:CD2	1:A:212:ALA:HB2	2.51	0.45
1:A:306:GLY:C	1:A:393:MET:CE	2.84	0.45
1:B:277:THR:HG22	1:B:321:ASP:HB3	1.99	0.45
1:B:498:HIS:C	1:B:500:PRO:HD2	2.41	0.45
1:A:307:PHE:N	1:A:393:MET:HE2	2.32	0.45
1:A:379:PRO:CB	1:A:388:ILE:HG22	2.46	0.45
1:A:404:SER:O	1:A:407:GLU:CD	2.59	0.45
1:B:307:PHE:CA	1:B:402:PHE:HE1	2.28	0.45
1:B:352:TYR:CE1	3:B:729:HOH:O	2.56	0.45
1:A:380:TYR:CD1	1:A:380:TYR:C	2.94	0.45
1:A:403:ALA:O	1:A:406:VAL:HG23	2.16	0.45
1:B:282:PHE:CD1	1:B:282:PHE:O	2.70	0.45
1:A:80:LYS:HE2	1:A:80:LYS:CA	2.46	0.45
1:A:158:LEU:HD22	1:A:159:PHE:N	2.31	0.45
1:A:202:MET:HA	3:A:714:HOH:O	2.15	0.45
1:A:216:ARG:N	1:A:216:ARG:NE	2.64	0.45
1:B:7:ILE:O	1:B:9:ILE:HG13	2.17	0.45
1:B:305:SER:C	1:B:393:MET:CE	2.89	0.45
1:A:129:ASP:OD1	1:A:129:ASP:O	2.34	0.45
1:A:180:PHE:CE2	1:A:242:TRP:CH2	2.92	0.45
1:A:380:TYR:O	1:A:380:TYR:CD1	2.70	0.45
1:A:446:TYR:CE1	1:A:450:ILE:HD12	2.51	0.45
1:B:328:LEU:HD23	1:B:331:MET:HE2	1.99	0.45
1:A:10:ALA:HA	3:A:736:HOH:O	2.15	0.45
1:A:406:VAL:C	1:A:408:THR:H	2.23	0.45
1:B:297:LEU:HA	1:B:297:LEU:HD22	1.61	0.45
1:A:159:PHE:CD1	1:A:159:PHE:C	2.94	0.45
1:A:288:GLY:H	1:A:505:HIS:CE1	2.34	0.45
1:A:129:ASP:OD1	1:A:129:ASP:C	2.60	0.45
1:A:261:ARG:HG3	1:A:261:ARG:NH1	2.22	0.45
1:A:299:TYR:CG	1:A:299:TYR:O	2.70	0.45
1:B:26:PHE:O	1:B:26:PHE:CD1	2.70	0.45
1:A:207:ALA:HA	1:A:210:LYS:CD	2.46	0.44
1:A:236:ARG:O	1:A:238:LYS:N	2.49	0.44
1:B:106:PRO:O	1:B:107:GLU:C	2.60	0.44
1:B:474:SER:OG	1:B:477:GLU:HB2	2.18	0.44
1:B:492:ASP:OD1	1:B:492:ASP:C	2.60	0.44
1:B:502:LEU:O	1:B:502:LEU:HD23	2.17	0.44
1:A:372:PHE:HB2	1:A:392:PRO:HA	1.99	0.44
1:B:291:MET:CA	1:B:291:MET:HE3	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:MET:CA	1:A:140:THR:HG22	2.47	0.44
1:A:406:VAL:HG13	1:A:441:VAL:HG21	1.98	0.44
1:B:39:ASN:OD1	1:B:41:ASP:HB2	2.18	0.44
1:B:502:LEU:HD23	1:B:502:LEU:C	2.42	0.44
1:B:36:LEU:HD11	1:B:90:LEU:HD21	2.00	0.44
1:B:202:MET:HE3	1:B:202:MET:HB3	1.62	0.44
1:B:258:ASN:HA	1:B:261:ARG:HD3	1.99	0.44
1:B:298:TYR:HB3	1:B:303:GLN:CB	2.48	0.44
1:A:33:GLU:HG3	1:A:70:LEU:HD22	1.99	0.44
1:A:74:LEU:C	1:A:76:GLU:H	2.26	0.44
1:A:264:ILE:HG22	1:A:265:PRO:N	2.32	0.44
1:A:282:PHE:O	1:A:282:PHE:CD1	2.70	0.44
1:A:374:HIS:CD2	1:A:374:HIS:O	2.70	0.44
1:A:325:ASN:HB3	1:A:481:PHE:HB3	1.99	0.44
1:A:16:LYS:O	1:A:43:GLY:C	2.61	0.44
1:A:132:TYR:OH	1:A:208:GLU:HG3	2.18	0.44
1:A:213:PHE:HA	1:A:216:ARG:HG2	2.00	0.44
1:A:297:LEU:HD22	1:A:297:LEU:HA	1.74	0.44
1:B:46:TYR:O	3:B:706:HOH:O	2.21	0.44
1:A:457:TYR:CE2	1:A:459:GLY:HA3	2.53	0.44
1:B:154:ARG:HH11	1:B:154:ARG:HG3	1.83	0.44
1:A:389:HIS:O	1:A:389:HIS:CD2	2.70	0.44
1:B:126:THR:HB	1:B:290:ARG:NH1	2.33	0.44
1:B:330:SER:CB	3:B:718:HOH:O	2.59	0.44
1:A:15:GLY:O	1:A:16:LYS:HG2	2.17	0.43
1:A:16:LYS:H	1:A:43:GLY:N	2.12	0.43
1:A:171:ARG:NH2	1:A:180:PHE:CZ	2.86	0.43
1:A:182:LEU:HA	1:A:255:MET:HB3	1.99	0.43
1:A:307:PHE:HA	1:A:402:PHE:CE1	2.53	0.43
1:A:463:ASN:O	1:A:466:THR:CG2	2.58	0.43
1:B:157:LYS:O	1:B:265:PRO:HG2	2.18	0.43
1:B:181:ARG:O	1:B:183:GLY:N	2.51	0.43
1:B:203:LEU:HA	1:B:203:LEU:HD23	1.69	0.43
1:B:388:ILE:HG22	1:B:390:VAL:HG23	1.98	0.43
1:A:170:GLN:O	1:A:172:GLN:OE1	2.35	0.43
1:A:278:TRP:CG	1:A:278:TRP:O	2.45	0.43
1:B:115:GLU:O	1:B:155:ARG:NE	2.50	0.43
1:A:216:ARG:O	1:A:217:ARG:C	2.62	0.43
1:A:374:HIS:O	1:A:374:HIS:CG	2.70	0.43
1:A:236:ARG:C	1:A:238:LYS:N	2.76	0.43
1:A:364:PHE:CE2	1:A:455:THR:HA	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ILE:CG2	1:A:473:MET:HA	2.49	0.43
1:B:372:PHE:HE1	1:B:390:VAL:CG1	2.15	0.43
1:A:61:LEU:O	1:A:66:VAL:HG22	2.18	0.43
1:A:314:VAL:HG23	1:A:460:ARG:NH1	2.34	0.43
1:A:372:PHE:HD1	1:A:391:PRO:C	2.26	0.43
1:B:74:LEU:C	1:B:76:GLU:H	2.27	0.43
1:B:101:ASN:C	1:B:102:VAL:HG22	2.44	0.43
1:B:417:LEU:HD22	1:B:417:LEU:O	2.19	0.43
1:A:47:VAL:O	1:A:48:LEU:C	2.60	0.43
1:A:271:PRO:HG2	1:A:271:PRO:O	2.19	0.43
1:A:395:LEU:HD13	3:A:732:HOH:O	2.17	0.43
1:B:304:LEU:HD22	1:B:304:LEU:N	2.33	0.43
1:A:164:THR:HB	1:A:166:TYR:N	2.34	0.43
1:A:222:SER:OG	1:A:224:SER:HB3	2.19	0.43
1:B:80:LYS:HA	3:B:702:HOH:O	2.17	0.43
1:B:291:MET:HE3	1:B:291:MET:N	2.33	0.43
1:A:60:ARG:O	1:A:64:GLU:HG3	2.19	0.42
1:A:71:PHE:HD1	1:A:74:LEU:HD12	1.82	0.42
1:A:295:VAL:O	1:A:296:VAL:C	2.62	0.42
1:B:113:ALA:O	1:B:153:PHE:HA	2.18	0.42
1:B:305:SER:O	1:B:393:MET:HA	2.18	0.42
1:A:277:THR:O	1:A:283:PRO:HA	2.19	0.42
1:B:28:ALA:O	1:B:31:LEU:CB	2.68	0.42
1:B:28:ALA:O	1:B:31:LEU:HB3	2.19	0.42
1:A:242:TRP:CD1	1:A:248:PHE:HD1	2.34	0.42
1:A:290:ARG:CG	1:A:290:ARG:HH11	2.33	0.42
1:A:307:PHE:O	1:A:395:LEU:HA	2.19	0.42
1:B:21:THR:CA	3:B:719:HOH:O	2.67	0.42
1:A:42:VAL:HB	1:A:43:GLY:O	2.19	0.42
1:A:167:VAL:HG22	1:A:251:ALA:HB2	2.02	0.42
1:A:182:LEU:CD2	1:A:205:ILE:CG1	2.88	0.42
1:A:205:ILE:N	1:A:205:ILE:CD1	2.58	0.42
1:A:502:LEU:C	1:A:502:LEU:HD23	2.45	0.42
1:B:203:LEU:C	1:B:203:LEU:HD22	2.44	0.42
1:B:473:MET:HB3	1:B:477:GLU:HB3	2.01	0.42
1:A:274:ILE:N	2:A:601:NAP:O7N	2.52	0.42
1:A:322:MET:HE1	1:A:485:VAL:CA	2.31	0.42
1:A:128:PHE:CE2	1:A:291:MET:SD	3.13	0.42
1:A:146:ILE:HG22	1:A:159:PHE:HE2	1.85	0.42
1:A:187:ALA:HB1	1:A:199:LYS:HD3	2.02	0.42
1:A:478:LYS:HB3	3:A:735:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:LEU:HD23	3:B:710:HOH:O	2.18	0.42
1:B:306:GLY:N	1:B:393:MET:CE	2.63	0.42
1:B:352:TYR:CD1	3:B:729:HOH:O	2.73	0.42
1:A:319:PRO:HG2	1:A:322:MET:HG3	2.00	0.42
1:B:20:ILE:HG12	1:B:120:VAL:HB	2.02	0.42
1:B:31:LEU:HA	1:B:324:VAL:HG13	2.02	0.42
1:B:174:VAL:HA	1:B:460:ARG:O	2.20	0.42
1:B:393:MET:HE3	1:B:393:MET:C	2.44	0.42
1:A:61:LEU:HD11	1:A:90:LEU:HD13	2.01	0.42
1:A:65:VAL:CG1	1:A:71:PHE:CZ	2.99	0.42
1:A:396:PHE:CD2	1:A:402:PHE:HA	2.54	0.42
1:A:203:LEU:HD12	1:A:255:MET:HE1	1.99	0.41
1:B:26:PHE:CZ	1:B:320:ALA:HB2	2.55	0.41
1:B:315:LEU:HD12	1:B:315:LEU:HA	1.89	0.41
1:B:396:PHE:HD1	1:B:396:PHE:N	2.18	0.41
1:B:507:MET:HE3	1:B:507:MET:HA	2.01	0.41
1:A:45:ILE:HG22	1:A:47:VAL:CG2	2.49	0.41
1:B:437:CYS:SG	1:B:438:ALA:N	2.90	0.41
1:A:79:GLY:O	1:A:80:LYS:CD	2.60	0.41
1:A:186:ILE:HG13	1:A:242:TRP:CZ3	2.55	0.41
1:A:209:ILE:O	1:A:212:ALA:O	2.38	0.41
1:A:282:PHE:CD1	1:A:282:PHE:C	2.98	0.41
1:A:403:ALA:C	1:A:405:TYR:H	2.28	0.41
1:B:13:LEU:O	1:B:39:ASN:ND2	2.54	0.41
2:B:601:NAP:H2N	2:B:601:NAP:H2D	1.81	0.41
1:A:20:ILE:HA	1:A:120:VAL:O	2.19	0.41
1:A:65:VAL:O	1:A:71:PHE:HE2	1.88	0.41
1:A:216:ARG:NE	1:A:216:ARG:CA	2.83	0.41
1:B:61:LEU:O	1:B:65:VAL:HB	2.21	0.41
1:B:182:LEU:HB2	1:B:259:SER:OG	2.20	0.41
1:B:333:LYS:HE3	1:B:472:GLU:OE1	2.20	0.41
1:A:362:LEU:HD12	1:A:490:TRP:HB3	2.01	0.41
1:B:182:LEU:HD11	1:B:205:ILE:CD1	2.50	0.41
1:B:171:ARG:HD2	1:B:175:VAL:CG1	2.50	0.41
1:B:239:LEU:HD13	1:B:239:LEU:O	2.20	0.41
1:B:302:GLY:C	1:B:303:GLN:HG2	2.45	0.41
1:B:302:GLY:O	1:B:303:GLN:C	2.63	0.41
1:A:147:MET:HE2	1:A:159:PHE:CG	2.56	0.41
1:A:7:ILE:CG2	1:A:477:GLU:OE1	2.61	0.41
1:A:396:PHE:HE2	1:A:405:TYR:CD1	2.38	0.41
1:B:182:LEU:HD21	1:B:205:ILE:CG1	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:LEU:C	1:B:502:LEU:CD2	2.94	0.41
1:A:74:LEU:C	1:A:76:GLU:N	2.76	0.41
1:A:164:THR:CG2	1:A:246:TYR:OH	2.66	0.41
1:A:213:PHE:HA	1:A:216:ARG:CD	2.51	0.41
1:A:264:ILE:HA	1:A:265:PRO:HD3	1.88	0.41
1:A:274:ILE:HD13	1:A:323:VAL:HG21	1.90	0.41
1:B:62:HIS:C	1:B:66:VAL:HG23	2.42	0.41
1:B:136:MET:CE	1:B:209:ILE:HG13	2.51	0.41
1:B:307:PHE:C	1:B:402:PHE:CE1	2.99	0.41
1:B:340:ALA:CB	3:B:738:HOH:O	2.68	0.41
1:B:340:ALA:HA	1:B:343:ALA:HB3	2.02	0.41
1:B:483:PHE:N	1:B:483:PHE:CD1	2.89	0.41
1:A:41:ASP:C	1:A:42:VAL:O	2.63	0.41
1:A:396:PHE:HD2	1:A:402:PHE:HA	1.86	0.41
1:A:411:LEU:C	1:A:413:ARG:N	2.79	0.41
1:A:446:TYR:O	1:A:447:LEU:C	2.63	0.41
1:A:278:TRP:O	1:A:279:ARG:HG2	2.20	0.40
1:B:127:THR:HB	1:B:130:GLU:HG2	2.03	0.40
1:A:393:MET:HE3	1:A:393:MET:HA	2.02	0.40
1:B:287:GLU:HA	1:B:505:HIS:CD2	2.56	0.40
1:A:198:HIS:ND1	1:A:198:HIS:N	2.69	0.40
1:A:474:SER:O	1:A:477:GLU:N	2.53	0.40
1:A:502:LEU:C	1:A:502:LEU:CD2	2.95	0.40
1:B:62:HIS:O	1:B:66:VAL:HG23	2.21	0.40
1:B:285:TRP:CZ2	1:B:287:GLU:CG	3.04	0.40
1:B:364:PHE:O	1:B:395:LEU:HD13	2.22	0.40
1:A:208:GLU:OE2	1:A:208:GLU:HA	2.22	0.40
1:B:182:LEU:CD1	1:B:205:ILE:HD11	2.52	0.40
1:B:223:ALA:C	1:B:225:PHE:N	2.79	0.40
1:B:286:MET:HE3	1:B:287:GLU:N	2.36	0.40
1:B:404:SER:O	1:B:407:GLU:CD	2.61	0.40
1:A:212:ALA:O	1:A:213:PHE:CD1	2.74	0.40
1:B:7:ILE:O	1:B:7:ILE:CG1	2.69	0.40
1:B:295:VAL:O	1:B:297:LEU:N	2.54	0.40
1:B:388:ILE:O	1:B:389:HIS:C	2.60	0.40

All (2) 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:A:417:LEU:CB	1:B:303:GLN:OE1[5_554]	1.82	0.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:ARG:NH2	1:B:437:CYS:O[5_554]	2.15	0.05

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	476/532 (90%)	375 (79%)	91 (19%)	10 (2%)	5	24
1	B	467/532 (88%)	391 (84%)	68 (15%)	8 (2%)	7	28
All	All	943/1064 (89%)	766 (81%)	159 (17%)	18 (2%)	6	26

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	280	ASP
1	B	296	VAL
1	A	442	GLU
1	A	75	GLN
1	A	144	PHE
1	A	296	VAL
1	B	182	LEU
1	A	237	ALA
1	B	224	SER
1	A	218	HIS
1	A	248	PHE
1	A	321	ASP
1	B	491	THR
1	A	391	PRO
1	B	43	GLY
1	B	359	VAL
1	A	359	VAL
1	B	354	VAL

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	391/422 (93%)	277 (71%)	114 (29%)	0	1
1	B	384/422 (91%)	276 (72%)	108 (28%)	0	1
All	All	775/844 (92%)	553 (71%)	222 (29%)	0	1

All (222) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	16	LYS
1	A	17	ASN
1	A	21	THR
1	A	24	THR
1	A	27	LEU
1	A	31	LEU
1	A	34	LYS
1	A	35	ILE
1	A	42	VAL
1	A	55	ASP
1	A	58	LEU
1	A	64	GLU
1	A	66	VAL
1	A	69	GLU
1	A	73	ARG
1	A	77	ILE
1	A	80	LYS
1	A	94	VAL
1	A	97	VAL
1	A	102	VAL
1	A	117	ASP
1	A	122	SER
1	A	125	ASN
1	A	127	THR
1	A	130	GLU
1	A	133	ASP

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Mol	Chain	Res	Type
1	A	136	MET
1	A	147	MET
1	A	152	ARG
1	A	154	ARG
1	A	155	ARG
1	A	158	LEU
1	A	164	THR
1	A	167	VAL
1	A	172	GLN
1	A	174	VAL
1	A	175	VAL
1	A	178	LYS
1	A	181	ARG
1	A	186	ILE
1	A	188	LYS
1	A	197	GLN
1	A	198	HIS
1	A	202	MET
1	A	203	LEU
1	A	205	ILE
1	A	208	GLU
1	A	209	ILE
1	A	210	LYS
1	A	216	ARG
1	A	217	ARG
1	A	221	ASP
1	A	224	SER
1	A	230	LYS
1	A	232	LEU
1	A	234	LEU
1	A	239	LEU
1	A	245	THR
1	A	247	VAL
1	A	250	LYS
1	A	254	GLU
1	A	261	ARG
1	A	265	PRO
1	A	266	VAL
1	A	269	ILE
1	A	275	GLU
1	A	277	THR
1	A	279	ARG

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Mol	Chain	Res	Type
1	A	290	ARG
1	A	291	MET
1	A	295	VAL
1	A	297	LEU
1	A	301	LYS
1	A	304	LEU
1	A	305	SER
1	A	307	PHE
1	A	312	GLU
1	A	318	VAL
1	A	336	ARG
1	A	347	GLU
1	A	353	HIS
1	A	356	SER
1	A	362	LEU
1	A	366	ASP
1	A	367	LEU
1	A	371	LEU
1	A	375	PHE
1	A	386	ARG
1	A	388	ILE
1	A	398	THR
1	A	405	TYR
1	A	407	GLU
1	A	408	THR
1	A	411	LEU
1	A	412	LEU
1	A	413	ARG
1	A	436	LEU
1	A	437	CYS
1	A	439	LYS
1	A	441	VAL
1	A	443	GLN
1	A	445	ILE
1	A	447	LEU
1	A	449	SER
1	A	452	GLN
1	A	460	ARG
1	A	466	THR
1	A	467	GLU
1	A	469	LEU
1	A	475	GLU

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Mol	Chain	Res	Type
1	A	480	ARG
1	A	485	VAL
1	A	506	VAL
1	B	17	ASN
1	B	21	THR
1	B	26	PHE
1	B	27	LEU
1	B	31	LEU
1	B	34	LYS
1	B	35	ILE
1	B	37	ARG
1	B	38	THR
1	B	42	VAL
1	B	44	LYS
1	B	45	ILE
1	B	50	LYS
1	B	55	ASP
1	B	58	LEU
1	B	66	VAL
1	B	70	LEU
1	B	73	ARG
1	B	77	ILE
1	B	84	SER
1	B	97	VAL
1	B	111	VAL
1	B	117	ASP
1	B	118	ILE
1	B	122	SER
1	B	125	ASN
1	B	130	GLU
1	B	131	ARG
1	B	146	ILE
1	B	152	ARG
1	B	154	ARG
1	B	158	LEU
1	B	160	LEU
1	B	164	THR
1	B	167	VAL
1	B	172	GLN
1	B	175	VAL
1	B	177	GLU
1	B	178	LYS

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Mol	Chain	Res	Type
1	B	186	ILE
1	B	201	THR
1	B	202	MET
1	B	203	LEU
1	B	205	ILE
1	B	208	GLU
1	B	211	LEU
1	B	217	ARG
1	B	221	ASP
1	B	230	LYS
1	B	232	LEU
1	B	236	ARG
1	B	239	LEU
1	B	247	VAL
1	B	250	LYS
1	B	261	ARG
1	B	263	ASP
1	B	269	ILE
1	B	274	ILE
1	B	275	GLU
1	B	277	THR
1	B	279	ARG
1	B	286	MET
1	B	291	MET
1	B	295	VAL
1	B	297	LEU
1	B	301	LYS
1	B	304	LEU
1	B	307	PHE
1	B	318	VAL
1	B	349	MET
1	B	353	HIS
1	B	359	VAL
1	B	362	LEU
1	B	367	LEU
1	B	369	ARG
1	B	371	LEU
1	B	388	ILE
1	B	389	HIS
1	B	391	PRO
1	B	393	MET
1	B	394	ARG

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Mol	Chain	Res	Type
1	B	399	MET
1	B	400	GLU
1	B	406	VAL
1	B	408	THR
1	B	409	ASP
1	B	411	LEU
1	B	413	ARG
1	B	416	ARG
1	B	417	LEU
1	B	439	LYS
1	B	441	VAL
1	B	445	ILE
1	B	447	LEU
1	B	450	ILE
1	B	466	THR
1	B	469	LEU
1	B	470	ILE
1	B	475	GLU
1	B	476	GLU
1	B	477	GLU
1	B	478	LYS
1	B	480	ARG
1	B	483	PHE
1	B	499	ILE
1	B	502	LEU
1	B	506	VAL
1	B	508	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	125	ASN
1	A	168	ASN
1	A	170	GLN
1	A	197	GLN
1	A	303	GLN
1	A	350	HIS
1	A	353	HIS
1	A	389	HIS
1	A	443	GLN
1	A	465	ASN

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Mol	Chain	Res	Type
1	A	505	HIS
1	B	17	ASN
1	B	83	HIS
1	B	125	ASN
1	B	172	GLN
1	B	373	GLN
1	B	401	GLN
1	B	463	ASN
1	B	465	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](#)

2 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	$\# Z > 2$
2	NAP	B	601	-	50,52,52	1.06	2 (4%)	71,80,80	1.78	15 (21%)
2	NAP	A	601	-	50,52,52	0.94	2 (4%)	71,80,80	1.65	11 (15%)

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
2	NAP	B	601	-	-	21/35/67/67	0/5/5/5
2	NAP	A	601	-	-	15/35/67/67	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	NAP	C2N-N1N	5.91	1.41	1.35
2	A	601	NAP	C2N-N1N	4.51	1.39	1.35
2	A	601	NAP	O4D-C1D	3.17	1.45	1.40
2	B	601	NAP	P2B-O2B	2.33	1.63	1.59

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	NAP	C6N-N1N-C2N	-6.51	116.34	121.88
2	B	601	NAP	P2B-O2B-C2B	-6.08	107.20	123.43
2	B	601	NAP	O2X-P2B-O2B	5.25	126.30	105.85
2	B	601	NAP	O2B-P2B-O1X	-4.51	93.25	109.33
2	A	601	NAP	C5N-C4N-C3N	-4.36	116.08	120.36
2	A	601	NAP	O2B-P2B-O1X	-4.33	93.88	109.33
2	B	601	NAP	C6N-N1N-C2N	-4.08	118.40	121.88
2	B	601	NAP	O3B-C3B-C2B	3.88	122.05	111.19
2	A	601	NAP	O2X-P2B-O2B	3.82	120.74	105.85
2	A	601	NAP	P2B-O2B-C2B	-3.82	113.23	123.43
2	B	601	NAP	C5N-C4N-C3N	-3.28	117.14	120.36
2	B	601	NAP	C3B-C2B-C1B	-3.26	96.57	102.81
2	A	601	NAP	O3-PN-O1N	-3.09	101.42	110.70
2	A	601	NAP	C3B-C2B-C1B	-2.88	97.28	102.81
2	A	601	NAP	O4B-C1B-N9A	2.85	113.56	108.09
2	B	601	NAP	O3B-C3B-C4B	-2.75	103.17	111.08
2	A	601	NAP	O2B-C2B-C3B	2.56	120.86	111.68
2	B	601	NAP	C2N-C3N-C4N	-2.52	115.33	118.26
2	B	601	NAP	O2N-PN-O1N	2.42	123.69	112.44
2	A	601	NAP	O3B-C3B-C2B	2.39	117.89	111.19
2	A	601	NAP	O2N-PN-O1N	2.37	123.45	112.44
2	B	601	NAP	O3X-P2B-O2B	-2.33	96.75	105.85
2	B	601	NAP	O2A-PA-O1A	2.26	122.95	112.44
2	B	601	NAP	C2B-C3B-C4B	-2.18	97.32	101.99
2	B	601	NAP	O2A-PA-O3	-2.14	101.49	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	NAP	O2B-C2B-C3B	2.10	119.21	111.68

There are no chirality outliers.

All (36) torsion outliers are listed below:

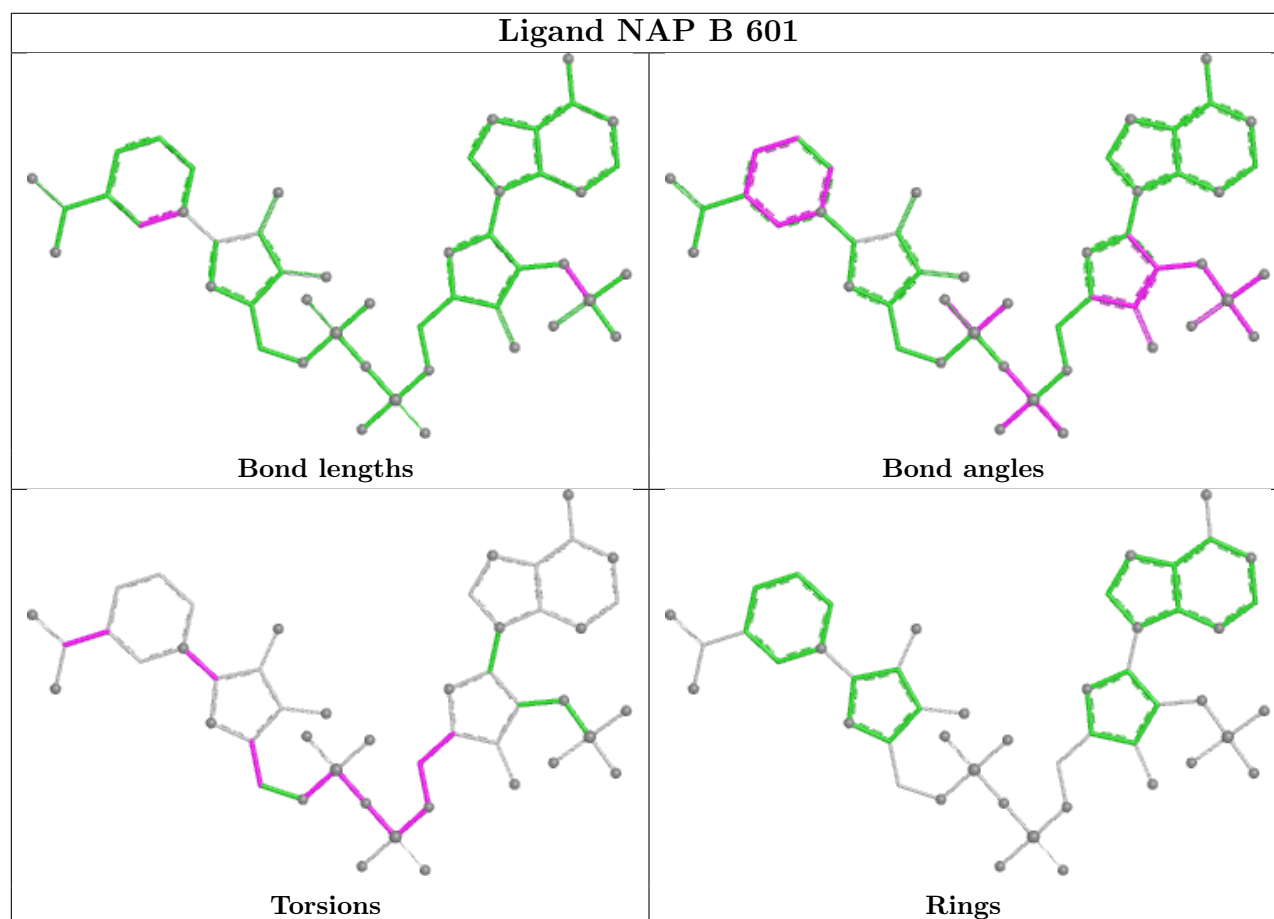
Mol	Chain	Res	Type	Atoms
2	A	601	NAP	C5B-O5B-PA-O3
2	A	601	NAP	O4B-C4B-C5B-O5B
2	A	601	NAP	C3B-C4B-C5B-O5B
2	A	601	NAP	C5D-O5D-PN-O3
2	A	601	NAP	C5D-O5D-PN-O2N
2	A	601	NAP	O4D-C1D-N1N-C2N
2	A	601	NAP	C2N-C3N-C7N-O7N
2	A	601	NAP	C2N-C3N-C7N-N7N
2	B	601	NAP	C5B-O5B-PA-O2A
2	B	601	NAP	C5B-O5B-PA-O3
2	B	601	NAP	C5D-O5D-PN-O3
2	B	601	NAP	C5D-O5D-PN-O2N
2	B	601	NAP	O4D-C1D-N1N-C2N
2	B	601	NAP	O4D-C1D-N1N-C6N
2	B	601	NAP	C2D-C1D-N1N-C6N
2	A	601	NAP	C4N-C3N-C7N-O7N
2	A	601	NAP	C4N-C3N-C7N-N7N
2	B	601	NAP	C3B-C4B-C5B-O5B
2	B	601	NAP	O4D-C4D-C5D-O5D
2	B	601	NAP	C4N-C3N-C7N-O7N
2	B	601	NAP	C4N-C3N-C7N-N7N
2	A	601	NAP	O4D-C4D-C5D-O5D
2	B	601	NAP	O4B-C4B-C5B-O5B
2	B	601	NAP	C3D-C4D-C5D-O5D
2	B	601	NAP	C2N-C3N-C7N-O7N
2	A	601	NAP	C3D-C4D-C5D-O5D
2	B	601	NAP	C2N-C3N-C7N-N7N
2	B	601	NAP	PN-O3-PA-O1A
2	B	601	NAP	C4B-C5B-O5B-PA
2	A	601	NAP	C5B-O5B-PA-O1A
2	B	601	NAP	C5B-O5B-PA-O1A
2	B	601	NAP	PA-O3-PN-O2N
2	B	601	NAP	C2D-C1D-N1N-C2N
2	A	601	NAP	O4D-C1D-N1N-C6N
2	A	601	NAP	C1B-C2B-O2B-P2B
2	B	601	NAP	PA-O3-PN-O1N

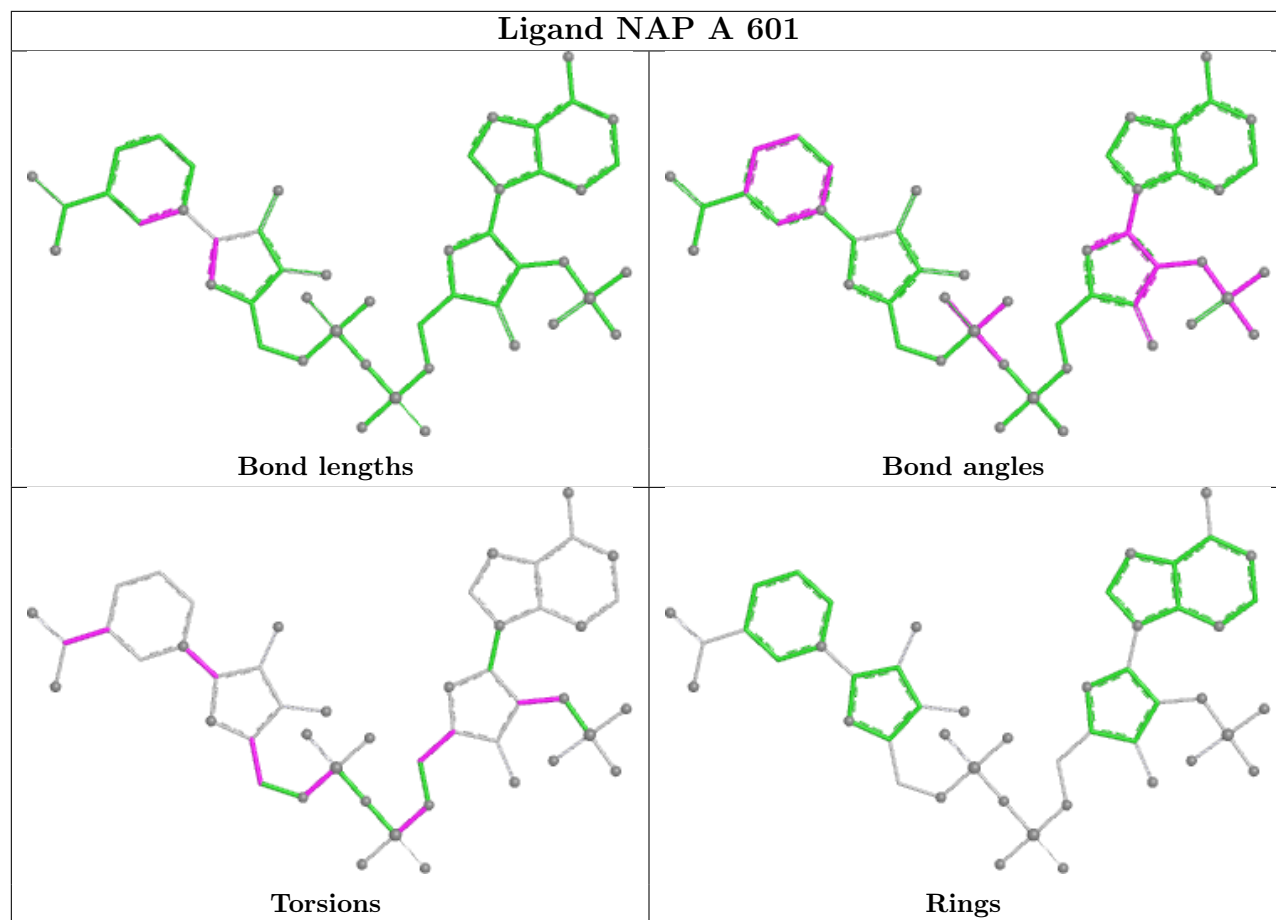
There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	NAP	3	0
2	A	601	NAP	10	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	482/532 (90%)	0.08	13 (2%) 56 42	30, 97, 152, 190	0
1	B	473/532 (88%)	0.05	7 (1%) 72 57	60, 95, 144, 195	0
All	All	955/1064 (89%)	0.07	20 (2%) 63 48	30, 96, 149, 195	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	471	GLY	3.8
1	B	216	ARG	3.8
1	A	387	PRO	3.4
1	A	414	ALA	3.2
1	A	415	GLY	3.0
1	B	107	GLU	3.0
1	A	389	HIS	2.8
1	A	412	LEU	2.6
1	B	412	LEU	2.6
1	A	440	SER	2.5
1	B	410	ALA	2.5
1	A	377	GLY	2.3
1	B	201	THR	2.2
1	A	438	ALA	2.2
1	A	214	ASP	2.2
1	A	313	GLY	2.1
1	A	129	ASP	2.1
1	B	440	SER	2.1
1	A	107	GLU	2.1
1	B	396	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

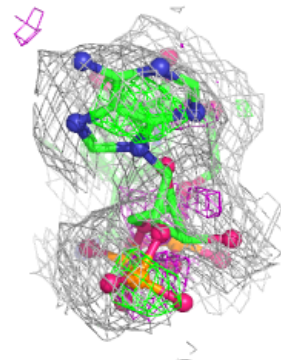
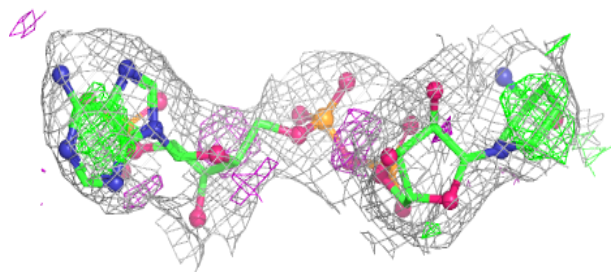
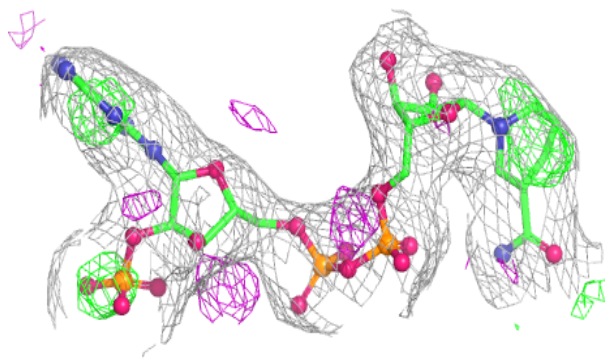
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAP	A	601	48/48	0.98	0.09	65,80,113,136	0
2	NAP	B	601	48/48	0.98	0.09	55,81,112,122	0

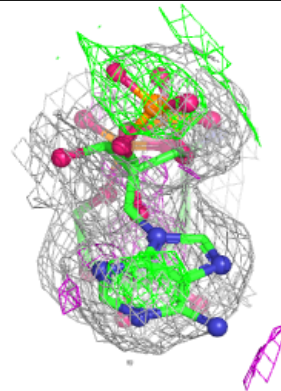
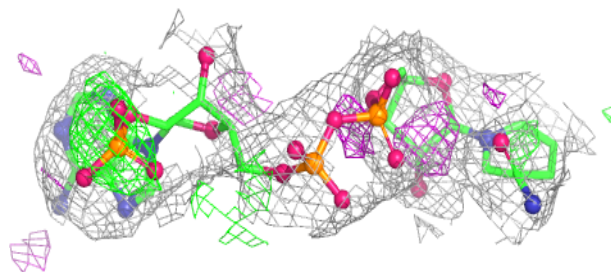
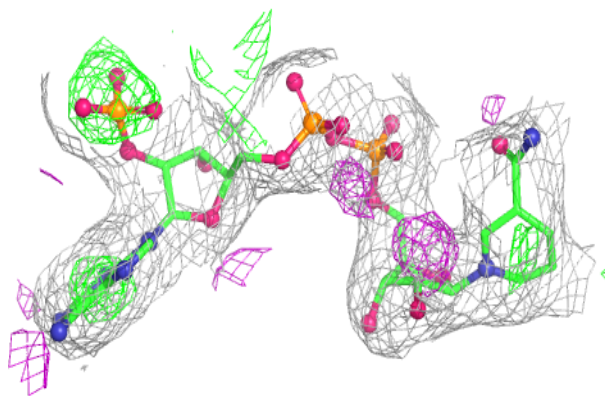
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP A 601:

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

**Electron density around NAP B 601:**

$2mF_o-DF_c$ (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.