



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 09:25 PM UTC

PDB ID : 9Q64 / pdb_00009q64
Title : Human prolyl endopeptidase (PREP) - complex with KT-2-59
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Deposited on : 2025-08-21
Resolution : 1.94 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

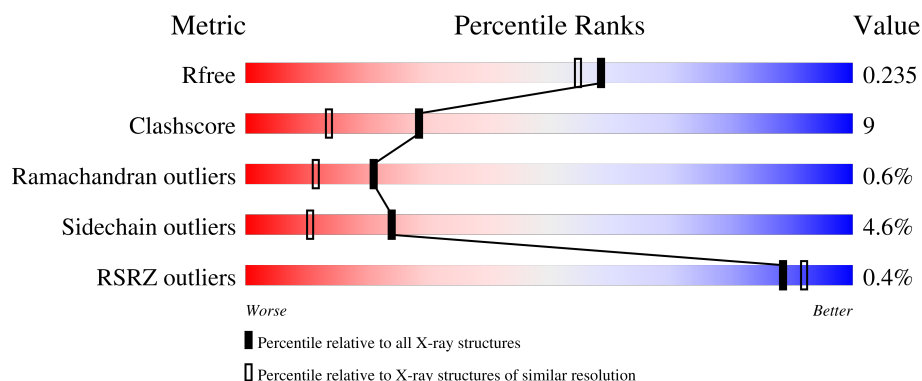
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	711	 73% 20% 5% ..
1	B	711	 76% 19% ..
1	C	711	 68% 25% 5% ..

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	B	802	-	X	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 18610 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.

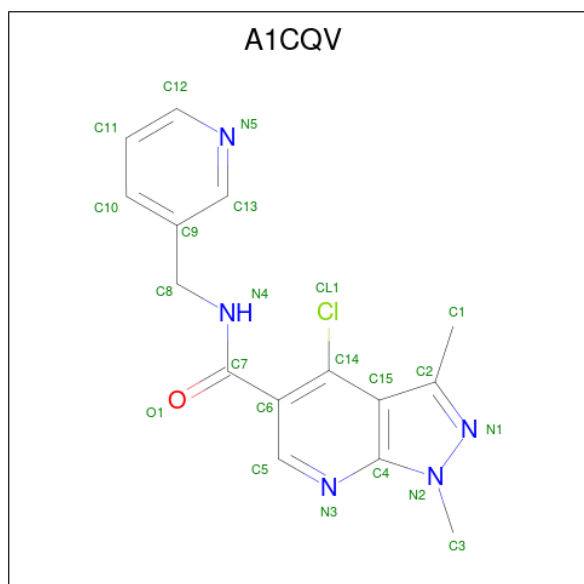
- Molecule 1 is a protein called Prolyl endopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	707	Total	C	N	O	S	0	0	0
			5673	3639	941	1066	27			
1	B	707	Total	C	N	O	S	0	2	0
			5686	3647	944	1068	27			
1	C	707	Total	C	N	O	S	0	1	0
			5681	3644	944	1066	27			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P48147
B	0	GLY	-	expression tag	UNP P48147
C	0	GLY	-	expression tag	UNP P48147

- Molecule 2 is 1,3-dimethyl-N-[(pyridin-3-yl)methyl]-1H-pyrazolo[3,4-b]pyridine-5-carboxamide (CCD ID: A1CQV) (formula: C₁₅H₁₄ClN₅O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			21	15	5	1		
2	B	1	Total	C	N	O	0	0
			21	15	5	1		
2	C	1	Total	C	N	O	0	0
			21	15	5	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



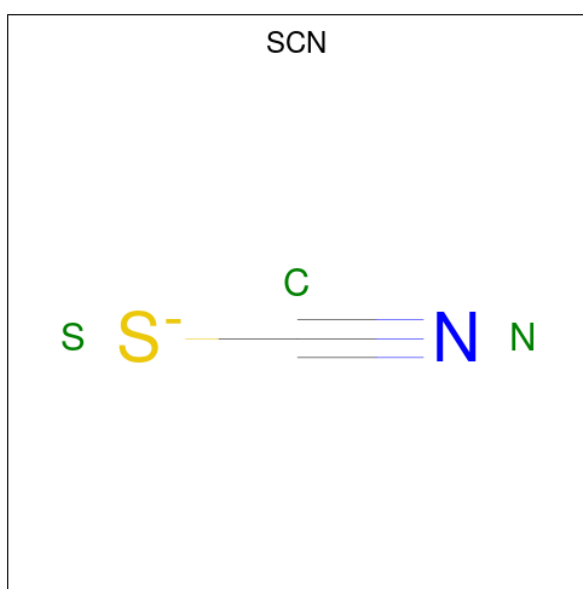
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



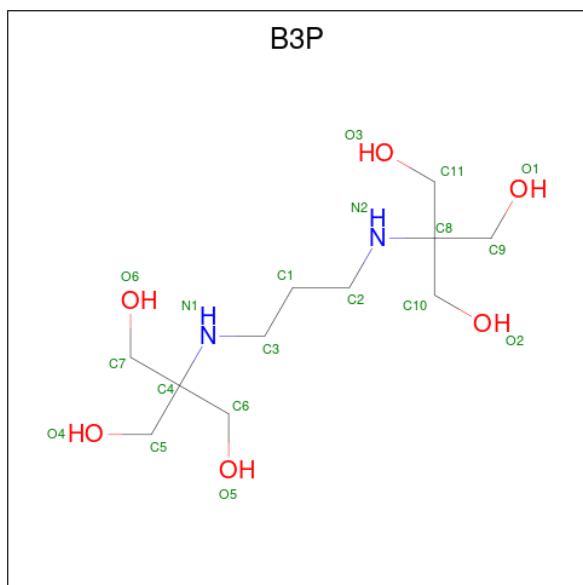
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	S	0	0
			3	1	1	1		
4	B	1	Total	C	N	S	0	0
			3	1	1	1		
4	B	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	1
			14	8	6		
5	B	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYLAMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: B3P) (formula: $C_{11}H_{26}N_2O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			19	11	2	6		

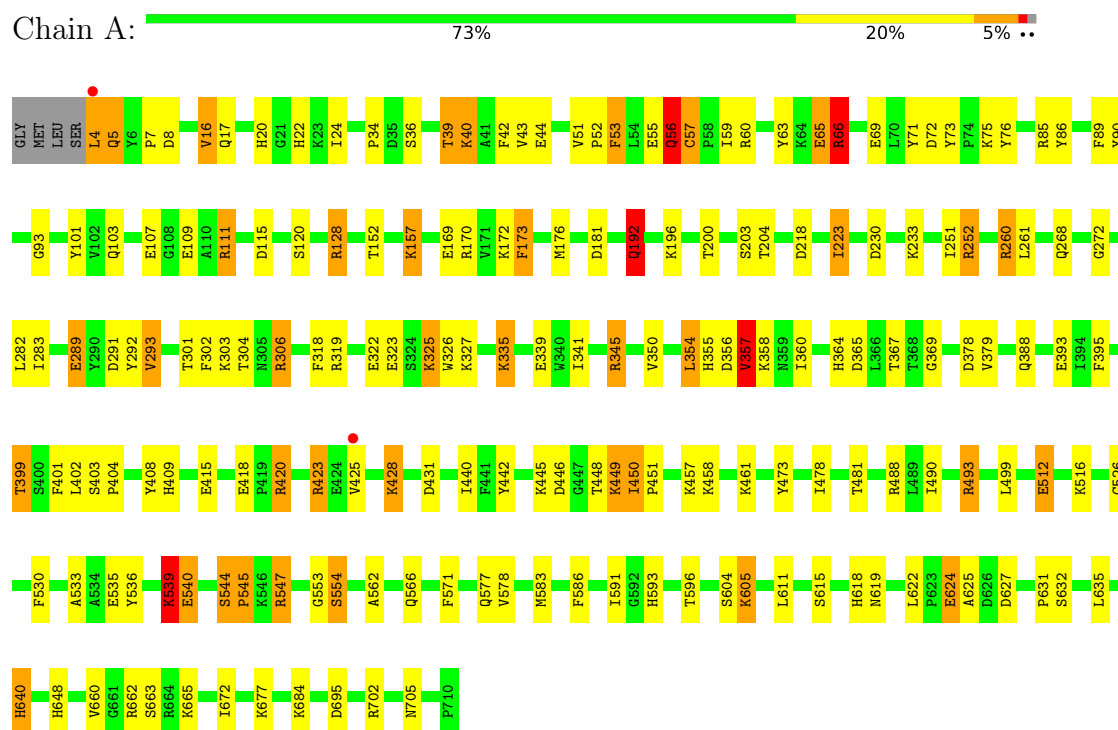
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	451	Total	O	0	1
			452	452		
7	B	560	Total	O	0	0
			560	560		
7	C	361	Total	O	0	0
			361	361		

3 Residue-property plots

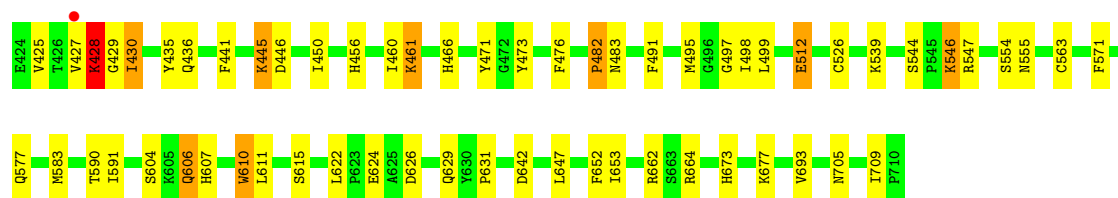
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Prolyl endopeptidase

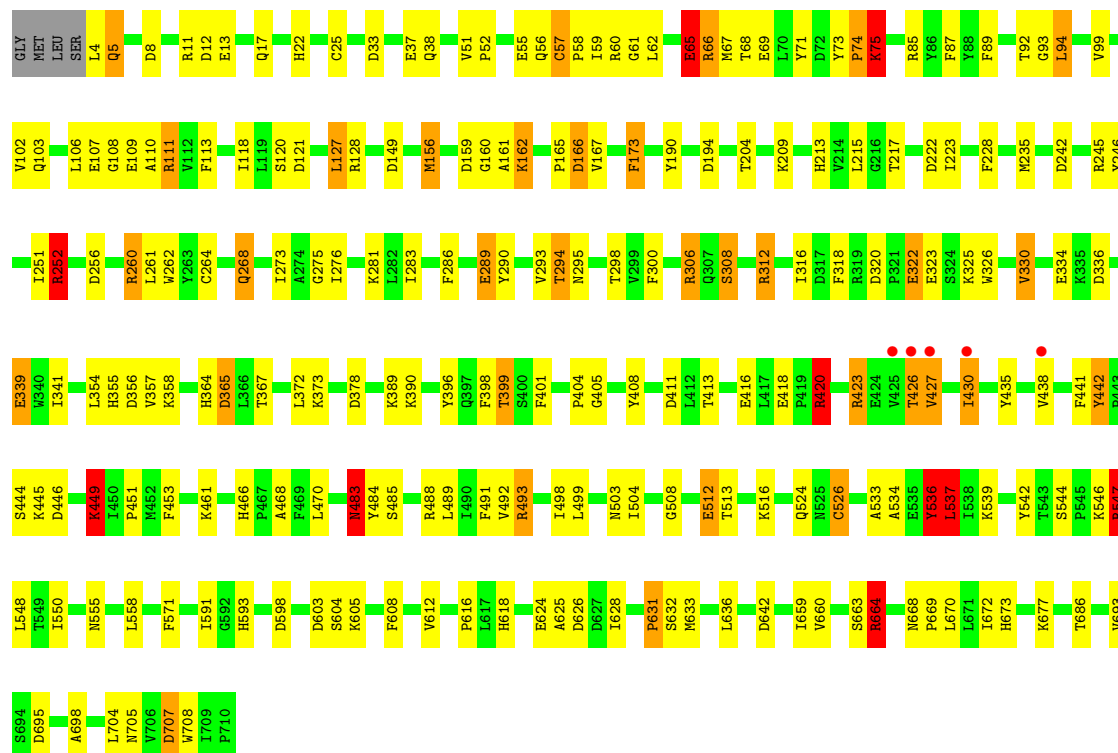


• Molecule 1: Prolyl endopeptidase





• Molecule 1: Prolyl endopeptidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.89Å 67.03Å 157.39Å 90.00° 99.41° 90.00°	Depositor
Resolution (Å)	34.10 – 1.94 34.10 – 1.94	Depositor EDS
% Data completeness (in resolution range)	70.0 (34.10-1.94) 70.0 (34.10-1.94)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.155 , 0.233 0.165 , 0.235	Depositor DCC
R_{free} test set	7960 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18610	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, B3P, A1CQV, SCN, GOL

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	1.00	3/5825 (0.1%)	1.71	103/7897 (1.3%)
1	B	1.08	6/5844 (0.1%)	1.64	74/7922 (0.9%)
1	C	0.98	1/5836 (0.0%)	1.70	111/7911 (1.4%)
All	All	1.02	10/17505 (0.1%)	1.68	288/23730 (1.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	8
1	C	0	11
All	All	0	26

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	252	ARG	NE-CZ	6.78	1.40	1.33
1	B	482	PRO	CA-CB	-6.13	1.45	1.53
1	B	105	SER	CA-CB	-5.96	1.45	1.53
1	A	593	HIS	CE1-NE2	5.66	1.38	1.32
1	A	632	SER	CA-CB	-5.55	1.44	1.53
1	B	624	GLU	C-O	-5.47	1.17	1.24
1	C	252	ARG	NE-CZ	5.26	1.38	1.33
1	B	673	HIS	CG-CD2	-5.19	1.30	1.35
1	A	615	SER	CA-CB	-5.12	1.45	1.53
1	B	577	GLN	C-O	-5.03	1.17	1.24

All (288) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	GLU	CB-CA-C	16.23	137.41	109.65
1	A	109	GLU	N-CA-CB	-12.61	91.44	109.97
1	C	322	GLU	CB-CG-CD	-12.31	91.67	112.60
1	C	526	CYS	CB-CA-C	-11.18	91.84	110.85
1	C	57	CYS	N-CA-CB	10.49	123.98	110.23
1	B	14	THR	CA-CB-OG1	-10.12	94.42	109.60
1	A	65	GLU	CB-CG-CD	10.08	129.74	112.60
1	C	546	LYS	N-CA-CB	9.86	125.41	110.22
1	A	318	PHE	CA-CB-CG	9.80	123.60	113.80
1	C	113	PHE	N-CA-CB	-9.74	96.28	110.40
1	C	512	GLU	CB-CG-CD	9.49	128.73	112.60
1	B	526	CYS	N-CA-CB	9.13	123.55	109.94
1	A	404	PRO	CB-CA-C	9.02	126.44	111.56
1	C	624	GLU	N-CA-CB	8.92	123.49	110.20
1	A	539	LYS	CB-CA-C	8.81	125.41	110.79
1	C	107	GLU	N-CA-CB	8.79	123.14	110.13
1	C	107	GLU	CB-CA-C	-8.76	96.07	110.79
1	A	512	GLU	CB-CG-CD	8.74	127.46	112.60
1	C	705	ASN	CB-CA-C	-8.65	100.27	111.86
1	C	373	LYS	N-CA-CB	-8.63	97.93	111.56
1	A	306	ARG	CB-CA-C	8.43	122.90	110.26
1	A	488	ARG	NE-CZ-NH2	8.42	126.78	119.20
1	B	512	GLU	CB-CG-CD	8.40	126.88	112.60
1	A	69	GLU	N-CA-CB	8.40	122.25	110.07
1	A	488	ARG	NE-CZ-NH1	-8.40	113.10	121.50
1	C	336	ASP	CA-CB-CG	8.12	120.72	112.60
1	C	268	GLN	CB-CA-C	-8.12	96.77	110.81
1	C	547	ARG	CB-CA-C	-8.09	98.56	111.18
1	C	416	GLU	CB-CA-C	8.03	123.63	110.78
1	B	320	ASP	CA-CB-CG	8.00	120.60	112.60
1	B	252	ARG	CD-NE-CZ	7.99	135.59	124.40
1	A	450	ILE	CA-C-O	7.98	124.38	119.19
1	A	499	LEU	N-CA-CB	7.95	123.58	110.63
1	A	293	VAL	N-CA-CB	-7.94	102.68	111.41
1	B	84	LYS	CB-CA-C	7.91	125.14	110.11
1	B	420	ARG	CB-CA-C	-7.86	94.99	109.37
1	A	60	ARG	NE-CZ-NH2	7.85	126.27	119.20
1	C	149	ASP	CA-CB-CG	7.82	120.42	112.60
1	B	705	ASN	CB-CA-C	-7.74	98.06	112.30
1	C	442	TYR	CB-CA-C	7.74	120.48	108.88
1	C	235	MET	CG-SD-CE	7.72	117.89	100.90
1	A	684	LYS	O-C-N	-7.70	115.07	121.38
1	A	327	LYS	CB-CA-C	-7.67	96.60	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	GLU	CB-CG-CD	7.64	125.59	112.60
1	C	642	ASP	CA-CB-CG	7.60	120.20	112.60
1	A	56	GLN	CB-CA-C	-7.48	94.68	110.31
1	A	252	ARG	CD-NE-CZ	7.47	134.86	124.40
1	C	686	THR	CA-CB-OG1	-7.40	98.51	109.60
1	B	420	ARG	CA-CB-CG	7.38	128.86	114.10
1	A	109	GLU	CB-CG-CD	-7.34	100.12	112.60
1	C	624	GLU	CB-CA-C	-7.33	97.29	110.70
1	C	322	GLU	N-CA-CB	7.30	120.79	110.36
1	A	596	THR	CA-CB-OG1	-7.29	98.66	109.60
1	C	526	CYS	N-CA-CB	7.29	120.95	110.16
1	C	8	ASP	CB-CA-C	-7.28	98.54	109.90
1	B	237	GLY	O-C-N	-7.25	118.03	123.61
1	C	252	ARG	CD-NE-CZ	7.22	134.51	124.40
1	A	490	ILE	N-CA-C	-7.22	103.43	110.72
1	B	482	PRO	CB-CA-C	-7.18	102.20	111.46
1	A	662	ARG	CD-NE-CZ	7.17	134.44	124.40
1	C	5	GLN	CB-CA-C	7.13	122.21	109.38
1	C	537	LEU	N-CA-CB	7.11	122.51	110.49
1	A	402	LEU	N-CA-CB	-7.10	99.88	110.61
1	C	289	GLU	CG-CD-OE2	-7.08	102.12	118.40
1	A	526	CYS	N-CA-CB	7.05	120.30	110.07
1	B	201	GLU	CB-CG-CD	7.04	124.56	112.60
1	B	526	CYS	CB-CA-C	-7.04	99.55	110.81
1	C	103	GLN	CB-CA-C	6.99	123.98	109.38
1	C	445	LYS	N-CA-CB	-6.99	99.79	110.20
1	A	181	ASP	CA-CB-CG	6.98	119.58	112.60
1	B	367	THR	OG1-CB-CG2	-6.97	95.35	109.30
1	C	547	ARG	N-CA-CB	6.97	121.65	111.54
1	B	109	GLU	CB-CA-C	6.93	121.22	109.72
1	C	56	GLN	CA-C-N	-6.92	111.99	121.61
1	C	56	GLN	C-N-CA	-6.92	111.99	121.61
1	A	204	THR	CA-CB-OG1	-6.89	99.26	109.60
1	C	693	VAL	N-CA-CB	6.83	120.83	110.58
1	A	230	ASP	CA-CB-CG	6.82	119.42	112.60
1	B	624	GLU	CB-CA-C	-6.81	99.35	110.79
1	B	336	ASP	CA-CB-CG	6.80	119.40	112.60
1	A	72	ASP	CA-CB-CG	6.77	119.37	112.60
1	C	670	LEU	N-CA-CB	-6.76	99.97	110.65
1	B	626	ASP	CB-CA-C	-6.75	99.38	110.85
1	C	446	ASP	CA-CB-CG	6.70	119.30	112.60
1	A	57	CYS	CB-CA-C	-6.68	98.82	109.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	GLN	N-CA-CB	6.68	123.52	111.37
1	B	420	ARG	N-CA-CB	6.67	121.52	110.85
1	A	399	THR	OG1-CB-CG2	-6.66	95.98	109.30
1	B	231	GLU	CB-CA-C	6.64	121.50	111.14
1	A	401	PHE	N-CA-CB	-6.64	100.11	110.06
1	B	179	THR	CA-CB-OG1	6.60	119.50	109.60
1	B	149	ASP	CA-CB-CG	6.58	119.18	112.60
1	C	546	LYS	CB-CA-C	-6.55	98.50	110.63
1	A	169	GLU	CB-CA-C	6.55	122.37	109.66
1	C	339	GLU	CB-CA-C	-6.54	99.80	110.79
1	A	128	ARG	NE-CZ-NH1	-6.52	114.98	121.50
1	A	69	GLU	CB-CA-C	-6.48	100.67	110.90
1	A	55	GLU	CB-CA-C	6.47	123.59	110.38
1	A	539	LYS	N-CA-CB	-6.47	100.60	110.12
1	C	4	LEU	CA-C-N	-6.42	113.62	122.93
1	C	4	LEU	C-N-CA	-6.42	113.62	122.93
1	A	335	LYS	CB-CA-C	6.41	120.43	109.65
1	A	16	VAL	N-CA-CB	-6.39	100.97	111.45
1	B	269	GLU	N-CA-CB	6.37	119.92	110.49
1	B	107	GLU	CB-CA-C	-6.33	97.76	109.29
1	C	190	TYR	CB-CA-C	6.33	117.48	108.68
1	A	403	SER	CB-CA-C	-6.32	102.88	110.15
1	C	442	TYR	O-C-N	-6.32	115.72	121.66
1	B	128	ARG	NE-CZ-NH1	-6.30	115.20	121.50
1	B	365	ASP	CB-CA-C	6.29	120.11	109.80
1	A	40	LYS	CB-CG-CD	6.27	125.72	111.30
1	B	260	ARG	NE-CZ-NH2	6.24	124.81	119.20
1	C	330	VAL	N-CA-CB	6.20	119.89	111.21
1	B	461	LYS	CB-CA-C	-6.20	99.64	109.80
1	C	618	HIS	N-CA-C	-6.16	105.05	113.30
1	A	448	THR	CA-CB-OG1	-6.15	100.38	109.60
1	C	55	GLU	CB-CA-C	-6.12	100.62	110.79
1	B	215	LEU	CA-C-O	-6.10	114.91	121.56
1	C	426	THR	CA-CB-OG1	-6.08	100.49	109.60
1	C	37	GLU	CB-CA-C	-6.05	100.40	110.68
1	B	495	MET	CG-SD-CE	-6.04	87.60	100.90
1	A	7	PRO	CB-CA-C	-6.04	103.50	111.23
1	A	39	THR	CA-C-N	6.04	128.69	120.54
1	A	39	THR	C-N-CA	6.04	128.69	120.54
1	B	416	GLU	CB-CA-C	-6.04	99.90	109.80
1	C	173	PHE	CA-CB-CG	-6.04	107.77	113.80
1	C	608	PHE	CA-CB-CG	-6.03	107.77	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	695	ASP	CA-CB-CG	6.03	118.63	112.60
1	B	652	PHE	CA-CB-CG	6.01	119.81	113.80
1	A	540	GLU	CB-CG-CD	6.00	122.81	112.60
1	A	291	ASP	CA-CB-CG	6.00	118.60	112.60
1	C	228	PHE	CA-C-N	5.99	126.15	119.32
1	C	228	PHE	C-N-CA	5.99	126.15	119.32
1	A	335	LYS	N-CA-CB	-5.96	100.38	110.51
1	B	16	VAL	N-CA-CB	-5.96	100.77	111.92
1	B	112	VAL	N-CA-C	-5.96	101.86	109.30
1	B	476	PHE	CA-CB-CG	-5.96	107.84	113.80
1	C	636	LEU	CA-C-O	-5.94	113.95	120.30
1	C	294	THR	CA-CB-OG1	-5.92	100.72	109.60
1	B	546	LYS	CB-CG-CD	5.91	124.89	111.30
1	C	121	ASP	CA-CB-CG	5.90	118.50	112.60
1	C	430	ILE	CA-C-N	-5.90	114.57	122.42
1	C	430	ILE	C-N-CA	-5.90	114.57	122.42
1	A	192	GLN	CB-CA-C	5.89	119.09	109.90
1	B	499	LEU	N-CA-CB	5.89	120.24	110.52
1	B	96	ASN	CA-CB-CG	-5.89	106.71	112.60
1	B	39	THR	N-CA-C	-5.88	104.95	111.36
1	A	89	PHE	CA-CB-CG	-5.88	107.92	113.80
1	A	461	LYS	CB-CA-C	-5.87	100.18	109.80
1	C	289	GLU	CG-CD-OE1	5.86	131.89	118.40
1	C	593	HIS	CA-CB-CG	5.86	119.66	113.80
1	A	152	THR	CA-CB-OG1	-5.84	100.84	109.60
1	C	312	ARG	CD-NE-CZ	-5.84	116.22	124.40
1	B	59	ILE	CA-CB-CG2	5.82	120.40	110.50
1	B	642	ASP	CA-CB-CG	5.79	118.39	112.60
1	C	57	CYS	CB-CA-C	-5.79	101.04	109.38
1	C	449	LYS	CB-CG-CD	5.78	124.58	111.30
1	A	499	LEU	CB-CA-C	-5.77	99.75	109.50
1	B	403	SER	CB-CA-C	-5.76	103.78	110.17
1	C	113	PHE	CA-CB-CG	-5.76	108.04	113.80
1	C	293	VAL	O-C-N	5.76	127.10	121.98
1	B	664	ARG	N-CA-CB	5.75	118.68	110.16
1	A	428	LYS	N-CA-CB	5.75	120.20	110.49
1	A	56	GLN	N-CA-CB	5.74	119.92	110.39
1	C	322	GLU	CB-CA-C	-5.74	97.91	109.68
1	B	435	TYR	CB-CA-C	5.72	120.54	110.36
1	C	364	HIS	CA-CB-CG	5.72	119.52	113.80
1	C	222	ASP	CA-CB-CG	5.69	118.29	112.60
1	A	55	GLU	CG-CD-OE2	-5.69	105.31	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	449	LYS	O-C-N	5.68	129.67	123.13
1	C	190	TYR	CA-C-O	5.68	125.47	120.19
1	B	22	HIS	CB-CA-C	5.67	119.37	110.19
1	C	298	THR	CA-CB-OG1	-5.66	101.11	109.60
1	C	341	ILE	CA-C-O	-5.66	114.59	120.64
1	C	33	ASP	CA-CB-CG	5.63	118.23	112.60
1	C	66	ARG	N-CA-CB	-5.61	101.58	110.28
1	C	286	PHE	CA-CB-CG	5.60	119.40	113.80
1	C	633	MET	CG-SD-CE	-5.58	88.62	100.90
1	A	43	VAL	N-CA-CB	-5.58	104.02	110.55
1	C	605	LYS	CB-CA-C	5.57	120.33	110.85
1	A	306	ARG	N-CA-CB	-5.57	101.14	109.71
1	B	445	LYS	CB-CA-C	-5.57	101.50	110.74
1	C	128	ARG	NE-CZ-NH1	-5.55	115.95	121.50
1	B	281	LYS	CB-CA-C	5.55	119.71	111.88
1	C	128	ARG	CA-CB-CG	-5.55	103.00	114.10
1	A	481	THR	CB-CA-C	5.53	117.45	109.09
1	C	11	ARG	CD-NE-CZ	5.53	132.15	124.40
1	C	209	LYS	N-CA-CB	-5.52	102.25	111.20
1	A	69	GLU	CB-CG-CD	5.52	121.99	112.60
1	A	418	GLU	CB-CG-CD	5.52	121.98	112.60
1	B	413	THR	N-CA-C	-5.52	106.55	113.28
1	B	693	VAL	N-CA-CB	5.52	120.76	110.77
1	C	365	ASP	CA-C-O	-5.51	115.56	121.56
1	A	409	HIS	CA-C-N	-5.51	115.01	122.77
1	A	409	HIS	C-N-CA	-5.51	115.01	122.77
1	B	14	THR	OG1-CB-CG2	5.50	120.30	109.30
1	C	92	THR	CA-CB-OG1	5.49	117.83	109.60
1	A	677	LYS	CD-CE-NZ	-5.48	94.35	111.90
1	B	92	THR	CA-CB-OG1	-5.48	101.38	109.60
1	A	107	GLU	N-CA-CB	5.47	118.41	110.47
1	C	603	ASP	CB-CA-C	-5.47	98.77	110.32
1	A	605	LYS	N-CA-CB	5.46	117.99	110.07
1	A	57	CYS	N-CA-CB	5.45	118.39	109.90
1	A	624	GLU	CB-CA-C	-5.43	99.30	110.38
1	A	289	GLU	CB-CA-C	-5.43	100.36	109.48
1	B	253	GLU	CB-CA-C	-5.42	102.82	111.17
1	C	261	LEU	N-CA-CB	5.42	119.08	110.84
1	C	65	GLU	CB-CA-C	5.42	119.48	110.81
1	B	134	GLU	CB-CA-C	5.42	119.79	110.79
1	A	34	PRO	CB-CA-C	-5.41	103.78	111.68
1	C	631	PRO	CB-CA-C	5.41	118.04	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	322	GLU	N-CA-CB	5.39	117.97	109.83
1	B	423	ARG	CA-CB-CG	-5.39	103.32	114.10
1	B	563	CYS	CB-CA-C	5.39	119.74	110.79
1	A	73	TYR	CB-CA-C	5.39	117.41	109.22
1	C	68	THR	CA-CB-OG1	-5.38	101.53	109.60
1	A	53	PHE	CA-CB-CG	-5.38	108.42	113.80
1	A	55	GLU	CA-CB-CG	-5.38	103.34	114.10
1	A	176	MET	CG-SD-CE	-5.34	89.15	100.90
1	A	619	ASN	CA-CB-CG	-5.34	107.26	112.60
1	C	74	PRO	CB-CA-C	-5.34	105.00	111.46
1	B	402	LEU	N-CA-CB	-5.33	102.82	110.65
1	B	267	GLN	CB-CA-C	-5.32	99.09	110.32
1	C	204	THR	O-C-N	-5.32	116.58	122.86
1	B	199	GLY	N-CA-C	-5.32	108.00	114.92
1	A	223	ILE	CB-CA-C	5.32	118.07	110.84
1	C	67	MET	CG-SD-CE	5.31	112.58	100.90
1	B	8	ASP	CA-CB-CG	-5.31	107.29	112.60
1	C	111	ARG	CG-CD-NE	-5.30	100.33	112.00
1	B	368	THR	CA-CB-OG1	-5.30	101.65	109.60
1	A	618	HIS	CA-CB-CG	-5.30	108.50	113.80
1	C	194	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	327	LYS	N-CA-CB	5.28	119.23	110.52
1	A	593	HIS	CB-CG-CD2	-5.28	124.34	131.20
1	B	242	ASP	CB-CA-C	-5.28	100.54	110.67
1	A	63	TYR	N-CA-CB	5.27	117.71	110.07
1	C	111	ARG	CA-C-N	5.27	127.63	120.63
1	C	111	ARG	C-N-CA	5.27	127.63	120.63
1	A	591	ILE	CA-C-N	5.25	126.74	120.13
1	A	591	ILE	C-N-CA	5.25	126.74	120.13
1	B	365	ASP	CA-CB-CG	5.24	117.84	112.60
1	C	408	TYR	CB-CA-C	-5.22	100.67	109.50
1	B	611	LEU	O-C-N	5.22	127.72	122.09
1	A	660	VAL	CA-C-N	5.21	126.65	120.14
1	A	660	VAL	C-N-CA	5.21	126.65	120.14
1	C	536	TYR	N-CA-CB	5.20	119.28	110.49
1	A	44	GLU	CB-CG-CD	5.20	121.43	112.60
1	A	440	ILE	N-CA-CB	-5.20	105.90	112.60
1	A	539	LYS	CA-CB-CG	5.20	124.49	114.10
1	B	26	ASP	CB-CA-C	5.20	119.24	111.14
1	A	292	TYR	CB-CA-C	-5.19	101.11	109.72
1	C	483	ASN	CA-CB-CG	-5.18	107.42	112.60
1	A	192	GLN	OE1-CD-NE2	-5.17	117.43	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	231	GLU	CB-CG-CD	5.17	121.39	112.60
1	C	420	ARG	N-CA-C	-5.17	102.54	110.14
1	A	157	LYS	CG-CD-CE	-5.17	99.42	111.30
1	C	396	TYR	CA-CB-CG	5.16	123.19	113.90
1	B	171	VAL	N-CA-CB	-5.16	105.10	110.72
1	C	492	VAL	N-CA-C	-5.16	105.30	110.30
1	B	261	LEU	N-CA-CB	5.15	118.67	110.84
1	C	318	PHE	CA-CB-CG	5.15	118.95	113.80
1	C	127	LEU	CB-CG-CD2	5.14	126.14	110.70
1	A	640	HIS	CB-CG-ND1	-5.13	115.00	122.70
1	A	17	GLN	CB-CA-C	-5.12	98.67	109.38
1	A	260	ARG	N-CA-CB	5.11	117.52	110.17
1	B	705	ASN	CA-CB-CG	-5.11	107.49	112.60
1	B	111	ARG	CB-CA-C	5.09	119.36	109.33
1	C	8	ASP	N-CA-CB	5.09	117.47	109.69
1	C	508	GLY	CA-C-N	5.08	127.80	120.38
1	C	508	GLY	C-N-CA	5.08	127.80	120.38
1	C	75	LYS	CB-CA-C	5.07	119.00	109.71
1	B	606	GLN	N-CA-C	-5.07	105.75	111.28
1	A	173	PHE	CA-CB-CG	-5.07	108.73	113.80
1	B	499	LEU	CB-CA-C	-5.06	100.98	109.48
1	A	66	ARG	N-CA-CB	-5.05	102.68	110.16
1	B	610	TRP	CB-CA-C	-5.05	102.95	110.88
1	A	66	ARG	NE-CZ-NH2	-5.05	114.66	119.20
1	C	598	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	449	LYS	CA-C-N	5.04	127.68	123.04
1	A	449	LYS	C-N-CA	5.04	127.68	123.04
1	A	695	ASP	CA-CB-CG	5.03	117.63	112.60
1	C	256	ASP	CA-CB-CG	5.02	117.62	112.60
1	C	69	GLU	CB-CG-CD	5.01	121.12	112.60
1	C	427	VAL	N-CA-CB	-5.01	106.10	111.46
1	C	94	LEU	CA-C-N	-5.01	113.19	120.75
1	C	94	LEU	C-N-CA	-5.01	113.19	120.75
1	A	648	HIS	CA-CB-CG	5.00	118.80	113.80
1	B	11	ARG	CB-CA-C	5.00	118.78	110.78

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	ARG	Sidechain
1	A	306	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	319	ARG	Sidechain
1	A	423	ARG	Sidechain
1	A	493	ARG	Sidechain
1	A	66	ARG	Sidechain
1	A	85	ARG	Sidechain
1	B	170[A]	ARG	Sidechain
1	B	170[B]	ARG	Sidechain
1	B	252	ARG	Sidechain
1	B	302	PHE	Peptide
1	B	319	ARG	Sidechain
1	B	405	GLY	Peptide
1	B	423	ARG	Sidechain
1	B	428	LYS	Peptide
1	C	111	ARG	Sidechain
1	C	156	MET	Peptide
1	C	252	ARG	Sidechain
1	C	260	ARG	Sidechain
1	C	306	ARG	Sidechain
1	C	420	ARG	Sidechain
1	C	423	ARG	Sidechain
1	C	493	ARG	Sidechain
1	C	547	ARG	Sidechain
1	C	60	ARG	Sidechain
1	C	664	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	5673	0	5490	88	0
1	B	5686	0	5507	88	0
1	C	5681	0	5503	121	0
2	A	21	0	0	0	0
2	B	21	0	0	0	0
2	C	21	0	0	0	0
3	A	18	0	23	0	0
3	B	42	0	55	4	0
3	C	18	0	23	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	3	0	0	0	0
4	B	6	0	0	0	0
5	A	14	0	20	2	0
5	B	14	0	20	0	0
6	B	19	0	26	2	0
7	A	452	0	0	23	0
7	B	560	0	0	29	0
7	C	361	0	0	25	0
All	All	18610	0	16667	298	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 9.

All (298) 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:B:709:ILE:CD1	7:B:1332:HOH:O	1.84	1.20
1:B:709:ILE:HG13	7:B:1332:HOH:O	1.45	1.15
1:B:252:ARG:HD2	7:B:1265:HOH:O	1.45	1.13
1:C:664:ARG:CZ	7:C:901:HOH:O	1.97	1.12
1:C:664:ARG:NE	7:C:901:HOH:O	1.81	1.11
1:C:17:GLN:HB3	7:C:1180:HOH:O	1.47	1.10
1:B:22:HIS:CD2	7:B:901:HOH:O	2.03	1.09
1:C:664:ARG:NH2	7:C:901:HOH:O	1.82	1.09
1:B:22:HIS:CE1	7:B:901:HOH:O	2.03	1.08
1:B:22:HIS:NE2	7:B:901:HOH:O	1.89	1.03
1:C:252:ARG:HD2	7:C:1062:HOH:O	1.57	1.03
1:A:252:ARG:HD2	7:A:1157:HOH:O	1.57	1.03
1:C:57:CYS:HB2	7:C:1166:HOH:O	1.63	0.98
1:C:273:ILE:O	7:C:902:HOH:O	1.83	0.94
1:A:445:LYS:HD3	7:A:1274:HOH:O	1.68	0.92
1:B:22:HIS:CG	7:B:901:HOH:O	2.20	0.91
1:A:345:ARG:HD2	1:A:345:ARG:O	1.70	0.89
1:B:345:ARG:HD2	1:B:345:ARG:O	1.75	0.86
1:C:533:ALA:O	1:C:536:TYR:O	1.94	0.86
1:A:261:LEU:HD23	1:A:282:LEU:HD23	1.57	0.85
1:C:547:ARG:NH1	1:C:547:ARG:HG2	1.92	0.82
1:B:218:ASP:HB3	7:B:902:HOH:O	1.81	0.81
1:A:345:ARG:O	1:A:345:ARG:CD	2.28	0.80
1:B:427:VAL:O	1:B:428:LYS:O	1.99	0.80
1:B:709:ILE:CG1	7:B:1332:HOH:O	1.93	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ILE:HD11	7:A:1316:HOH:O	1.85	0.76
1:A:663:SER:O	7:A:901:HOH:O	2.03	0.76
1:A:76:TYR:CD2	1:A:423:ARG:HD3	2.22	0.75
1:A:445:LYS:HB2	7:A:1274:HOH:O	1.86	0.73
1:C:399:THR:HG23	1:C:483:ASN:HA	1.69	0.73
1:C:547:ARG:HG2	1:C:547:ARG:HH11	1.53	0.73
1:A:388:GLN:HG3	7:A:1276:HOH:O	1.88	0.72
1:A:339:GLU:HG3	1:A:354:LEU:HD22	1.73	0.70
1:C:334:GLU:HB2	7:C:1011:HOH:O	1.92	0.70
1:B:38:GLN:N	1:B:38:GLN:OE1	2.25	0.69
1:B:427:VAL:C	1:B:428:LYS:O	2.35	0.69
1:A:20:HIS:N	7:A:905:HOH:O	2.24	0.69
1:A:625:ALA:HB1	1:A:627:ASP:OD1	1.92	0.68
1:B:70:LEU:HD22	1:B:429:GLY:HA3	1.76	0.68
1:C:513:THR:OG1	7:C:903:HOH:O	2.11	0.68
1:C:404:PRO:HD3	1:C:427:VAL:HG22	1.76	0.68
1:A:103:GLN:HB2	7:A:956:HOH:O	1.95	0.66
1:A:622:LEU:HD21	1:A:663:SER:CB	2.25	0.66
1:A:120:SER:O	7:A:902:HOH:O	2.13	0.65
1:C:524:GLN:OE1	7:C:904:HOH:O	2.13	0.65
1:A:20:HIS:CG	7:A:905:HOH:O	2.50	0.65
1:B:571:PHE:O	1:B:631:PRO:HB3	1.98	0.64
1:C:159:ASP:HB3	7:C:965:HOH:O	1.97	0.64
1:B:59:ILE:HD12	7:B:1049:HOH:O	1.98	0.63
1:C:71:TYR:O	1:C:75:LYS:NZ	2.31	0.62
1:A:111:ARG:NH1	1:A:111:ARG:HG2	2.13	0.62
1:C:571:PHE:O	1:C:631:PRO:HB3	1.99	0.62
1:B:22:HIS:ND1	7:B:901:HOH:O	2.20	0.62
1:B:427:VAL:O	1:B:428:LYS:C	2.41	0.62
1:A:111:ARG:HG2	1:A:111:ARG:HH11	1.66	0.61
1:B:546:LYS:HG2	7:B:1188:HOH:O	1.99	0.61
1:A:53:PHE:O	1:A:702:ARG:NH1	2.34	0.61
1:A:170:ARG:HD3	1:A:192:GLN:HE21	1.66	0.60
1:B:345:ARG:O	1:B:345:ARG:CD	2.49	0.60
1:B:251:ILE:HB	1:B:260:ARG:HB2	1.83	0.60
1:C:323:GLU:HG3	1:C:326:TRP:CE3	2.36	0.60
1:C:591:ILE:HG12	3:C:802:GOL:H31	1.83	0.60
1:A:251:ILE:HB	1:A:260:ARG:HB2	1.83	0.59
1:A:512:GLU:OE1	1:A:516:LYS:HE3	2.01	0.59
1:C:251:ILE:HB	1:C:260:ARG:HB2	1.84	0.59
1:C:401:PHE:HE2	1:C:453:PHE:CD2	2.19	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:GLY:O	1:C:161:ALA:HB3	2.03	0.58
1:C:411:ASP:OD1	1:C:413:THR:OG1	2.20	0.58
1:C:625:ALA:HB3	1:C:628:ILE:HD12	1.85	0.58
1:C:534:ALA:O	1:C:537:LEU:HB2	2.03	0.58
1:A:36:SER:O	1:A:40:LYS:HG3	2.03	0.58
1:C:322:GLU:HG3	7:C:971:HOH:O	2.03	0.58
1:B:583:MET:HB2	1:B:615:SER:HB2	1.85	0.58
1:A:172:LYS:HD3	1:A:173:PHE:CE2	2.39	0.58
1:B:23:LYS:HE2	7:B:1277:HOH:O	2.04	0.58
1:C:466:HIS:HB2	1:C:498:ILE:HD12	1.86	0.57
1:C:499:LEU:HD23	1:C:499:LEU:N	2.20	0.57
1:A:512:GLU:O	1:A:516:LYS:HG3	2.05	0.56
1:C:323:GLU:HG3	1:C:326:TRP:CZ3	2.40	0.56
1:A:622:LEU:HD21	1:A:663:SER:OG	2.04	0.56
1:C:275:GLY:O	1:C:276:ILE:C	2.47	0.56
1:B:311:TYR:OH	7:B:903:HOH:O	2.18	0.56
1:C:441:PHE:HB3	1:C:449:LYS:HB3	1.87	0.56
1:A:355:HIS:HB2	1:A:360:ILE:HD12	1.88	0.56
1:B:38:GLN:H	1:B:38:GLN:CD	2.14	0.56
1:B:460:ILE:CD1	1:B:498:ILE:HD11	2.36	0.55
5:A:806[B]:PEG:H42	7:A:1215:HOH:O	2.07	0.55
1:C:430:ILE:HG23	1:C:435:TYR:CE2	2.41	0.55
1:A:431:ASP:C	1:A:431:ASP:OD1	2.50	0.55
1:C:62:LEU:HD13	1:C:708:TRP:CD1	2.42	0.55
1:C:17:GLN:CG	7:C:1232:HOH:O	2.55	0.54
1:A:56:GLN:HE21	1:C:626:ASP:HB2	1.72	0.54
1:A:90:TYR:HB3	1:A:101:TYR:CE1	2.42	0.54
1:A:473:TYR:CE2	1:A:478:ILE:HD12	2.43	0.54
1:C:398:PHE:O	1:C:405:GLY:HA2	2.08	0.54
1:B:709:ILE:HD11	7:B:1332:HOH:O	1.76	0.54
1:C:390:LYS:HG2	7:C:1115:HOH:O	2.08	0.54
1:B:71:TYR:CZ	1:B:75:LYS:HE2	2.43	0.53
1:A:20:HIS:CE1	1:A:605:LYS:HA	2.44	0.53
1:A:86:TYR:OH	1:A:393:GLU:OE1	2.25	0.53
1:B:320:ASP:OD1	7:B:904:HOH:O	2.18	0.53
1:C:57:CYS:HB3	1:C:698:ALA:HB1	1.91	0.53
1:A:562:ALA:O	1:A:566:GLN:HG3	2.09	0.53
3:B:807:GOL:H11	7:B:1266:HOH:O	2.09	0.53
1:B:103:GLN:NE2	1:B:108:GLY:O	2.42	0.52
1:A:635:LEU:HB2	1:A:672:ILE:HG13	1.91	0.52
1:C:87:PHE:CE1	1:C:102:VAL:HG23	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:PHE:O	1:A:533:ALA:HB3	2.09	0.52
1:C:245:ARG:HD3	1:C:246:TYR:CE1	2.45	0.52
1:A:51:VAL:HB	1:A:52:PRO:HD3	1.90	0.52
1:A:76:TYR:CG	1:A:423:ARG:HD3	2.44	0.52
1:A:157:LYS:HE3	7:A:1076:HOH:O	2.09	0.52
1:C:355:HIS:N	1:C:358:LYS:O	2.33	0.52
1:C:536:TYR:O	1:C:537:LEU:CB	2.57	0.52
1:C:57:CYS:SG	1:C:58:PRO:HD2	2.50	0.51
1:C:664:ARG:HG3	1:C:664:ARG:HH11	1.75	0.51
1:A:4:LEU:HD23	1:A:5:GLN:N	2.25	0.51
1:A:223:ILE:HD13	7:A:903:HOH:O	2.10	0.51
1:C:466:HIS:CB	1:C:498:ILE:HD12	2.39	0.51
1:B:70:LEU:CD2	1:B:429:GLY:HA3	2.39	0.51
1:B:427:VAL:O	1:B:427:VAL:HG12	2.10	0.51
1:A:571:PHE:O	1:A:631:PRO:HB3	2.10	0.51
1:B:22:HIS:CE1	6:B:806:B3P:H112	2.45	0.51
1:C:339:GLU:OE1	1:C:354:LEU:HD13	2.11	0.51
1:C:166:ASP:OD2	1:C:215:LEU:HD12	2.11	0.50
1:B:170[A]:ARG:HG2	1:B:170[A]:ARG:HH11	1.76	0.50
1:C:660:VAL:O	1:C:663:SER:HB3	2.12	0.50
1:B:335:LYS:NZ	7:B:919:HOH:O	2.39	0.50
1:A:22:HIS:NE2	7:A:906:HOH:O	2.28	0.50
1:C:516:LYS:O	7:C:906:HOH:O	2.20	0.49
1:C:547:ARG:HH11	1:C:547:ARG:CG	2.22	0.49
1:A:640:HIS:NE2	7:A:914:HOH:O	2.34	0.49
1:B:268:GLN:HG3	7:B:1036:HOH:O	2.13	0.49
1:A:449:LYS:HB2	5:A:806[A]:PEG:H11	1.94	0.49
1:C:493:ARG:O	1:C:493:ARG:HG3	2.11	0.49
1:B:181:ASP:OD1	1:B:183:LYS:HB2	2.12	0.49
1:C:444:SER:HB3	7:C:923:HOH:O	2.11	0.49
1:C:504:ILE:HD12	1:C:526:CYS:HB3	1.95	0.49
1:C:252:ARG:NH1	1:C:289:GLU:OE1	2.46	0.49
1:C:320:ASP:OD1	1:C:325:LYS:HG3	2.12	0.49
1:B:358:LYS:NZ	7:B:936:HOH:O	2.46	0.48
1:C:468:ALA:HB3	1:C:548:LEU:HD13	1.94	0.48
1:B:709:ILE:HD12	7:B:1332:HOH:O	1.79	0.48
1:C:306:ARG:O	1:C:308:SER:OG	2.32	0.47
1:B:256:ASP:HB2	7:B:1174:HOH:O	2.13	0.47
1:B:172:LYS:HD3	1:B:173:PHE:CE2	2.49	0.47
1:C:17:GLN:HG3	7:C:1232:HOH:O	2.15	0.47
1:B:107:GLU:OE2	1:B:107:GLU:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170[A]:ARG:HD2	1:B:192:GLN:CD	2.40	0.47
1:B:400:SER:OG	1:B:403:SER:HB2	2.15	0.47
1:B:429:GLY:O	1:B:430:ILE:C	2.56	0.47
1:B:228:PHE:N	1:B:229:PRO:HD3	2.30	0.47
1:C:165:PRO:O	1:C:167:VAL:HG23	2.15	0.47
1:C:378:ASP:O	1:C:398:PHE:CE2	2.68	0.47
1:C:632:SER:OG	1:C:668:ASN:HB3	2.14	0.47
1:A:365:ASP:OD2	1:A:367:THR:HB	2.15	0.47
1:A:536:TYR:CZ	1:A:540:GLU:HG3	2.49	0.46
1:C:13:GLU:OE2	1:C:13:GLU:HA	2.16	0.46
1:C:73:TYR:O	1:C:93:GLY:HA2	2.16	0.46
1:C:166:ASP:OD1	1:C:166:ASP:N	2.46	0.46
1:A:223:ILE:CD1	7:A:1316:HOH:O	2.51	0.46
1:C:707:ASP:OD1	1:C:707:ASP:N	2.48	0.46
1:B:115:ASP:O	1:B:118:ILE:HG12	2.15	0.46
1:C:242:ASP:OD2	1:C:294:THR:OG1	2.30	0.46
1:B:446:ASP:OD1	1:B:446:ASP:C	2.59	0.46
1:B:227:GLU:C	1:B:229:PRO:HD3	2.41	0.46
1:B:188:ASN:HA	1:B:209:LYS:O	2.15	0.46
1:C:451:PRO:HB2	1:C:503:ASN:HB2	1.98	0.46
1:C:488[B]:ARG:HB3	1:C:499:LEU:HD11	1.98	0.46
1:C:442:TYR:CZ	1:C:533:ALA:HB2	2.50	0.45
1:A:57:CYS:HB2	7:A:1196:HOH:O	2.17	0.45
1:A:289:GLU:O	1:A:304:THR:HA	2.15	0.45
1:A:544:SER:O	1:A:545:PRO:C	2.58	0.45
1:C:159:ASP:CB	7:C:965:HOH:O	2.62	0.45
1:B:28:TYR:HB3	1:B:31:LEU:HD12	1.98	0.45
1:B:154:LYS:HE3	7:B:1382:HOH:O	2.16	0.45
1:C:283:ILE:HG21	1:C:290:TYR:CE2	2.51	0.45
1:A:442:TYR:CZ	1:A:450:ILE:HB	2.52	0.45
1:A:8:ASP:HA	7:A:1003:HOH:O	2.16	0.45
1:C:127:LEU:HD12	1:C:127:LEU:HA	1.55	0.45
1:C:326:TRP:HB2	7:C:911:HOH:O	2.16	0.45
1:A:625:ALA:O	1:A:665:LYS:NZ	2.50	0.45
1:A:415:GLU:HB3	7:A:1131:HOH:O	2.16	0.44
1:B:272:GLY:O	1:B:274:ALA:N	2.50	0.44
1:A:115:ASP:C	1:A:115:ASP:OD1	2.58	0.44
1:C:22:HIS:ND1	7:C:909:HOH:O	2.36	0.44
1:A:341:ILE:HA	1:A:350:VAL:O	2.16	0.44
1:A:420:ARG:HG2	1:A:420:ARG:HH11	1.83	0.44
1:C:536:TYR:CD1	1:C:536:TYR:C	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:GLU:HB3	7:B:1198:HOH:O	2.18	0.44
1:C:262:TRP:CE2	1:C:281:LYS:HG2	2.51	0.44
1:C:316:ILE:HG12	1:C:326:TRP:CD1	2.53	0.44
1:C:672:ILE:HG12	1:C:673:HIS:N	2.32	0.44
1:C:294:THR:OG1	1:C:295:ASN:N	2.49	0.44
1:C:470:LEU:HD23	1:C:550:ILE:HG22	1.98	0.44
1:A:293:VAL:HB	1:A:301:THR:O	2.18	0.44
1:A:547:ARG:NH1	1:A:547:ARG:HG2	2.33	0.44
1:B:145:ALA:O	1:B:146:SER:HB2	2.18	0.44
1:B:471:TYR:OH	3:B:809:GOL:C3	2.65	0.44
1:A:364:HIS:ND1	1:A:369:GLY:O	2.51	0.43
1:A:75:LYS:NZ	1:A:93:GLY:O	2.51	0.43
1:A:272:GLY:HA2	7:A:1169:HOH:O	2.17	0.43
1:B:606:GLN:OE1	7:B:905:HOH:O	2.21	0.43
1:C:591:ILE:CG1	3:C:802:GOL:H31	2.48	0.43
1:A:395:PHE:HA	1:A:408:TYR:O	2.19	0.43
1:C:25:CYS:HB3	7:C:1146:HOH:O	2.18	0.43
1:C:173:PHE:CE2	1:C:591:ILE:HG12	2.54	0.43
1:A:622:LEU:HD21	1:A:663:SER:HB3	1.99	0.43
1:A:53:PHE:CD1	1:A:53:PHE:C	2.97	0.43
1:A:458:LYS:HA	7:A:987:HOH:O	2.19	0.43
1:C:223:ILE:CD1	7:C:1069:HOH:O	2.66	0.43
1:B:38:GLN:N	1:B:38:GLN:CD	2.76	0.43
1:B:356:ASP:C	1:B:357:VAL:HG23	2.44	0.43
1:C:268:GLN:OE1	1:C:268:GLN:HA	2.18	0.43
1:C:401:PHE:CE2	1:C:453:PHE:CD2	3.04	0.43
1:C:51:VAL:N	1:C:52:PRO:HD2	2.34	0.43
1:C:73:TYR:HB2	1:C:74:PRO:HD2	2.01	0.43
1:C:485:SER:OG	1:C:488[A]:ARG:HD3	2.19	0.43
1:B:212:TYR:CD2	1:B:273:ILE:HG21	2.54	0.43
1:A:553:GLY:HA2	1:A:577:GLN:O	2.19	0.42
1:B:466:HIS:C	1:B:547:ARG:HD3	2.44	0.42
1:B:483:ASN:N	1:B:483:ASN:ND2	2.66	0.42
1:C:466:HIS:HB2	1:C:542:TYR:O	2.19	0.42
1:A:399:THR:HG21	7:A:1216:HOH:O	2.18	0.42
1:C:555:ASN:O	1:C:558:LEU:HB3	2.19	0.42
1:A:446:ASP:OD1	1:A:446:ASP:C	2.63	0.42
1:A:325:LYS:HA	1:A:325:LYS:HD3	1.64	0.42
1:B:179:THR:OG1	1:B:212:TYR:OH	2.32	0.42
1:C:488[A]:ARG:HB3	1:C:499:LEU:CD1	2.49	0.42
1:C:427:VAL:HG13	1:C:484:TYR:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:444:SER:CB	7:C:923:HOH:O	2.68	0.42
1:C:536:TYR:O	1:C:537:LEU:HB2	2.19	0.42
1:C:632:SER:OG	1:C:669:PRO:HD2	2.19	0.42
1:A:16:VAL:HA	1:A:24:ILE:O	2.20	0.42
1:B:607:HIS:CD2	1:B:610:TRP:CH2	3.08	0.42
1:C:312:ARG:HB2	1:C:330:VAL:O	2.20	0.42
1:C:488[A]:ARG:HB3	1:C:499:LEU:HD11	2.00	0.42
1:A:39:THR:O	1:A:42:PHE:HB3	2.19	0.42
1:B:629:GLN:O	3:B:805:GOL:H31	2.19	0.42
1:C:93:GLY:O	1:C:94:LEU:HD23	2.20	0.42
1:B:365:ASP:HB2	1:B:372:LEU:HD11	2.01	0.42
1:B:653:ILE:HD12	1:B:653:ILE:HA	1.92	0.42
1:C:17:GLN:CB	7:C:1232:HOH:O	2.68	0.42
1:C:38:GLN:HG2	7:C:1200:HOH:O	2.19	0.42
1:C:430:ILE:HD13	1:C:489:LEU:HD13	2.01	0.42
1:A:554:SER:HA	1:A:578:VAL:O	2.20	0.42
1:C:213:HIS:HE1	1:C:217:THR:O	2.03	0.42
1:C:365:ASP:HB2	1:C:372:LEU:HD11	2.01	0.42
1:B:647:LEU:C	1:B:647:LEU:HD12	2.45	0.41
1:C:12:ASP:OD1	1:C:12:ASP:C	2.61	0.41
1:A:583:MET:HB3	1:A:611:LEU:HD22	2.01	0.41
1:B:356:ASP:O	1:B:358:LYS:HE3	2.20	0.41
1:C:61:GLY:O	1:C:65:GLU:HB3	2.20	0.41
1:A:268:GLN:HB2	7:A:1010:HOH:O	2.19	0.41
1:B:268:GLN:CG	7:B:1036:HOH:O	2.68	0.41
1:B:473:TYR:CE1	1:B:555:ASN:HB3	2.56	0.41
1:B:583:MET:HB2	1:B:615:SER:CB	2.50	0.41
1:B:379:VAL:HG12	7:B:1407:HOH:O	2.20	0.41
1:C:355:HIS:O	1:C:356:ASP:C	2.63	0.41
1:C:483:ASN:N	1:C:483:ASN:HD22	2.17	0.41
1:B:415:GLU:CB	7:B:1198:HOH:O	2.68	0.41
1:A:323:GLU:HA	1:A:326:TRP:CE2	2.56	0.41
1:A:535:GLU:O	1:A:539:LYS:HB3	2.21	0.41
1:C:295:ASN:HB3	1:C:300:PHE:CD2	2.55	0.41
1:A:196:LYS:HE3	1:A:200:THR:OG1	2.20	0.41
1:A:355:HIS:O	1:A:356:ASP:C	2.63	0.41
1:B:22:HIS:CD2	1:B:22:HIS:C	2.98	0.41
1:B:213:HIS:HD1	1:B:222:ASP:CG	2.28	0.41
1:B:491:PHE:CE2	1:B:497:GLY:HA3	2.56	0.41
1:A:71:TYR:CZ	1:A:75:LYS:HE2	2.56	0.41
1:B:5:GLN:NE2	1:B:5:GLN:HA	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:LYS:HB2	1:B:428:LYS:HE3	1.86	0.41
1:B:591:ILE:HG12	3:B:802:GOL:H11	2.03	0.41
1:B:662:ARG:NH2	7:B:976:HOH:O	2.54	0.41
1:C:109:GLU:CG	1:C:110:ALA:N	2.84	0.41
1:C:468:ALA:HB3	1:C:548:LEU:CD1	2.50	0.41
1:C:677:LYS:HB3	1:C:677:LYS:HE2	1.74	0.41
1:A:261:LEU:HD21	1:A:302:PHE:CZ	2.56	0.41
1:A:450:ILE:HA	1:A:451:PRO:HD3	1.92	0.41
1:A:493:ARG:O	1:A:493:ARG:NH1	2.49	0.41
1:B:102:VAL:HG22	1:B:103:GLN:N	2.36	0.41
1:B:172:LYS:CD	1:B:173:PHE:CE2	3.04	0.41
1:B:607:HIS:CD2	1:B:610:TRP:CZ3	3.09	0.41
1:B:436:GLN:NE2	1:B:456:HIS:CE1	2.89	0.40
1:B:441:PHE:HA	1:B:450:ILE:O	2.21	0.40
1:C:246:TYR:HA	1:C:264:CYS:O	2.20	0.40
1:C:659:ILE:O	1:C:659:ILE:HG22	2.21	0.40
1:B:22:HIS:HE1	6:B:806:B3P:H112	1.85	0.40
1:B:323:GLU:HA	1:B:326:TRP:CE2	2.56	0.40
1:C:66:ARG:HD2	1:C:66:ARG:HA	1.90	0.40
1:A:357:VAL:HG12	1:A:357:VAL:O	2.21	0.40
1:A:358:LYS:HD3	1:A:379:VAL:HG13	2.03	0.40
1:C:106:LEU:HA	1:C:106:LEU:HD23	1.79	0.40
1:C:156:MET:HA	1:C:162:LYS:O	2.22	0.40
1:C:547:ARG:HA	1:C:704:LEU:HD13	2.03	0.40
1:A:586:PHE:CD1	1:A:586:PHE:C	2.99	0.40
1:C:89:PHE:HA	1:C:99:VAL:O	2.21	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	705/711 (99%)	673 (96%)	29 (4%)	3 (0%)	30	22
1	B	707/711 (99%)	682 (96%)	20 (3%)	5 (1%)	18	9
1	C	706/711 (99%)	665 (94%)	37 (5%)	4 (1%)	21	11
All	All	2118/2133 (99%)	2020 (95%)	86 (4%)	12 (1%)	21	11

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	405	GLY
1	B	428	LYS
1	C	537	LEU
1	A	357	VAL
1	B	554	SER
1	A	378	ASP
1	A	554	SER
1	B	357	VAL
1	B	590	THR
1	C	357	VAL
1	C	389	LYS
1	C	108	GLY

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	614/617 (100%)	584 (95%)	30 (5%)	22	9
1	B	616/617 (100%)	591 (96%)	25 (4%)	27	14
1	C	615/617 (100%)	585 (95%)	30 (5%)	22	9
All	All	1845/1851 (100%)	1760 (95%)	85 (5%)	24	10

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU

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Mol	Chain	Res	Type
1	A	5	GLN
1	A	56	GLN
1	A	59	ILE
1	A	65	GLU
1	A	66	ARG
1	A	111	ARG
1	A	192	GLN
1	A	203	SER
1	A	218	ASP
1	A	233	LYS
1	A	283	ILE
1	A	303	LYS
1	A	322	GLU
1	A	325	LYS
1	A	335	LYS
1	A	345	ARG
1	A	354	LEU
1	A	357	VAL
1	A	420	ARG
1	A	425	VAL
1	A	428	LYS
1	A	457	LYS
1	A	539	LYS
1	A	544	SER
1	A	545	PRO
1	A	547	ARG
1	A	604	SER
1	A	624	GLU
1	A	705	ASN
1	B	8	ASP
1	B	16	VAL
1	B	44	GLU
1	B	49	ILE
1	B	58	PRO
1	B	59	ILE
1	B	65	GLU
1	B	66	ARG
1	B	261	LEU
1	B	271	SER
1	B	345	ARG
1	B	357	VAL
1	B	415	GLU

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Mol	Chain	Res	Type
1	B	416	GLU
1	B	425	VAL
1	B	430	ILE
1	B	445	LYS
1	B	461	LYS
1	B	482	PRO
1	B	512	GLU
1	B	539	LYS
1	B	544	SER
1	B	604	SER
1	B	622	LEU
1	B	677	LYS
1	C	5	GLN
1	C	59	ILE
1	C	65	GLU
1	C	75	LYS
1	C	85	ARG
1	C	118	ILE
1	C	120	SER
1	C	162	LYS
1	C	166	ASP
1	C	308	SER
1	C	367	THR
1	C	399	THR
1	C	418	GLU
1	C	420	ARG
1	C	423	ARG
1	C	426	THR
1	C	438	VAL
1	C	449	LYS
1	C	461	LYS
1	C	483	ASN
1	C	512	GLU
1	C	536	TYR
1	C	539	LYS
1	C	544	SER
1	C	547	ARG
1	C	604	SER
1	C	612	VAL
1	C	616	PRO
1	C	664	ARG
1	C	707	ASP

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

Mol	Chain	Res	Type
1	A	5	GLN
1	A	192	GLN
1	A	193	GLN
1	A	524	GLN
1	A	531	GLN
1	A	551	ASN
1	A	555	ASN
1	A	566	GLN
1	A	619	ASN
1	B	5	GLN
1	B	17	GLN
1	B	22	HIS
1	B	362	GLN
1	B	388	GLN
1	B	436	GLN
1	B	477	ASN
1	B	483	ASN
1	B	503	ASN
1	B	551	ASN
1	B	577	GLN
1	C	483	ASN
1	C	524	GLN
1	C	531	GLN
1	C	566	GLN
1	C	606	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

24 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
4	SCN	B	808	-	1,2,2	1.06	0	0,1,1	-	-
3	GOL	B	803	-	5,5,5	0.36	0	5,5,5	0.75	0
3	GOL	B	807	-	5,5,5	0.16	0	5,5,5	0.36	0
5	PEG	A	806[A]	-	6,6,6	0.63	0	5,5,5	0.58	0
3	GOL	B	809	-	5,5,5	0.20	0	5,5,5	0.38	0
5	PEG	B	810	-	6,6,6	0.41	0	5,5,5	0.30	0
2	A1CQV	B	801	1	23,23,24	0.87	1 (4%)	29,32,34	1.06	3 (10%)
3	GOL	C	802	-	5,5,5	1.12	1 (20%)	5,5,5	1.24	0
2	A1CQV	A	801	1	23,23,24	0.89	1 (4%)	29,32,34	1.06	3 (10%)
3	GOL	A	803	-	5,5,5	0.20	0	5,5,5	0.56	0
2	A1CQV	C	801	1	23,23,24	0.84	1 (4%)	29,32,34	1.05	3 (10%)
3	GOL	B	805	-	5,5,5	0.19	0	5,5,5	0.70	0
4	SCN	A	805	-	1,2,2	1.14	0	0,1,1	-	-
3	GOL	A	802	-	5,5,5	0.37	0	5,5,5	0.86	0
3	GOL	B	802	-	5,5,5	1.39	2 (40%)	5,5,5	1.35	1 (20%)
3	GOL	B	811	-	5,5,5	0.32	0	5,5,5	0.85	0
5	PEG	B	813	-	6,6,6	1.19	1 (16%)	5,5,5	0.96	0
3	GOL	B	804	-	5,5,5	0.23	0	5,5,5	0.58	0
4	SCN	B	812	-	1,2,2	0.45	0	0,1,1	-	-
3	GOL	C	803	-	5,5,5	0.46	0	5,5,5	0.72	0
3	GOL	C	804	-	5,5,5	0.21	0	5,5,5	0.66	0
6	B3P	B	806	-	18,18,18	0.74	0	23,23,23	1.54	4 (17%)
5	PEG	A	806[B]	-	6,6,6	0.40	0	5,5,5	0.37	0
3	GOL	A	804	-	5,5,5	1.37	1 (20%)	5,5,5	2.20	2 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	803	-	-	4/4/4/4	-
3	GOL	B	807	-	-	4/4/4/4	-
5	PEG	A	806[A]	-	-	1/4/4/4	-
3	GOL	B	809	-	-	2/4/4/4	-
5	PEG	B	810	-	-	3/4/4/4	-
2	A1CQV	B	801	1	-	4/9/9/9	0/3/3/3
3	GOL	C	802	-	-	2/4/4/4	-
2	A1CQV	A	801	1	-	4/9/9/9	0/3/3/3
3	GOL	A	803	-	-	1/4/4/4	-
2	A1CQV	C	801	1	-	3/9/9/9	0/3/3/3
3	GOL	B	805	-	-	2/4/4/4	-
3	GOL	A	802	-	-	2/4/4/4	-
3	GOL	B	802	-	-	3/4/4/4	-
3	GOL	B	811	-	-	0/4/4/4	-
5	PEG	B	813	-	-	2/4/4/4	-
3	GOL	B	804	-	-	3/4/4/4	-
3	GOL	C	803	-	-	2/4/4/4	-
3	GOL	C	804	-	-	2/4/4/4	-
6	B3P	B	806	-	-	7/28/28/28	-
5	PEG	A	806[B]	-	-	3/4/4/4	-
3	GOL	A	804	-	-	0/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	A1CQV	C2-N1	3.24	1.35	1.32
2	B	801	A1CQV	C2-N1	3.08	1.35	1.32
2	C	801	A1CQV	C2-N1	2.94	1.35	1.32
3	A	804	GOL	C3-C2	-2.46	1.42	1.51
3	B	802	GOL	C3-C2	-2.33	1.42	1.51
3	C	802	GOL	O2-C2	-2.25	1.36	1.43
5	B	813	PEG	O4-C4	2.22	1.53	1.42
3	B	802	GOL	O3-C3	-2.03	1.33	1.42

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	806	B3P	C11-C8-C9	4.78	120.50	110.02
3	A	804	GOL	O3-C3-C2	-3.73	93.59	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	A1CQV	C4-C15-C2	-3.07	104.16	105.15
2	A	801	A1CQV	C4-C15-C2	-2.84	104.23	105.15
6	B	806	B3P	O1-C9-C8	-2.79	106.01	111.68
2	C	801	A1CQV	C4-C15-C2	-2.72	104.27	105.15
6	B	806	B3P	C11-C8-C10	-2.51	104.51	110.02
6	B	806	B3P	C10-C8-C9	-2.39	104.78	110.02
2	A	801	A1CQV	C15-C2-N1	-2.32	109.85	110.76
2	C	801	A1CQV	C15-C2-N1	-2.29	109.86	110.76
2	C	801	A1CQV	C15-C14-C6	-2.25	116.99	120.70
3	A	804	GOL	O2-C2-C3	-2.21	100.02	109.18
2	A	801	A1CQV	C15-C14-C6	-2.19	117.08	120.70
2	B	801	A1CQV	C15-C2-N1	-2.19	109.90	110.76
2	B	801	A1CQV	C15-C14-C6	-2.17	117.12	120.70
3	B	802	GOL	O2-C2-C1	2.14	118.03	109.18

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	803	GOL	O1-C1-C2-C3
3	B	803	GOL	O2-C2-C3-O3
3	B	804	GOL	O1-C1-C2-C3
3	B	805	GOL	C1-C2-C3-O3
3	B	807	GOL	O1-C1-C2-C3
3	B	809	GOL	C1-C2-C3-O3
3	C	802	GOL	O1-C1-C2-C3
3	C	803	GOL	O1-C1-C2-O2
3	C	803	GOL	O1-C1-C2-C3
3	C	804	GOL	O1-C1-C2-C3
6	B	806	B3P	O3-C11-C8-C10
6	B	806	B3P	O3-C11-C8-C9
5	A	806[A]	PEG	O2-C3-C4-O4
5	B	810	PEG	O1-C1-C2-O2
3	A	802	GOL	O1-C1-C2-C3
3	B	802	GOL	O1-C1-C2-C3
3	B	803	GOL	C1-C2-C3-O3
3	B	807	GOL	C1-C2-C3-O3
3	A	802	GOL	O1-C1-C2-O2
3	B	802	GOL	O1-C1-C2-O2
3	B	803	GOL	O1-C1-C2-O2
3	B	804	GOL	O1-C1-C2-O2
3	B	805	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	B	807	GOL	O1-C1-C2-O2
3	B	807	GOL	O2-C2-C3-O3
3	C	804	GOL	O1-C1-C2-O2
6	B	806	B3P	O3-C11-C8-N2
5	A	806[B]	PEG	O1-C1-C2-O2
3	B	809	GOL	O2-C2-C3-O3
5	B	813	PEG	O2-C3-C4-O4
2	B	801	A1CQV	C5-C6-C7-N4
2	A	801	A1CQV	C5-C6-C7-N4
2	C	801	A1CQV	C5-C6-C7-N4
5	B	810	PEG	O2-C3-C4-O4
3	A	803	GOL	O2-C2-C3-O3
2	B	801	A1CQV	C14-C6-C7-N4
5	B	810	PEG	C4-C3-O2-C2
5	B	813	PEG	C1-C2-O2-C3
2	A	801	A1CQV	C5-C6-C7-O1
2	B	801	A1CQV	C5-C6-C7-O1
2	A	801	A1CQV	C14-C6-C7-N4
5	A	806[B]	PEG	O2-C3-C4-O4
6	B	806	B3P	C7-C4-C5-O4
2	C	801	A1CQV	C5-C6-C7-O1
2	C	801	A1CQV	C14-C6-C7-N4
3	B	802	GOL	O2-C2-C3-O3
3	C	802	GOL	O1-C1-C2-O2
6	B	806	B3P	C3-C1-C2-N2
5	A	806[B]	PEG	C1-C2-O2-C3
3	B	804	GOL	O2-C2-C3-O3
6	B	806	B3P	N1-C4-C5-O4
2	A	801	A1CQV	C14-C6-C7-O1
2	B	801	A1CQV	C14-C6-C7-O1
6	B	806	B3P	C2-C1-C3-N1

There are no ring outliers.

8 monomers are involved in 10 short contacts:

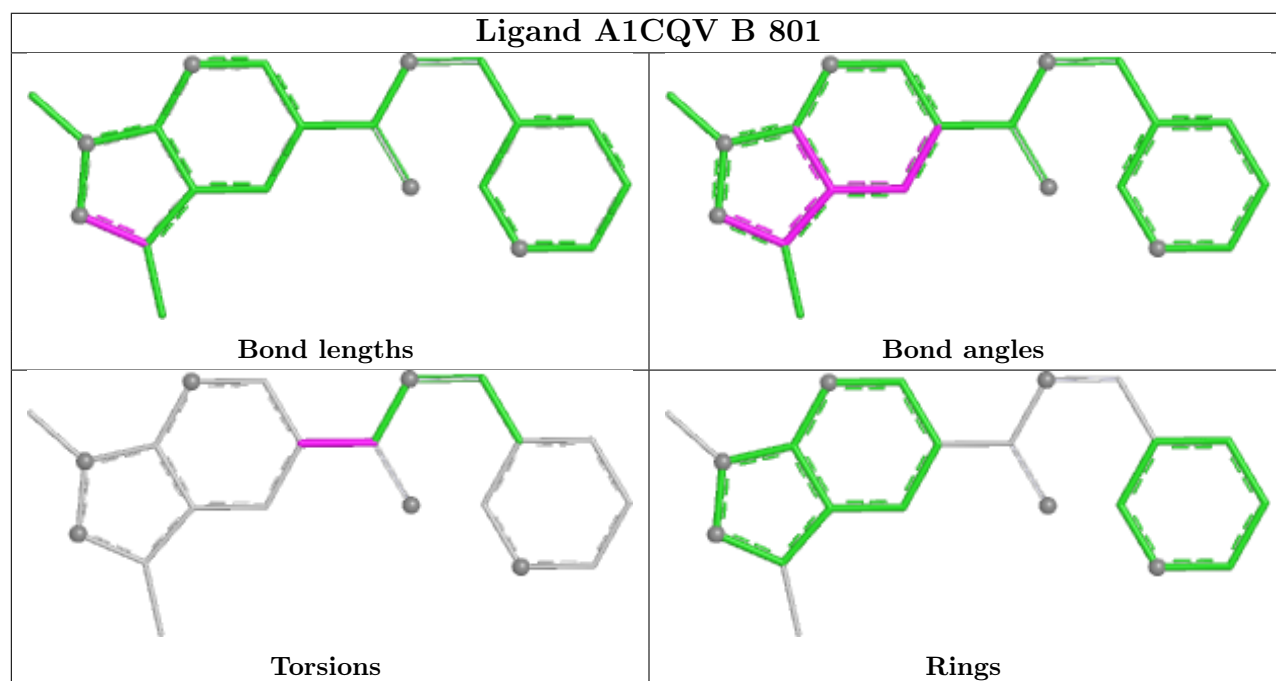
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	807	GOL	1	0
5	A	806[A]	PEG	1	0
3	B	809	GOL	1	0
3	C	802	GOL	2	0
3	B	805	GOL	1	0
3	B	802	GOL	1	0

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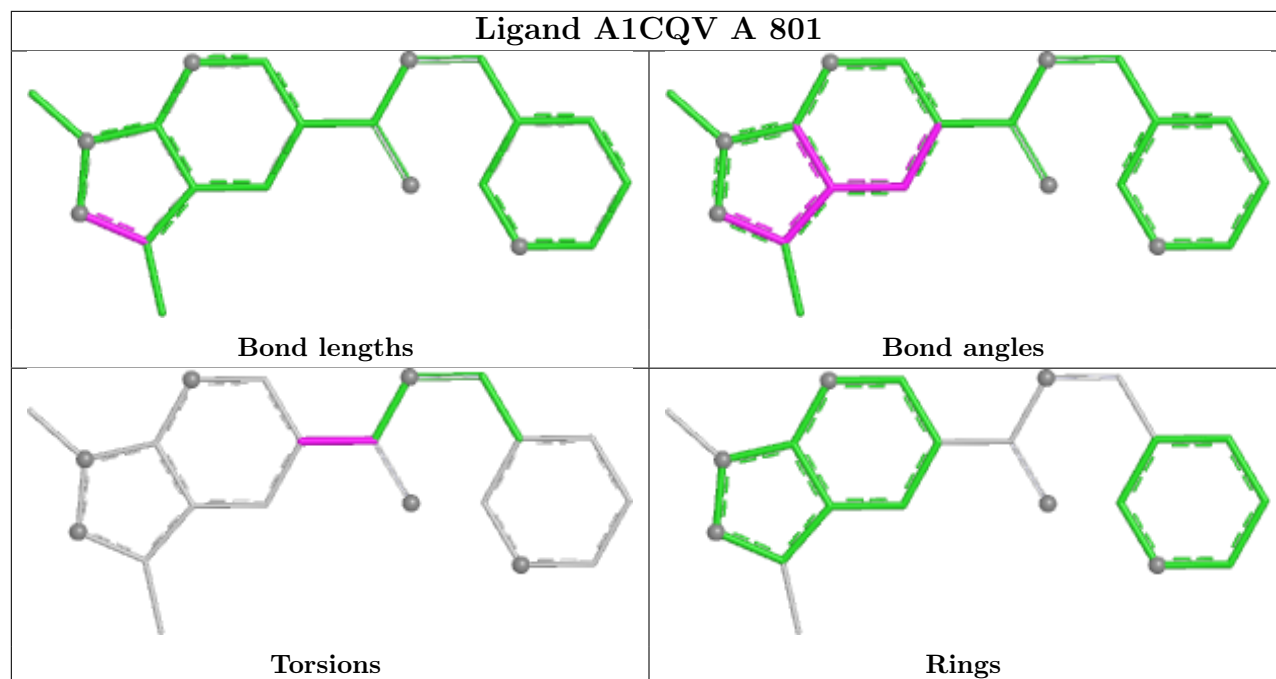
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	806	B3P	2	0
5	A	806[B]	PEG	1	0

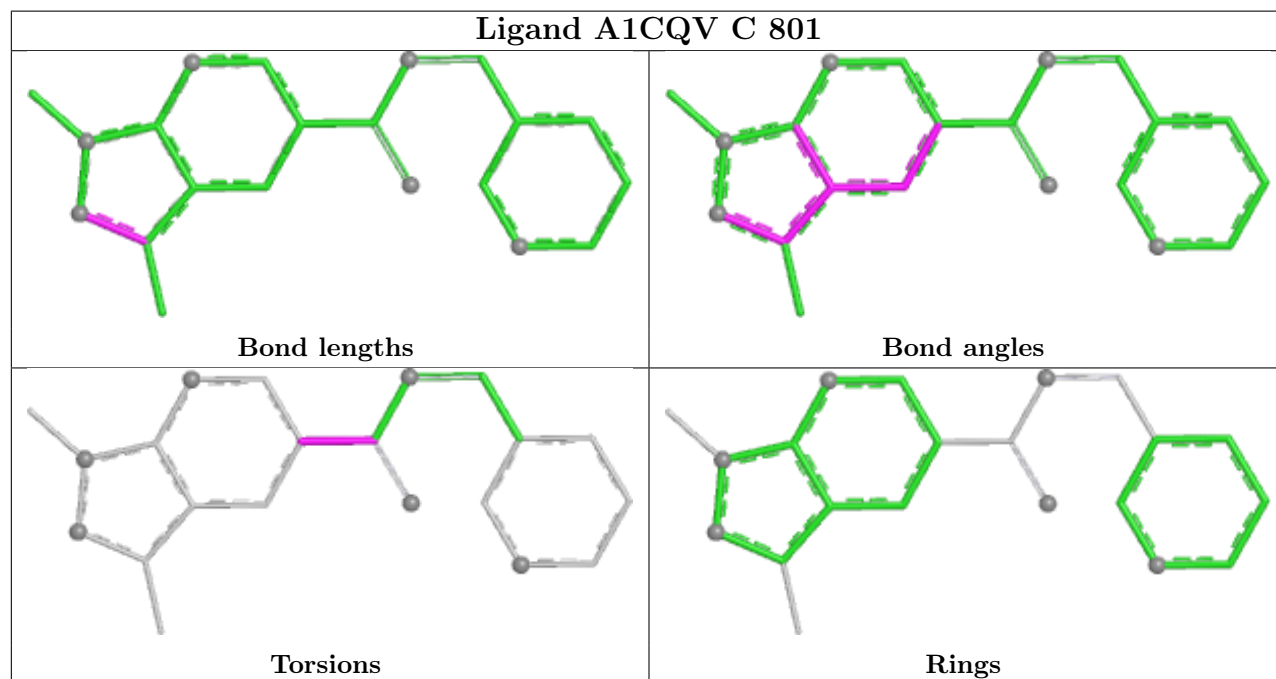
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

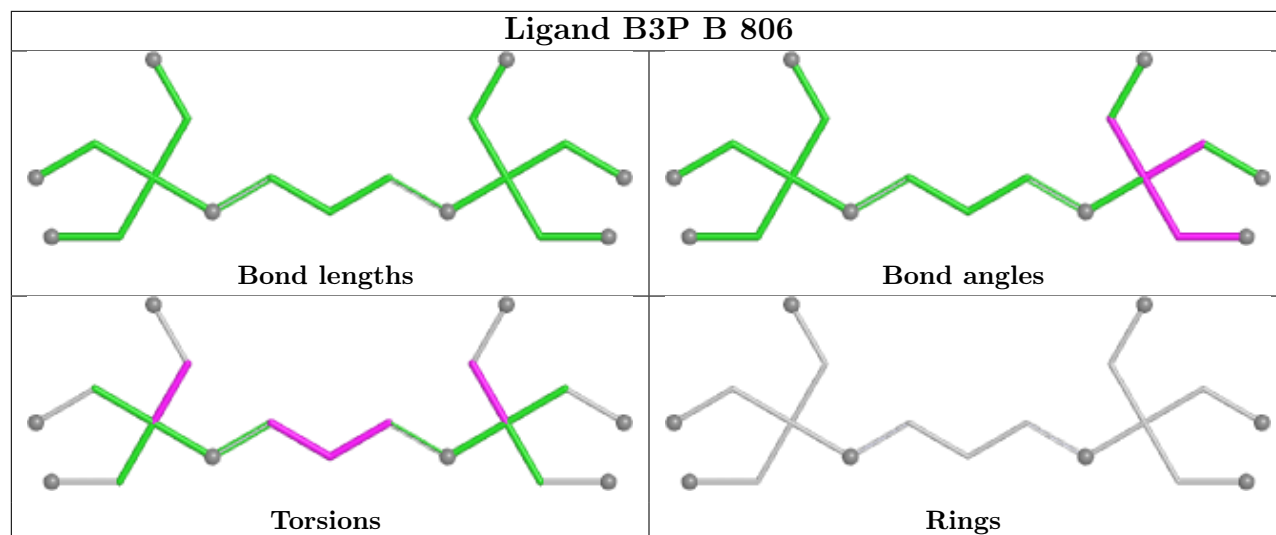


Ligand A1CQV A 801



Ligand A1CQV C 801





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	707/711 (99%)	-0.36	2 (0%)	90 93	19, 34, 55, 82	0
1	B	707/711 (99%)	-0.61	1 (0%)	92 94	14, 28, 50, 84	2 (0%)
1	C	707/711 (99%)	-0.13	5 (0%)	84 88	17, 39, 70, 96	1 (0%)
All	All	2121/2133 (99%)	-0.37	8 (0%)	88 92	14, 33, 60, 96	3 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	425	VAL	2.6
1	C	425	VAL	2.4
1	B	427	VAL	2.3
1	C	430	ILE	2.3
1	C	438	VAL	2.3
1	A	4	LEU	2.3
1	C	426	THR	2.0
1	C	427	VAL	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

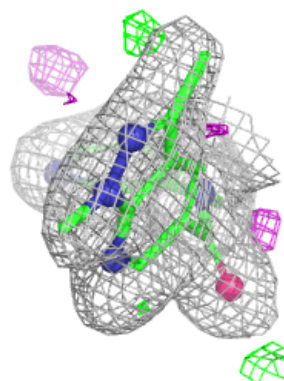
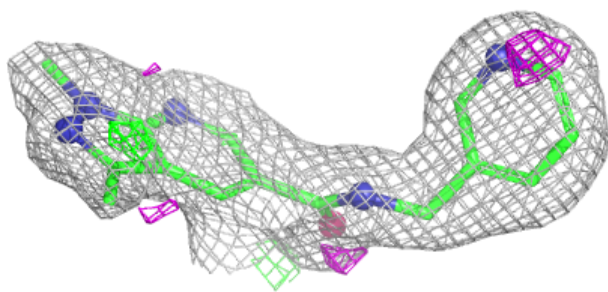
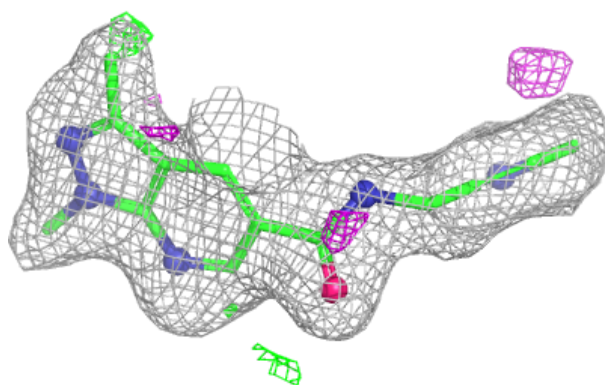
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	C	803	6/6	0.63	0.26	26,27,28,31	6
3	GOL	B	809	6/6	0.85	0.10	42,49,57,61	0
5	PEG	B	813	7/7	0.87	0.11	37,44,49,54	0
3	GOL	A	803	6/6	0.88	0.11	51,52,57,62	0
5	PEG	A	806[A]	7/7	0.88	0.12	26,29,35,37	7
5	PEG	A	806[B]	7/7	0.88	0.12	35,37,60,66	7
3	GOL	B	811	6/6	0.88	0.12	47,50,51,51	6
5	PEG	B	810	7/7	0.89	0.11	41,48,52,57	0
3	GOL	B	803	6/6	0.89	0.10	37,43,48,65	0
4	SCN	A	805	3/3	0.90	0.14	54,54,61,65	0
4	SCN	B	812	3/3	0.90	0.12	50,50,61,61	0
3	GOL	B	805	6/6	0.91	0.08	32,35,39,41	0
3	GOL	A	802	6/6	0.91	0.08	33,42,50,52	0
4	SCN	B	808	3/3	0.93	0.08	48,48,51,60	0
3	GOL	B	807	6/6	0.93	0.06	37,41,44,45	0
3	GOL	C	802	6/6	0.94	0.14	19,35,43,46	0
2	A1CQV	C	801	21/22	0.94	0.07	18,25,32,33	0
3	GOL	C	804	6/6	0.94	0.07	41,43,50,52	0
3	GOL	B	804	6/6	0.94	0.07	31,36,39,40	0
3	GOL	A	804	6/6	0.94	0.11	18,24,46,58	0
6	B3P	B	806	19/19	0.94	0.07	26,29,39,42	0
3	GOL	B	802	6/6	0.95	0.12	16,28,38,56	0
2	A1CQV	A	801	21/22	0.95	0.06	21,28,33,45	0
2	A1CQV	B	801	21/22	0.95	0.06	17,22,28,30	0

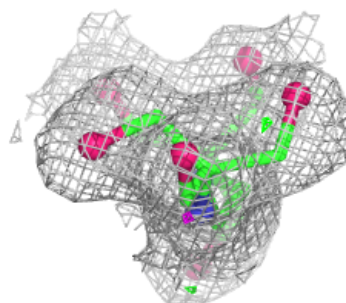
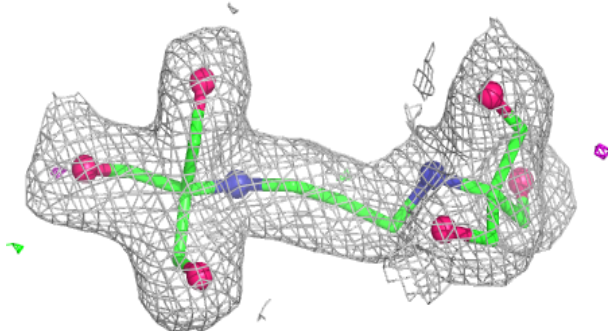
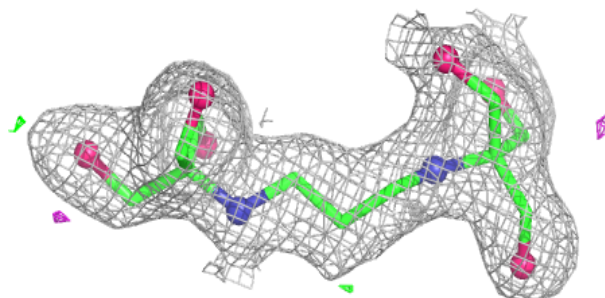
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1CQV C 801:

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

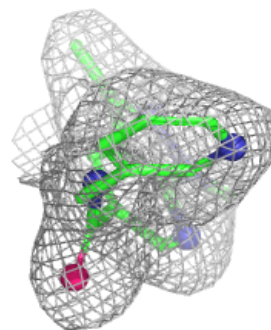
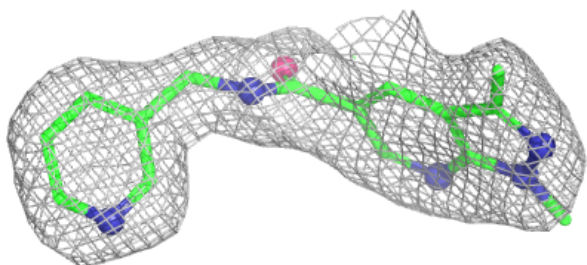
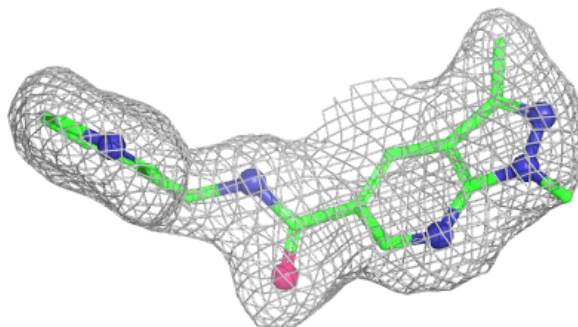
**Electron density around B3P B 806:**

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

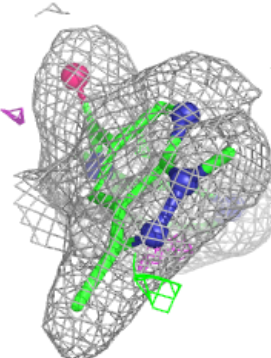
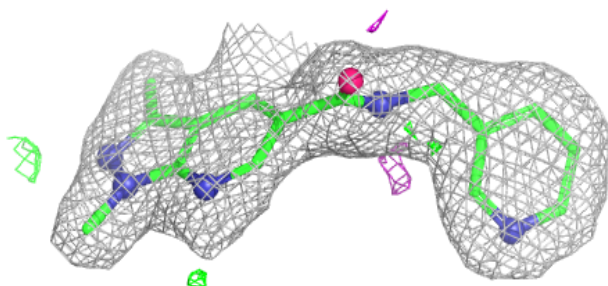
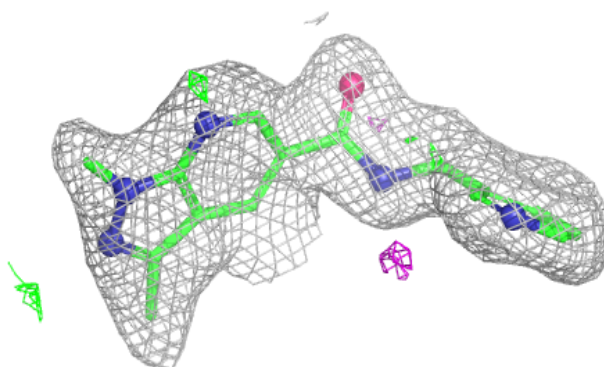


Electron density around A1CQV A 801:

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

**Electron density around A1CQV B 801:**

$2mF_o-DF_c$ (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.