



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:55 AM UTC

PDB ID : 9Q6K / pdb_00009q6k
Title : Human prolyl endopeptidase (PREP) - complex with JP-2-1-7
Authors : Fucci, I.J.; Thakur, K.; Pandian, J.; Yoo, E.; Monteiro, D.C.F.
Deposited on : 2025-08-22
Resolution : 1.85 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

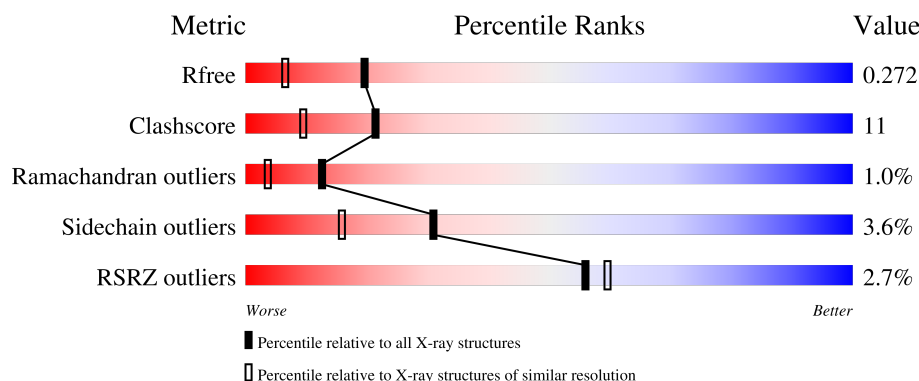
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	 77% 21% ..
1	B	711	 71% 25% ..
1	C	711	 8% 56% 32% 9% ..

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
4	GOL	A	806	-	-	X	-
4	GOL	A	807	-	-	X	-
5	PEG	A	805	-	-	X	-
6	SCN	B	810	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 35085 atoms, of which 16811 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.

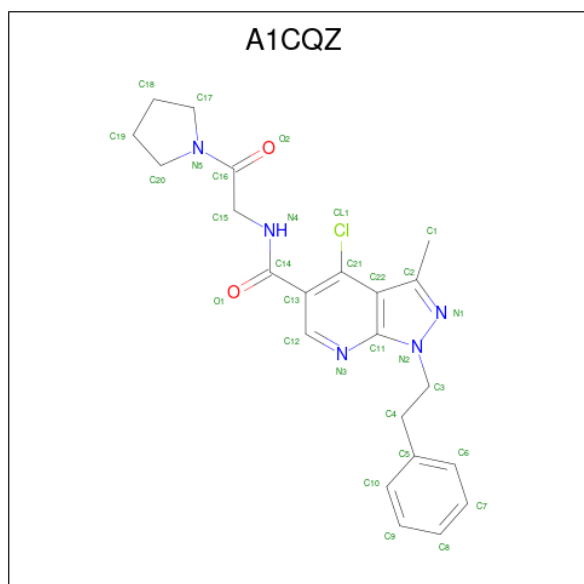
- Molecule 1 is a protein called Prolyl endopeptidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	707	Total	C	H	N	O	S	177	0	0
			11187	3639	5514	941	1066	27			
1	B	707	Total	C	H	N	O	S	177	2	0
			11229	3649	5540	947	1066	27			
1	C	707	Total	C	H	N	O	S	177	1	0
			11208	3644	5527	944	1066	27			

There are 3 discrepancies between the modelled and reference sequences:

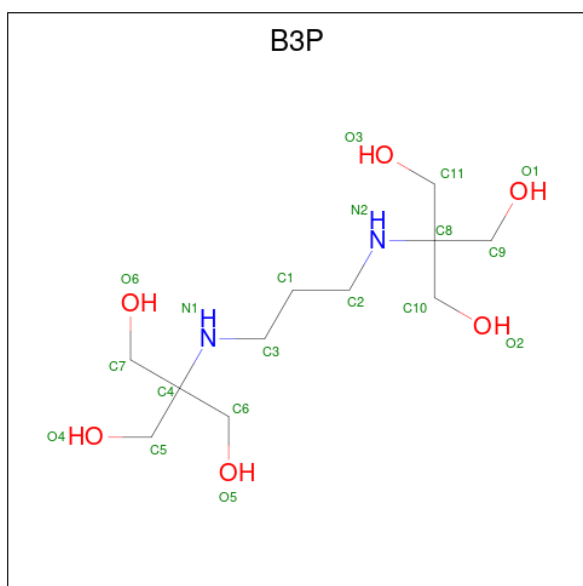
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P48147
B	0	GLY	-	expression tag	UNP P48147
C	0	GLY	-	expression tag	UNP P48147

- Molecule 2 is 4-chloro-3-methyl-N-[2-oxo-2-(pyrrolidin-1-yl)ethyl]-1-(2-phenylethyl)-1H-pyrazolo[3,4-b]pyridine-5-carboxamide (CCD ID: A1CQZ) (formula: C₂₂H₂₄ClN₅O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	3	0
			53	22	24	5	2		
2	B	1	Total	C	H	N	O	3	0
			53	22	24	5	2		
2	C	1	Total	C	H	N	O	3	0
			53	22	24	5	2		

- Molecule 3 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
3	A	1	Total	C	H	N	O	8	0
			45	11	26	2	6		
3	A	1	Total	C	H	N	O	8	0
			45	11	26	2	6		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



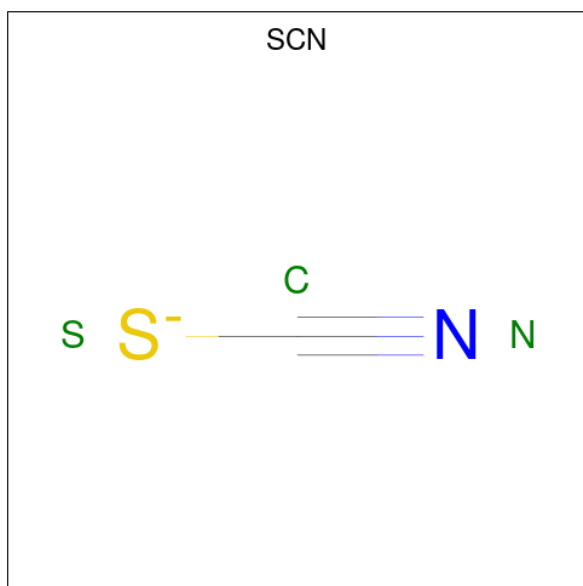
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	3	0
			14	3	8	3		
4	A	1	Total	C	H	O	3	0
			14	3	8	3		
4	A	1	Total	C	H	O	3	0
			14	3	8	3		
4	A	1	Total	C	H	O	3	0
			14	3	8	3		
4	A	1	Total	C	H	O	3	0
			14	3	8	3		
4	B	1	Total	C	H	O	3	0
			14	3	8	3		
4	B	1	Total	C	H	O	3	0
			14	3	8	3		
4	B	1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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	2	0
			17	4	10	3		

- Molecule 6 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



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

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	453	Total 453	O 453	0	0
7	B	383	Total 383	O 383	0	0

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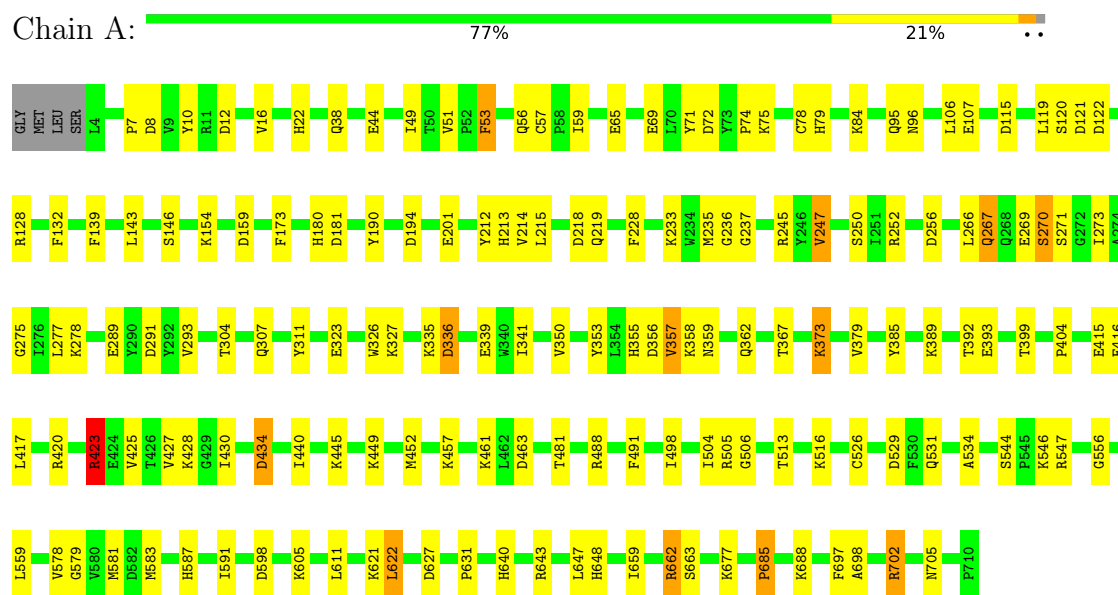
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	131	Total 131	O 131	0	0

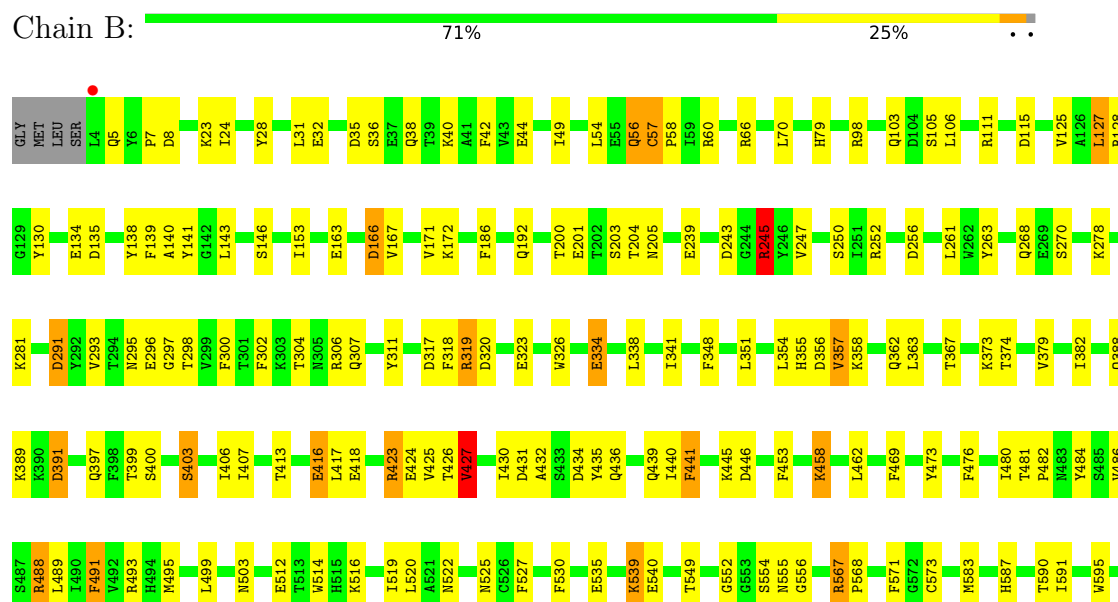
3 Residue-property plots

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: Prolyl endopeptidase

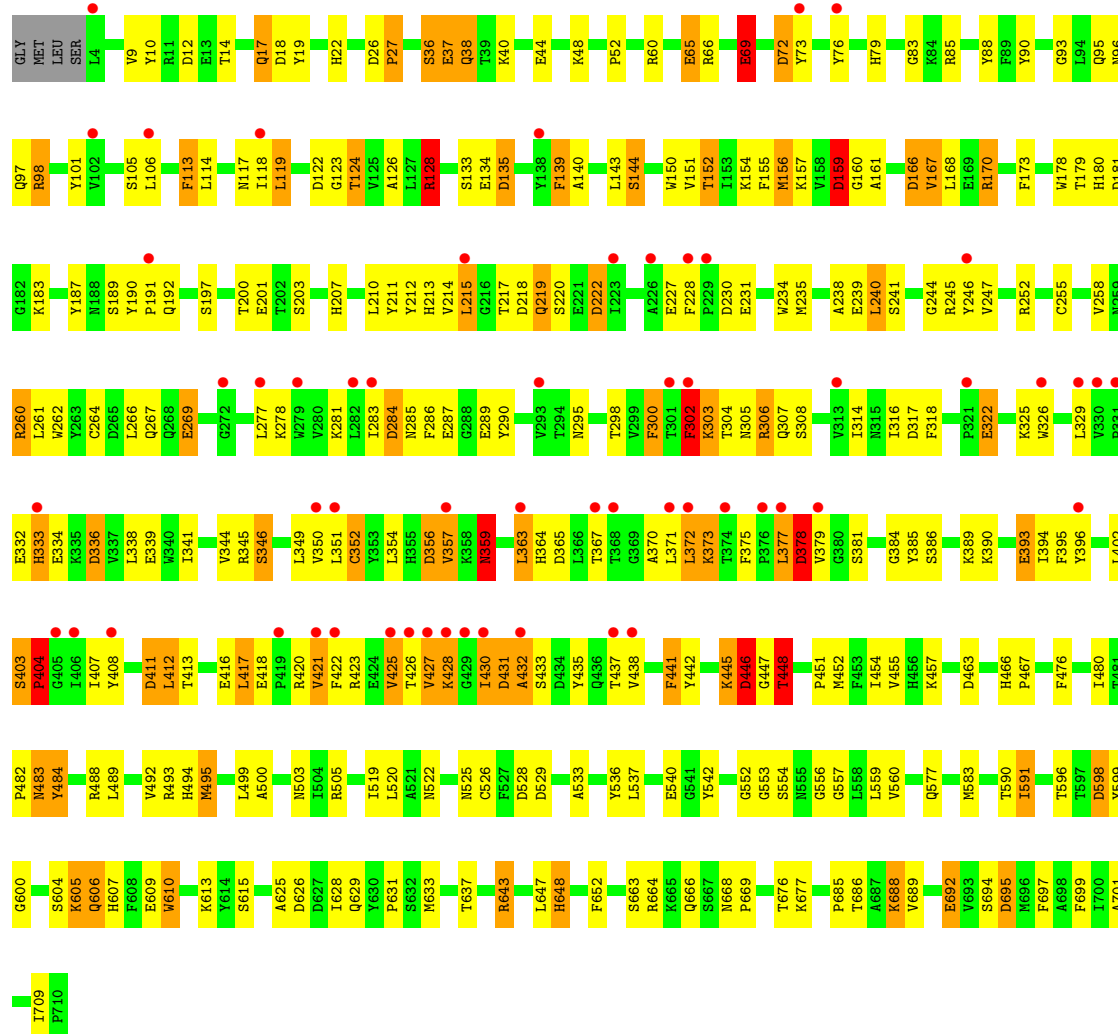


• Molecule 1: Prolyl endopeptidase





- 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	103.34Å 66.84Å 155.64Å 90.00° 102.07° 90.00°	Depositor
Resolution (Å)	42.70 – 1.85 42.70 – 1.85	Depositor EDS
% Data completeness (in resolution range)	74.4 (42.70-1.85) 74.4 (42.70-1.85)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.100)	Depositor
R, R_{free}	0.196 , 0.272 0.196 , 0.272	Depositor DCC
R_{free} test set	8707 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	20.7	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 35.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	35085	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.67% 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, GOL, SCN, B3P, A1CQZ

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	4/5825 (0.1%)	1.69	88/7897 (1.1%)
1	B	1.13	4/5847 (0.1%)	1.71	93/7925 (1.2%)
1	C	0.92	3/5836 (0.1%)	1.68	91/7911 (1.2%)
All	All	1.07	11/17508 (0.1%)	1.69	272/23733 (1.1%)

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	3
1	B	0	8
1	C	0	7
All	All	0	18

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	587	HIS	CG-CD2	-7.80	1.27	1.35
1	C	663	SER	CA-CB	-7.76	1.41	1.53
1	A	22	HIS	CG-CD2	7.45	1.44	1.35
1	A	22	HIS	CE1-NE2	6.17	1.38	1.32
1	B	250	SER	CA-CB	-5.85	1.45	1.53
1	B	673	HIS	CG-CD2	5.26	1.41	1.35
1	B	512	GLU	CD-OE2	5.25	1.35	1.25
1	C	648	HIS	CG-CD2	-5.15	1.30	1.35
1	A	481	THR	C-O	-5.05	1.19	1.24
1	C	139	PHE	C-O	-5.03	1.18	1.23
1	A	587	HIS	ND1-CE1	5.01	1.37	1.32

All (272) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	596	THR	CA-CB-OG1	-13.99	88.61	109.60
1	A	65	GLU	CB-CG-CD	11.12	131.51	112.60
1	B	426	THR	CA-CB-OG1	-10.49	93.87	109.60
1	C	200	THR	CA-CB-OG1	-10.29	94.16	109.60
1	C	336	ASP	CA-CB-CG	9.92	122.52	112.60
1	A	293	VAL	O-C-N	9.14	128.80	121.85
1	C	446	ASP	CA-CB-CG	9.06	121.66	112.60
1	B	427	VAL	N-CA-CB	-8.78	102.13	112.40
1	B	98	ARG	CD-NE-CZ	8.67	136.54	124.40
1	B	618	HIS	CA-CB-CG	-8.63	105.17	113.80
1	C	300	PHE	CA-CB-CG	-8.36	105.44	113.80
1	A	627	ASP	CA-CB-CG	8.31	120.92	112.60
1	B	293	VAL	N-CA-C	-8.19	104.52	111.56
1	B	603	ASP	CA-CB-CG	8.08	120.68	112.60
1	B	403	SER	CB-CA-C	-8.07	100.87	110.15
1	B	686	THR	CA-CB-OG1	-8.06	97.51	109.60
1	C	437	THR	CA-CB-OG1	-8.06	97.51	109.60
1	A	423	ARG	CD-NE-CZ	-8.05	113.13	124.40
1	C	38	GLN	CB-CA-C	-8.04	98.26	110.88
1	B	304	THR	OG1-CB-CG2	-7.88	93.55	109.30
1	C	483	ASN	CA-CB-CG	-7.87	104.73	112.60
1	C	528	ASP	CA-CB-CG	7.81	120.41	112.60
1	C	333	HIS	CB-CA-C	7.69	123.61	109.46
1	B	567	ARG	N-CA-CB	7.68	124.05	110.37
1	C	552	GLY	CA-C-N	7.61	126.83	121.65
1	C	552	GLY	C-N-CA	7.61	126.83	121.65
1	C	484	TYR	N-CA-CB	-7.48	98.35	109.95
1	B	535	GLU	O-C-N	7.41	129.97	122.12
1	A	434	ASP	CB-CA-C	-7.40	97.19	110.37
1	C	22	HIS	CA-CB-CG	-7.40	106.40	113.80
1	C	26	ASP	CA-CB-CG	7.38	119.98	112.60
1	A	415	GLU	N-CA-CB	-7.29	99.08	109.94
1	B	111	ARG	NE-CZ-NH2	7.24	125.71	119.20
1	A	697	PHE	CA-CB-CG	-7.22	106.58	113.80
1	A	293	VAL	N-CA-CB	7.21	118.70	111.57
1	C	359	ASN	CA-CB-CG	7.17	119.77	112.60
1	A	107	GLU	CB-CA-C	-7.17	95.96	109.72
1	A	128	ARG	NE-CZ-NH1	-7.15	114.35	121.50
1	C	441	PHE	CA-CB-CG	-7.14	106.66	113.80
1	C	356	ASP	CA-CB-CG	7.13	119.73	112.60
1	C	222	ASP	CA-CB-CG	7.08	119.68	112.60
1	B	354	LEU	CB-CG-CD2	-7.07	89.49	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	415	GLU	CG-CD-OE2	-7.06	102.16	118.40
1	C	69	GLU	CB-CA-C	7.05	121.88	110.95
1	A	423	ARG	CB-CA-C	-7.04	95.08	109.38
1	B	530	PHE	CA-CB-CG	7.03	120.83	113.80
1	C	697	PHE	CA-CB-CG	-6.99	106.81	113.80
1	C	215	LEU	N-CA-CB	-6.97	98.70	110.49
1	B	128	ARG	NE-CZ-NH1	-6.95	114.56	121.50
1	C	306	ARG	CB-CA-C	6.92	118.32	109.80
1	B	204	THR	CA-CB-OG1	-6.92	99.22	109.60
1	A	457	LYS	CB-CA-C	6.90	121.45	109.65
1	A	269	GLU	CB-CG-CD	6.89	124.31	112.60
1	B	318	PHE	N-CA-CB	6.86	120.35	110.06
1	B	514	TRP	N-CA-C	-6.84	103.90	111.36
1	A	51	VAL	O-C-N	-6.84	116.04	120.42
1	B	539	LYS	N-CA-CB	6.83	120.73	110.22
1	C	590	THR	CA-CB-OG1	6.78	119.77	109.60
1	C	375	PHE	CB-CA-C	6.74	118.38	108.87
1	C	467	PRO	CB-CA-C	6.74	120.18	111.21
1	B	626	ASP	CA-CB-CG	6.74	119.34	112.60
1	A	367	THR	CA-CB-OG1	-6.71	99.53	109.60
1	C	17	GLN	CB-CA-C	6.70	121.22	109.89
1	A	65	GLU	N-CA-CB	6.70	120.11	110.06
1	A	190	TYR	CB-CA-C	6.70	117.99	108.68
1	C	284	ASP	CA-CB-CG	-6.67	105.92	112.60
1	B	200	THR	OG1-CB-CG2	6.61	122.53	109.30
1	B	555	ASN	N-CA-C	-6.55	104.22	111.82
1	B	674	VAL	N-CA-CB	6.51	120.11	111.90
1	A	215	LEU	N-CA-CB	-6.51	100.00	109.83
1	B	57	CYS	CA-C-O	6.50	125.24	119.59
1	B	520	LEU	N-CA-CB	-6.48	99.54	110.49
1	C	303	LYS	CB-CG-CD	6.48	126.20	111.30
1	A	428	LYS	N-CA-CB	6.44	119.47	110.26
1	B	298	THR	CA-CB-OG1	-6.41	99.98	109.60
1	A	393	GLU	CB-CG-CD	6.39	123.46	112.60
1	C	278	LYS	CB-CA-C	6.39	121.35	110.81
1	C	27	PRO	CB-CA-C	-6.38	101.60	112.26
1	B	391	ASP	CA-CB-CG	6.37	118.97	112.60
1	A	247	VAL	N-CA-CB	6.36	118.25	111.00
1	A	143	LEU	N-CA-CB	-6.36	100.46	110.69
1	A	463	ASP	CA-CB-CG	6.34	118.94	112.60
1	C	227	GLU	O-C-N	-6.33	116.61	123.26
1	B	139	PHE	CB-CA-C	6.33	120.27	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	705	ASN	CB-CA-C	-6.27	100.76	112.30
1	B	453	PHE	CB-CA-C	-6.26	98.91	109.50
1	B	367	THR	CA-CB-OG1	6.25	118.97	109.60
1	B	525	ASN	N-CA-C	-6.25	104.55	111.36
1	C	269	GLU	CB-CA-C	6.24	121.82	111.83
1	A	622	LEU	CB-CA-C	6.23	120.10	109.82
1	A	132	PHE	CA-CB-CG	6.23	120.03	113.80
1	B	166	ASP	CA-CB-CG	6.21	118.81	112.60
1	C	302	PHE	CA-CB-CG	-6.21	107.59	113.80
1	A	139	PHE	CA-CB-CG	6.20	120.00	113.80
1	C	695	ASP	CA-CB-CG	6.20	118.80	112.60
1	B	476	PHE	CA-CB-CG	-6.20	107.61	113.80
1	A	247	VAL	CB-CA-C	-6.17	103.50	110.96
1	B	245	ARG	CB-CA-C	-6.16	98.46	109.24
1	A	236	GLY	CA-C-N	6.16	128.05	122.20
1	A	236	GLY	C-N-CA	6.16	128.05	122.20
1	A	72	ASP	CA-CB-CG	6.15	118.75	112.60
1	A	702	ARG	CB-CA-C	-6.11	101.25	110.90
1	A	685	PRO	CB-CA-C	-6.08	103.62	111.46
1	C	495	MET	CG-SD-CE	6.07	114.26	100.90
1	C	689	VAL	N-CA-CB	6.06	117.22	110.62
1	B	527	PHE	CB-CA-C	6.05	121.13	110.85
1	B	291	ASP	CA-CB-CG	6.04	118.64	112.60
1	A	392	THR	CA-CB-CG2	6.04	120.76	110.50
1	A	159	ASP	CA-CB-CG	6.02	118.62	112.60
1	C	448	THR	CA-CB-OG1	-6.00	100.60	109.60
1	C	372	LEU	N-CA-CB	5.99	118.75	110.07
1	A	526	CYS	CB-CA-C	-5.99	101.48	110.88
1	B	642	ASP	CA-CB-CG	5.99	118.58	112.60
1	C	637	THR	OG1-CB-CG2	-5.98	97.34	109.30
1	B	702	ARG	NE-CZ-NH2	-5.98	113.82	119.20
1	C	37	GLU	CB-CG-CD	-5.97	102.45	112.60
1	B	270	SER	CA-C-N	-5.95	112.92	122.62
1	B	270	SER	C-N-CA	-5.95	112.92	122.62
1	B	138	TYR	CA-CB-CG	-5.92	103.23	113.90
1	B	446	ASP	CA-CB-CG	5.92	118.52	112.60
1	C	610	TRP	O-C-N	5.91	128.47	122.09
1	C	235	MET	CG-SD-CE	-5.91	87.90	100.90
1	C	385	TYR	CA-C-O	-5.91	114.37	120.99
1	B	334	GLU	CB-CA-C	5.90	122.00	110.67
1	C	217	THR	CA-CB-OG1	5.90	118.45	109.60
1	A	425	VAL	N-CA-CB	5.88	117.54	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	448	THR	OG1-CB-CG2	5.87	121.04	109.30
1	C	577	GLN	CB-CA-C	5.86	119.41	109.80
1	A	201	GLU	CB-CG-CD	5.86	122.56	112.60
1	B	281	LYS	CG-CD-CE	-5.83	97.89	111.30
1	A	84	LYS	N-CA-CB	-5.82	102.04	110.47
1	B	389	LYS	CB-CA-C	5.81	120.56	110.68
1	A	74	PRO	CB-CA-C	5.80	118.93	111.21
1	B	143	LEU	N-CA-CB	-5.80	100.73	110.83
1	B	252	ARG	CB-CA-C	-5.79	97.92	109.33
1	B	613	LYS	CG-CD-CE	-5.79	97.99	111.30
1	C	606	GLN	CB-CA-C	5.78	121.92	110.42
1	B	462	LEU	N-CA-CB	-5.78	103.48	110.53
1	B	245	ARG	NE-CZ-NH2	5.78	124.40	119.20
1	C	688	LYS	N-CA-CB	5.77	119.22	110.28
1	C	431	ASP	CA-CB-CG	5.76	118.36	112.60
1	C	159	ASP	CA-CB-CG	5.75	118.35	112.60
1	C	170	ARG	N-CA-CB	5.75	121.20	112.47
1	A	389	LYS	CG-CD-CE	5.74	124.49	111.30
1	A	218	ASP	CB-CA-C	5.73	119.19	109.50
1	A	336	ASP	CA-CB-CG	5.73	118.33	112.60
1	B	658	TYR	N-CA-CB	5.73	118.61	110.13
1	B	163	GLU	N-CA-CB	5.72	118.44	109.69
1	C	98	ARG	CD-NE-CZ	-5.70	116.42	124.40
1	B	512	GLU	N-CA-CB	5.68	118.58	110.06
1	C	476	PHE	CA-CB-CG	-5.68	108.12	113.80
1	B	427	VAL	CB-CA-C	5.68	118.17	111.59
1	B	481	THR	OG1-CB-CG2	-5.67	97.96	109.30
1	B	441	PHE	CA-CB-CG	-5.66	108.14	113.80
1	B	491	PHE	CA-CB-CG	-5.64	108.16	113.80
1	A	121	ASP	CA-CB-CG	5.64	118.24	112.60
1	B	115	ASP	CA-C-O	-5.63	114.57	120.09
1	A	233	LYS	CB-CA-C	-5.61	99.90	109.65
1	A	359	ASN	CA-C-O	-5.60	114.66	121.05
1	B	42	PHE	CA-CB-CG	-5.60	108.20	113.80
1	B	382	ILE	CA-C-N	-5.60	115.93	122.14
1	B	382	ILE	C-N-CA	-5.60	115.93	122.14
1	C	352	CYS	O-C-N	5.59	129.59	123.27
1	A	53	PHE	CA-CB-CG	-5.59	108.21	113.80
1	C	166	ASP	CB-CA-C	5.58	118.61	109.90
1	A	8	ASP	CB-CA-C	5.57	118.19	109.84
1	C	322	GLU	N-CA-CB	5.57	121.09	111.13
1	C	600	GLY	CA-C-O	-5.55	118.14	122.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	598	ASP	N-CA-C	-5.54	106.19	113.12
1	C	38	GLN	N-CA-CB	5.54	118.04	110.01
1	C	113	PHE	N-CA-CB	5.53	119.83	110.49
1	C	260	ARG	CA-CB-CG	-5.52	103.06	114.10
1	C	375	PHE	N-CA-CB	-5.51	102.85	110.29
1	C	652	PHE	N-CA-C	-5.51	104.91	111.69
1	A	621	LYS	CB-CA-C	5.50	119.76	109.86
1	A	452	MET	CG-SD-CE	5.46	112.92	100.90
1	C	445	LYS	CB-CA-C	5.46	121.28	110.42
1	A	416	GLU	CB-CA-C	-5.45	98.60	109.99
1	A	526	CYS	N-CA-CB	5.45	117.91	110.01
1	B	503	ASN	N-CA-CB	5.44	116.61	110.35
1	B	652	PHE	CA-CB-CG	5.44	119.24	113.80
1	A	95	GLN	N-CA-CB	-5.43	102.06	110.04
1	B	186	PHE	CB-CA-C	-5.43	99.47	109.46
1	A	373	LYS	CB-CA-C	-5.42	101.26	109.99
1	A	291	ASP	CA-CB-CG	5.42	118.02	112.60
1	B	469	PHE	CA-CB-CG	5.41	119.21	113.80
1	B	488	ARG	CB-CG-CD	-5.41	98.86	111.30
1	C	69	GLU	CB-CG-CD	5.41	121.79	112.60
1	A	218	ASP	CA-CB-CG	5.41	118.01	112.60
1	A	631	PRO	CB-CA-C	-5.40	104.31	111.23
1	B	134	GLU	CB-CA-C	5.40	119.36	110.88
1	A	488	ARG	O-C-N	-5.40	116.00	122.15
1	C	411	ASP	CA-CB-CG	5.39	118.00	112.60
1	A	56	GLN	CG-CD-NE2	-5.39	108.31	116.40
1	C	451	PRO	CB-CA-C	-5.39	105.69	111.56
1	B	98	ARG	CG-CD-NE	-5.38	100.17	112.00
1	B	44	GLU	CB-CG-CD	5.38	121.74	112.60
1	A	213	HIS	CB-CA-C	-5.37	100.89	109.75
1	C	505	ARG	N-CA-C	-5.37	103.31	110.55
1	C	277	LEU	N-CA-CB	5.35	117.71	110.38
1	B	111	ARG	NE-CZ-NH1	-5.34	116.16	121.50
1	B	130	TYR	CA-C-O	-5.34	115.52	121.23
1	A	228	PHE	CA-C-N	5.33	125.15	119.28
1	A	228	PHE	C-N-CA	5.33	125.15	119.28
1	A	327	LYS	N-CA-CB	5.33	120.11	110.83
1	B	482	PRO	N-CA-CB	5.33	107.94	103.25
1	B	697	PHE	CB-CA-C	5.30	120.33	109.67
1	C	90	TYR	CB-CA-C	5.30	120.14	109.38
1	B	192	GLN	CB-CA-C	5.30	118.51	109.72
1	B	662	ARG	NE-CZ-NH1	-5.30	116.20	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	526	CYS	CB-CA-C	-5.29	102.01	110.79
1	C	375	PHE	CA-CB-CG	5.28	119.08	113.80
1	A	640	HIS	CA-CB-CG	5.28	119.08	113.80
1	A	267	GLN	N-CA-C	-5.28	104.95	111.33
1	B	622	LEU	CA-C-O	5.28	124.18	119.59
1	C	505	ARG	CA-C-O	-5.27	115.60	121.81
1	A	78	CYS	CB-CA-C	-5.26	100.98	109.72
1	C	66	ARG	NE-CZ-NH1	-5.26	116.24	121.50
1	C	36	SER	CA-C-N	5.24	127.57	120.44
1	C	36	SER	C-N-CA	5.24	127.57	120.44
1	A	705	ASN	CA-CB-CG	-5.24	107.36	112.60
1	A	491	PHE	N-CA-C	-5.23	105.75	111.82
1	C	425	VAL	CB-CA-C	5.23	118.19	110.77
1	A	180	HIS	CA-CB-CG	-5.22	108.58	113.80
1	A	181	ASP	CA-CB-CG	5.22	117.82	112.60
1	B	458	LYS	CB-CA-C	5.21	118.23	109.89
1	A	434	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	505	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	B	125	VAL	N-CA-CB	5.19	117.22	110.99
1	A	659	ILE	CB-CA-C	-5.19	105.06	112.22
1	C	128	ARG	NE-CZ-NH1	-5.19	116.31	121.50
1	A	214	VAL	N-CA-CB	5.18	116.91	111.00
1	B	60	ARG	CA-CB-CG	-5.18	103.74	114.10
1	A	513	THR	N-CA-CB	5.17	118.29	110.28
1	B	135	ASP	CA-CB-CG	5.16	117.76	112.60
1	B	293	VAL	O-C-N	5.15	126.56	121.98
1	C	152	THR	CA-CB-OG1	-5.15	101.87	109.60
1	A	194	ASP	CA-CB-CG	5.15	117.75	112.60
1	C	505	ARG	O-C-N	5.15	128.72	122.85
1	A	128	ARG	CB-CG-CD	5.15	123.14	111.30
1	C	286	PHE	N-CA-C	-5.14	107.17	112.93
1	C	156	MET	CG-SD-CE	5.14	112.21	100.90
1	B	56	GLN	N-CA-C	-5.14	106.52	112.89
1	B	399	THR	CA-CB-OG1	-5.14	101.89	109.60
1	A	275	GLY	CA-C-O	-5.13	115.78	120.97
1	B	239	GLU	N-CA-CB	-5.13	103.31	111.62
1	A	685	PRO	N-CA-CB	5.12	107.87	103.31
1	C	258	VAL	CA-C-O	-5.12	115.86	121.28
1	A	461	LYS	N-CA-CB	-5.12	102.08	110.52
1	B	571	PHE	CA-CB-CG	-5.11	108.69	113.80
1	B	28	TYR	N-CA-CB	-5.10	102.76	110.92
1	A	212	TYR	CB-CA-C	5.09	118.61	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	201	GLU	CB-CG-CD	5.09	121.25	112.60
1	C	699	PHE	CA-CB-CG	5.09	118.89	113.80
1	A	44	GLU	CB-CA-C	5.08	120.43	110.67
1	B	24	ILE	CA-C-O	5.08	124.74	120.22
1	C	19	TYR	CB-CA-C	-5.08	104.02	111.23
1	A	506	GLY	CA-C-N	-5.08	114.96	121.96
1	A	506	GLY	C-N-CA	-5.08	114.96	121.96
1	B	491	PHE	CB-CA-C	5.07	119.21	110.79
1	C	519	ILE	CA-C-O	-5.07	116.67	121.64
1	B	669	PRO	CA-C-O	-5.06	115.60	122.08
1	A	516	LYS	CG-CD-CE	5.05	122.92	111.30
1	C	200	THR	OG1-CB-CG2	5.05	119.39	109.30
1	C	484	TYR	CB-CA-C	5.04	118.05	109.84
1	C	285	ASN	N-CA-C	-5.03	100.82	108.76
1	B	140	ALA	O-C-N	-5.02	117.31	123.19
1	C	372	LEU	N-CA-C	-5.02	105.72	111.14
1	A	702	ARG	NE-CZ-NH2	-5.02	114.69	119.20
1	A	622	LEU	N-CA-CB	-5.01	99.87	109.44
1	B	302	PHE	CB-CA-C	-5.01	99.76	109.68
1	B	127	LEU	N-CA-CB	-5.00	102.96	110.17

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	420	ARG	Sidechain
1	A	643	ARG	Sidechain
1	A	662	ARG	Sidechain
1	B	245	ARG	Sidechain
1	B	319	ARG	Sidechain
1	B	423[A]	ARG	Sidechain
1	B	423[B]	ARG	Sidechain
1	B	643	ARG	Sidechain
1	B	66	ARG	Sidechain
1	B	662	ARG	Sidechain
1	B	702	ARG	Sidechain
1	C	128	ARG	Sidechain
1	C	302	PHE	Peptide
1	C	378	ASP	Peptide
1	C	404	PRO	Peptide
1	C	493	ARG	Sidechain
1	C	643	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	664	ARG	Sidechain

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	5673	5514	5490	77	0
1	B	5689	5540	5516	86	0
1	C	5681	5527	5503	205	0
2	A	29	24	0	0	0
2	B	29	24	0	0	0
2	C	29	24	0	0	0
3	A	38	52	52	3	0
4	A	30	40	40	11	0
4	B	24	32	32	2	0
4	C	18	24	24	0	0
5	A	7	10	10	5	0
6	A	27	0	0	3	0
6	B	24	0	0	5	0
6	C	9	0	0	2	0
7	A	453	0	0	12	0
7	B	383	0	0	10	0
7	C	131	0	0	21	0
All	All	18274	16811	16667	369	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 11.

All (369) 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:C:377:LEU:C	1:C:378:ASP:OD1	1.98	1.06
1:C:181:ASP:CG	1:C:183:LYS:HG3	1.89	0.98
1:B:166:ASP:HA	6:B:810:SCN:N	1.86	0.91
1:C:170:ARG:NE	1:C:190:TYR:O	2.06	0.88
1:C:318:PHE:O	7:C:901:HOH:O	1.93	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:811:SCN:N	7:A:901:HOH:O	2.08	0.85
1:B:58:PRO:O	7:B:901:HOH:O	1.95	0.84
1:A:449:LYS:HE3	7:A:1041:HOH:O	1.76	0.84
1:C:377:LEU:O	1:C:378:ASP:OD1	1.95	0.83
1:A:662:ARG:HD3	7:A:1290:HOH:O	1.82	0.79
1:A:423:ARG:CG	1:A:423:ARG:HH21	1.96	0.77
1:B:317:ASP:O	1:B:320:ASP:N	2.15	0.77
1:C:403:SER:O	1:C:404:PRO:O	2.04	0.76
1:C:407:ILE:HD12	1:C:423:ARG:HD2	1.66	0.76
1:C:18:ASP:O	7:C:902:HOH:O	2.05	0.73
1:B:416:GLU:O	1:B:417:LEU:C	2.32	0.71
1:B:291:ASP:OD1	6:B:806:SCN:S	2.49	0.71
1:C:322:GLU:HA	7:C:916:HOH:O	1.88	0.71
1:C:283:ILE:HG21	1:C:290:TYR:HE2	1.57	0.70
1:A:237:GLY:H	4:A:806:GOL:H12	1.56	0.70
1:C:181:ASP:OD1	1:C:183:LYS:HG3	1.92	0.69
1:C:252[B]:ARG:HG3	7:C:939:HOH:O	1.92	0.69
1:A:38:GLN:HG2	5:A:805:PEG:H12	1.75	0.69
1:B:245:ARG:HD2	7:B:1049:HOH:O	1.92	0.69
1:C:60:ARG:HH11	1:C:60:ARG:HG2	1.58	0.68
1:A:256:ASP:HB2	7:A:952:HOH:O	1.94	0.68
1:C:168:LEU:HD23	1:C:219:GLN:HG2	1.76	0.67
1:A:38:GLN:CG	5:A:805:PEG:H12	2.24	0.67
1:C:495:MET:HE3	1:C:701:ALA:HB2	1.77	0.67
1:C:283:ILE:HG21	1:C:290:TYR:CE2	2.29	0.66
6:A:815:SCN:N	7:A:905:HOH:O	2.27	0.66
1:C:44:GLU:O	1:C:48:LYS:HG3	1.95	0.66
1:A:591:ILE:HG12	4:A:803:GOL:H11	1.77	0.66
1:C:178:TRP:O	1:C:240:LEU:HD23	1.95	0.66
1:B:348:PHE:HB3	1:B:363:LEU:HD11	1.77	0.66
1:B:407:ILE:HD13	1:B:423[B]:ARG:NH1	2.12	0.65
1:B:431:ASP:HB3	1:B:434:ASP:OD2	1.97	0.65
1:A:307:GLN:H	3:A:812:B3P:H92	1.63	0.64
1:C:213:HIS:ND1	1:C:222:ASP:OD1	2.31	0.64
1:C:284:ASP:OD2	6:C:806:SCN:N	2.30	0.64
1:C:213:HIS:HA	1:C:222:ASP:OD1	1.97	0.64
1:C:135:ASP:OD1	1:C:135:ASP:N	2.28	0.63
1:C:173:PHE:CE2	1:C:591:ILE:HG12	2.33	0.63
1:C:295:ASN:CG	1:C:300:PHE:CZ	2.77	0.63
1:C:260:ARG:NH1	1:C:284:ASP:OD2	2.32	0.62
1:A:57:CYS:HB3	7:A:1248:HOH:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:HIS:HE1	1:C:423:ARG:HH11	1.46	0.61
1:A:245:ARG:HG3	1:A:267:GLN:HG2	1.83	0.61
1:A:423:ARG:CG	1:A:423:ARG:NH2	2.64	0.61
1:A:237:GLY:N	4:A:806:GOL:H12	2.16	0.61
1:C:676:THR:O	1:C:688:LYS:NZ	2.33	0.61
1:B:406:ILE:HG12	1:B:424:GLU:HG3	1.83	0.60
1:B:79:HIS:NE2	1:B:103:GLN:NE2	2.49	0.60
1:C:105:SER:O	1:C:106:LEU:C	2.45	0.60
1:C:694:SER:O	1:C:695:ASP:C	2.43	0.60
1:C:122:ASP:OD1	1:C:122:ASP:N	2.33	0.60
1:C:133:SER:HA	1:C:178:TRP:CG	2.36	0.60
1:C:334:GLU:O	1:C:334:GLU:HG2	2.01	0.60
1:C:166:ASP:O	1:C:167:VAL:HG23	2.02	0.59
1:C:333:HIS:CD2	1:C:336:ASP:HB2	2.38	0.59
1:C:264:CYS:SG	1:C:269:GLU:HG3	2.42	0.59
1:B:427:VAL:HG11	1:B:484:TYR:OH	2.03	0.59
1:C:338:LEU:HD12	1:C:352:CYS:O	2.02	0.58
1:A:531:GLN:O	1:A:534:ALA:HB3	2.04	0.58
1:B:605:LYS:HE2	1:B:609:GLU:OE2	2.04	0.58
1:A:154:LYS:HD3	7:A:1271:HOH:O	2.03	0.58
1:B:358:LYS:HD2	1:B:379:VAL:HG13	1.84	0.58
1:B:567:ARG:N	1:B:568:PRO:CD	2.67	0.58
1:C:341:ILE:HD11	1:C:349:LEU:HD13	1.86	0.57
1:C:403:SER:O	1:C:404:PRO:C	2.46	0.57
1:A:362:GLN:HE22	4:A:807:GOL:H2	1.69	0.57
1:B:358:LYS:CD	1:B:379:VAL:HG13	2.34	0.57
1:B:268:GLN:O	1:B:278:LYS:NZ	2.33	0.57
1:A:423:ARG:HH21	1:A:423:ARG:HG2	1.69	0.57
1:C:160:GLY:O	1:C:161:ALA:HB3	2.03	0.57
1:C:446:ASP:OD1	1:C:448:THR:OG1	2.18	0.57
1:C:396:TYR:CE2	1:C:408:TYR:CD1	2.93	0.57
1:B:355:HIS:O	1:B:356:ASP:C	2.48	0.57
1:C:345:ARG:HD3	1:C:412:LEU:HB3	1.87	0.57
1:C:97:GLN:NE2	1:C:126:ALA:HB2	2.21	0.56
1:C:144:SER:OG	1:C:150:TRP:O	2.23	0.56
1:C:287:GLU:OE1	1:C:306:ARG:NH1	2.37	0.56
1:B:32:GLU:OE2	1:B:651:LYS:NZ	2.36	0.56
1:C:332:GLU:HG2	1:C:333:HIS:O	2.04	0.56
1:C:402:LEU:O	1:C:404:PRO:HD3	2.05	0.56
1:C:17:GLN:HB3	7:C:909:HOH:O	2.06	0.56
1:A:38:GLN:HB3	5:A:805:PEG:H12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:LYS:HD2	1:A:379:VAL:HG13	1.87	0.56
1:C:298:THR:HB	1:C:318:PHE:HB2	1.88	0.56
1:C:605:LYS:O	1:C:606:GLN:C	2.49	0.56
1:C:322:GLU:OE1	1:C:325:LYS:HG3	2.06	0.56
1:C:365:ASP:HB2	1:C:372:LEU:HD21	1.87	0.56
1:C:378:ASP:OD1	1:C:378:ASP:N	2.37	0.56
1:C:647:LEU:HD12	1:C:648:HIS:N	2.21	0.55
1:B:413:THR:O	7:B:902:HOH:O	2.18	0.55
1:A:434:ASP:HB3	7:A:1097:HOH:O	2.06	0.55
1:B:519:ILE:O	1:B:522:ASN:HB2	2.07	0.55
1:C:241:SER:HB2	1:C:295:ASN:OD1	2.07	0.55
1:A:647:LEU:HD12	1:A:648:HIS:N	2.22	0.55
1:C:48:LYS:O	1:C:52:PRO:HG2	2.06	0.55
1:C:609:GLU:O	1:C:613:LYS:HE3	2.05	0.55
1:B:388:GLN:O	1:B:391:ASP:HB2	2.06	0.54
1:C:346:SER:HA	1:C:389:LYS:HG2	1.89	0.54
1:A:69:GLU:OE1	1:A:69:GLU:HA	2.06	0.54
1:C:123:GLY:O	1:C:685:PRO:HB3	2.07	0.54
1:C:252[B]:ARG:NE	7:C:906:HOH:O	2.38	0.54
1:C:431:ASP:CG	1:C:433:SER:OG	2.50	0.54
1:A:57:CYS:HB2	1:A:698:ALA:HB1	1.89	0.54
1:B:146:SER:HB3	1:B:677:LYS:HA	1.88	0.54
1:A:605:LYS:HE3	1:B:56:GLN:HE21	1.73	0.54
1:B:40:LYS:O	6:B:812:SCN:S	2.66	0.54
1:C:97:GLN:O	1:C:117:ASN:ND2	2.37	0.54
1:C:430:ILE:HG22	1:C:431:ASP:H	1.73	0.54
1:B:167:VAL:H	6:B:810:SCN:C	2.21	0.54
1:C:239:GLU:HG2	7:C:919:HOH:O	2.07	0.54
1:C:339:GLU:HG2	1:C:354:LEU:HD22	1.89	0.53
1:C:218:ASP:HB2	7:C:911:HOH:O	2.09	0.53
1:A:362:GLN:HE22	4:A:807:GOL:C3	2.22	0.53
1:C:244:GLY:O	1:C:266:LEU:HD12	2.09	0.53
1:C:483:ASN:OD1	1:C:483:ASN:N	2.42	0.53
1:B:591:ILE:O	1:B:591:ILE:HG13	2.09	0.53
1:C:12:ASP:OD1	1:C:14:THR:OG1	2.22	0.53
1:C:283:ILE:HD13	1:C:290:TYR:CD2	2.44	0.53
1:B:516:LYS:O	7:B:903:HOH:O	2.19	0.52
1:A:252:ARG:HG2	4:A:806:GOL:H11	1.91	0.52
1:B:7:PRO:HD3	1:B:49:ILE:CD1	2.39	0.52
1:B:306:ARG:HD2	1:B:307:GLN:HG3	1.91	0.52
1:B:358:LYS:NZ	1:B:439:GLN:OE1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:ASN:HB3	1:C:300:PHE:CE2	2.45	0.52
1:B:362:GLN:HE22	4:B:813:GOL:H2	1.75	0.52
1:C:420:ARG:O	1:C:421:VAL:C	2.53	0.52
1:C:466:HIS:HB2	1:C:542:TYR:O	2.10	0.51
1:C:350:VAL:C	1:C:351:LEU:HD12	2.35	0.51
1:B:341:ILE:HD12	1:B:351:LEU:HD11	1.93	0.51
1:B:416:GLU:CG	1:B:418:GLU:HB2	2.40	0.51
1:A:323:GLU:HA	1:A:326:TRP:CE2	2.46	0.51
1:B:407:ILE:CD1	1:B:423[B]:ARG:NH1	2.73	0.51
1:C:220:SER:N	7:C:911:HOH:O	2.44	0.51
1:C:157:LYS:NZ	1:C:159:ASP:HB3	2.26	0.51
1:B:323:GLU:HA	1:B:326:TRP:CE2	2.45	0.50
1:B:440:ILE:HD12	1:B:440:ILE:C	2.36	0.50
1:C:426:THR:O	1:C:427:VAL:O	2.29	0.50
1:C:441:PHE:CD1	1:C:441:PHE:N	2.77	0.50
1:C:36:SER:O	1:C:40:LYS:HG3	2.11	0.50
1:C:334:GLU:O	1:C:334:GLU:CG	2.60	0.50
1:C:396:TYR:CE2	1:C:408:TYR:HB2	2.47	0.50
1:C:201:GLU:CD	1:C:201:GLU:H	2.19	0.50
1:C:210:LEU:HD21	1:C:238:ALA:HB2	1.94	0.50
1:A:7:PRO:HD3	1:A:49:ILE:CD1	2.41	0.50
1:B:172:LYS:HZ1	1:B:205:ASN:HD21	1.60	0.50
1:C:533:ALA:O	1:C:537:LEU:HG	2.12	0.50
1:C:314:ILE:HD11	1:C:316:ILE:HD11	1.94	0.50
1:B:407:ILE:HD12	1:B:423[B]:ARG:HD2	1.94	0.50
1:C:124:THR:HB	7:C:967:HOH:O	2.12	0.50
1:C:583:MET:HB2	1:C:615:SER:HB2	1.94	0.49
1:B:493:ARG:HD2	1:B:493:ARG:O	2.12	0.49
1:C:245:ARG:O	1:C:266:LEU:HB2	2.12	0.49
1:A:235:MET:HB3	4:A:806:GOL:H2	1.93	0.49
1:C:154:LYS:HG2	1:C:167:VAL:HG22	1.95	0.49
1:C:83:GLY:HA2	1:C:135:ASP:O	2.12	0.49
1:B:58:PRO:HD2	7:B:1148:HOH:O	2.11	0.49
1:C:298:THR:O	1:C:317:ASP:HA	2.13	0.49
1:C:333:HIS:CG	1:C:336:ASP:HB2	2.47	0.49
1:A:96:ASN:HB3	1:A:685:PRO:HB3	1.93	0.49
1:B:416:GLU:HG2	1:B:418:GLU:HB2	1.95	0.49
1:C:95:GLN:O	1:C:686:THR:OG1	2.28	0.49
1:C:143:LEU:O	1:C:151:VAL:HA	2.13	0.49
1:C:647:LEU:HD12	1:C:647:LEU:C	2.37	0.48
1:C:98:ARG:NH2	6:C:805:SCN:N	2.58	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:TYR:CD1	1:A:385:TYR:C	2.92	0.48
1:A:688:LYS:HG2	7:A:916:HOH:O	2.12	0.48
1:B:623:PRO:O	1:B:665:LYS:NZ	2.46	0.48
1:C:240:LEU:HD11	1:C:247:VAL:HG22	1.94	0.48
1:A:38:GLN:CB	5:A:805:PEG:H12	2.44	0.48
1:B:436:GLN:HB3	1:B:458:LYS:HE2	1.94	0.48
1:C:351:LEU:HD22	1:C:364:HIS:CE1	2.49	0.48
1:C:431:ASP:CG	1:C:433:SER:HG	2.21	0.48
1:B:435:TYR:O	1:B:458:LYS:HE3	2.14	0.48
1:A:622:LEU:HD11	1:A:663:SER:HB3	1.96	0.48
1:C:402:LEU:O	1:C:404:PRO:CD	2.62	0.48
1:A:341:ILE:HA	1:A:350:VAL:O	2.13	0.48
1:C:295:ASN:HB3	1:C:300:PHE:CD2	2.49	0.48
1:C:427:VAL:HG21	1:C:484:TYR:OH	2.13	0.47
1:A:544:SER:HB2	1:A:547:ARG:HG3	1.95	0.47
1:B:127:LEU:HD11	1:B:141:TYR:HB2	1.96	0.47
1:C:281:LYS:HE3	7:C:914:HOH:O	2.14	0.47
1:A:647:LEU:HD12	1:A:647:LEU:C	2.39	0.47
1:B:491:PHE:CD1	1:B:495:MET:HE2	2.50	0.47
1:A:362:GLN:NE2	4:A:807:GOL:H2	2.29	0.47
1:B:54:LEU:HA	1:B:57:CYS:SG	2.54	0.47
1:B:38:GLN:H	1:B:38:GLN:CD	2.22	0.47
1:C:168:LEU:HD23	1:C:219:GLN:CG	2.44	0.47
1:B:397:GLN:NE2	7:B:937:HOH:O	2.47	0.47
1:C:384:GLY:HA3	7:C:987:HOH:O	2.14	0.47
1:C:556:GLY:O	1:C:559:LEU:HB3	2.15	0.47
1:C:386:SER:O	1:C:394:ILE:HA	2.15	0.47
1:A:12:ASP:C	1:A:12:ASP:OD1	2.57	0.47
1:B:637:THR:OG1	1:B:638:ALA:N	2.48	0.47
1:C:118:ILE:CG1	1:C:119:LEU:HD23	2.45	0.47
1:B:341:ILE:CD1	1:B:351:LEU:HD11	2.45	0.46
1:B:473:TYR:HB3	1:B:480:ILE:HD11	1.96	0.46
1:C:122:ASP:OD2	1:C:677:LYS:HD3	2.15	0.46
1:C:191:PRO:HG3	1:C:207:HIS:HB2	1.97	0.46
1:C:332:GLU:CG	1:C:333:HIS:O	2.63	0.46
1:A:10:TYR:CD2	5:A:805:PEG:H22	2.50	0.46
1:B:552:GLY:HA3	1:B:556:GLY:O	2.16	0.46
1:C:629:GLN:CD	1:C:668:ASN:ND2	2.73	0.46
1:C:113:PHE:O	1:C:156:MET:HE1	2.16	0.46
1:C:416:GLU:OE2	1:C:418:GLU:OE1	2.34	0.46
1:C:488:ARG:HB3	1:C:499:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:GLN:N	6:A:809:SCN:S	2.76	0.46
1:A:252:ARG:HD3	3:A:802:B3P:O6	2.15	0.46
1:C:536:TYR:CZ	1:C:540:GLU:HG3	2.50	0.46
1:A:579:GLY:HA3	1:A:581:MET:HE2	1.98	0.46
1:B:539:LYS:HE2	1:B:540:GLU:HG2	1.98	0.46
1:C:446:ASP:OD1	1:C:447:GLY:N	2.48	0.46
1:B:595:TRP:CD1	1:B:595:TRP:N	2.81	0.46
1:C:181:ASP:OD1	1:C:183:LYS:CG	2.62	0.46
1:A:122:ASP:OD2	1:A:677:LYS:NZ	2.41	0.45
1:C:12:ASP:O	1:C:27:PRO:HA	2.17	0.45
1:A:373:LYS:HE3	1:A:417:LEU:HB2	1.98	0.45
1:C:489:LEU:O	1:C:492:VAL:HB	2.15	0.45
1:A:266:LEU:O	1:A:267:GLN:C	2.57	0.45
1:C:344:VAL:HG21	1:C:394:ILE:HG22	1.98	0.45
1:A:546:LYS:HG2	7:A:1233:HOH:O	2.16	0.45
1:C:262:TRP:CD1	1:C:281:LYS:HA	2.51	0.45
1:C:306:ARG:HH21	1:C:307:GLN:HE21	1.64	0.45
1:C:354:LEU:HD13	1:C:359:ASN:ND2	2.30	0.45
1:A:440:ILE:C	1:A:440:ILE:HD12	2.42	0.45
1:C:246:TYR:OH	1:C:298:THR:HG22	2.17	0.45
1:C:96:ASN:HA	1:C:686:THR:HB	1.98	0.45
1:B:153:ILE:HD11	1:B:171:VAL:HG11	1.98	0.45
1:B:245:ARG:CD	7:B:1049:HOH:O	2.57	0.45
1:C:252[A]:ARG:NH1	1:C:255:CYS:HA	2.32	0.45
1:C:393:GLU:HA	1:C:412:LEU:HG	1.98	0.45
1:C:607:HIS:CD2	1:C:610:TRP:CH2	3.05	0.45
1:A:449:LYS:HA	1:A:449:LYS:HD3	1.86	0.45
1:A:556:GLY:O	1:A:559:LEU:HB3	2.17	0.45
1:B:247:VAL:O	1:B:263:TYR:HA	2.17	0.45
1:C:356:ASP:C	1:C:357:VAL:HG23	2.41	0.45
1:B:643:ARG:HD2	4:B:802:GOL:H11	1.99	0.44
1:C:191:PRO:O	1:C:192:GLN:C	2.60	0.44
1:C:281:LYS:HG3	7:C:914:HOH:O	2.17	0.44
1:C:373:LYS:HE2	1:C:417:LEU:HB2	1.98	0.44
1:C:454:ILE:C	1:C:455:VAL:HG23	2.43	0.44
1:C:395:PHE:HE2	1:C:422:PHE:CE2	2.35	0.44
1:C:452:MET:HE3	1:C:537:LEU:HD21	2.00	0.44
1:A:362:GLN:HE22	4:A:807:GOL:C2	2.30	0.44
1:C:179:THR:OG1	1:C:212:TYR:OH	2.22	0.44
1:A:289:GLU:OE2	3:A:802:B3P:O2	2.35	0.44
1:A:358:LYS:HB2	1:A:358:LYS:HE2	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:THR:HG21	7:A:1149:HOH:O	2.16	0.44
1:A:504:ILE:HG22	1:A:529:ASP:HB3	2.00	0.44
1:C:262:TRP:NE1	1:C:284:ASP:OD1	2.48	0.44
1:C:289:GLU:O	1:C:304:THR:OG1	2.34	0.44
1:C:114:LEU:HA	1:C:114:LEU:HD12	1.75	0.44
1:A:119:LEU:O	1:A:120:SER:HB3	2.18	0.44
1:A:449:LYS:HD2	7:A:1001:HOH:O	2.17	0.44
1:B:35:ASP:O	1:B:40:LYS:HE2	2.17	0.44
1:C:666:GLN:HG3	7:C:950:HOH:O	2.17	0.44
1:B:172:LYS:NZ	1:B:205:ASN:HD21	2.15	0.44
1:C:60:ARG:NH2	1:C:695:ASP:OD1	2.50	0.44
1:C:9:VAL:O	1:C:10:TYR:C	2.59	0.44
1:C:187:TYR:CE1	1:C:211:TYR:HB2	2.52	0.44
1:A:353:TYR:CD2	4:A:807:GOL:H11	2.53	0.43
1:A:583:MET:HB3	1:A:611:LEU:HD22	1.99	0.43
1:C:166:ASP:OD2	1:C:213:HIS:NE2	2.33	0.43
1:C:363:LEU:HB3	1:C:373:LYS:HB3	2.00	0.43
1:C:442:TYR:OH	1:C:529:ASP:O	2.27	0.43
1:C:267:GLN:NE2	7:C:924:HOH:O	2.51	0.43
1:C:231:GLU:HB3	1:C:234:TRP:CG	2.53	0.43
1:A:71:TYR:CZ	1:A:75:LYS:HE2	2.53	0.43
1:C:553:GLY:O	1:C:554:SER:HB3	2.19	0.43
1:A:323:GLU:HA	1:A:326:TRP:NE1	2.34	0.43
1:C:140:ALA:HB2	1:C:155:PHE:CE2	2.53	0.43
1:A:404:PRO:CG	1:A:427:VAL:HG23	2.48	0.43
1:C:134:GLU:HB2	1:C:180:HIS:HA	1.99	0.43
1:C:329:LEU:HD11	1:C:367:THR:C	2.43	0.43
1:B:407:ILE:CD1	1:B:423[B]:ARG:HH11	2.31	0.43
1:C:218:ASP:CB	7:C:911:HOH:O	2.64	0.43
1:A:273:ILE:HG23	1:A:277:LEU:HD21	2.01	0.43
1:C:168:LEU:HA	1:C:219:GLN:CD	2.43	0.43
1:C:591:ILE:HD12	1:C:591:ILE:HA	1.86	0.43
1:C:17:GLN:HG2	7:C:902:HOH:O	2.19	0.43
1:C:411:ASP:OD1	1:C:413:THR:OG1	2.30	0.43
1:B:243:ASP:OD1	1:B:243:ASP:C	2.61	0.42
1:B:583:MET:HE1	1:B:599:TYR:CD2	2.54	0.42
1:C:73:TYR:O	1:C:93:GLY:HA2	2.19	0.42
1:C:219:GLN:O	1:C:220:SER:C	2.62	0.42
1:C:499:LEU:HD12	1:C:500:ALA:N	2.34	0.42
1:A:79:HIS:HE1	1:A:423:ARG:HH11	1.67	0.42
1:B:296:GLU:O	1:B:297:GLY:C	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:TYR:HB2	1:B:338:LEU:HB3	2.01	0.42
1:C:128:ARG:HG3	1:C:128:ARG:HH11	1.84	0.42
1:C:170:ARG:NH1	1:C:189:SER:OG	2.52	0.42
1:A:69:GLU:OE1	1:A:69:GLU:CA	2.67	0.42
1:A:622:LEU:HD11	1:A:663:SER:CB	2.49	0.42
1:C:520:LEU:HB3	1:C:610:TRP:CH2	2.54	0.42
1:A:266:LEU:HA	1:A:266:LEU:HD23	1.71	0.42
1:B:416:GLU:O	1:B:416:GLU:HG2	2.17	0.42
1:B:441:PHE:CD1	1:B:441:PHE:N	2.86	0.42
1:C:326:TRP:CD1	1:C:326:TRP:N	2.86	0.42
1:C:344:VAL:HG21	1:C:394:ILE:CG2	2.49	0.42
1:C:631:PRO:O	1:C:633:MET:HG3	2.19	0.42
1:A:115:ASP:C	1:A:115:ASP:OD1	2.60	0.42
1:A:336:ASP:CG	1:A:355:HIS:HD1	2.23	0.42
1:C:118:ILE:HG12	1:C:119:LEU:HD23	2.02	0.42
1:C:370:ALA:O	1:C:372:LEU:HD23	2.19	0.42
1:C:432:ALA:O	1:C:435:TYR:O	2.38	0.42
1:C:480:ILE:O	1:C:503:ASN:ND2	2.43	0.42
1:B:295:ASN:ND2	1:B:300:PHE:CZ	2.87	0.42
1:C:83:GLY:CA	1:C:135:ASP:O	2.68	0.42
1:C:314:ILE:HG21	7:C:928:HOH:O	2.18	0.42
1:C:364:HIS:HA	1:C:370:ALA:O	2.20	0.42
1:C:88:TYR:CE1	1:C:101:TYR:HB2	2.55	0.41
1:C:605:LYS:C	1:C:607:HIS:N	2.78	0.41
1:A:250:SER:O	4:A:806:GOL:H12	2.20	0.41
1:C:427:VAL:HG22	1:C:428:LYS:N	2.34	0.41
1:C:65:GLU:C	1:C:65:GLU:OE2	2.63	0.41
1:C:69:GLU:O	1:C:72:ASP:HB3	2.20	0.41
1:C:197:SER:N	7:C:910:HOH:O	2.39	0.41
1:C:381:SER:OG	1:C:482:PRO:HD2	2.20	0.41
1:B:400:SER:OG	1:B:403:SER:HB2	2.21	0.41
1:A:427:VAL:HG11	1:A:430:ILE:HD12	2.01	0.41
1:C:231:GLU:HB3	1:C:234:TRP:CD1	2.56	0.41
1:C:557:GLY:HA2	1:C:560:VAL:HG22	2.02	0.41
1:A:173:PHE:CE2	1:A:591:ILE:HG12	2.55	0.41
1:B:7:PRO:HD3	1:B:49:ILE:HD11	2.02	0.41
1:B:36:SER:CB	7:B:908:HOH:O	2.68	0.41
1:C:494:HIS:HA	1:C:709:ILE:O	2.20	0.41
1:C:583:MET:HE1	1:C:599:TYR:CD2	2.55	0.41
1:C:668:ASN:HA	1:C:669:PRO:HD3	1.85	0.41
1:C:354:LEU:HD12	1:C:354:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:ILE:HG21	1:B:489:LEU:HD13	2.03	0.41
1:B:488:ARG:HB3	1:B:499:LEU:HD22	2.02	0.41
1:C:76:TYR:CD1	1:C:423:ARG:HD3	2.56	0.41
1:C:295:ASN:CG	1:C:300:PHE:CE2	2.98	0.41
1:A:304:THR:O	1:A:311:TYR:HA	2.21	0.41
1:B:31:LEU:HA	1:B:31:LEU:HD23	1.90	0.41
1:B:127:LEU:CD1	1:B:141:TYR:HB2	2.50	0.41
1:B:549:THR:HA	1:B:573:CYS:O	2.21	0.41
1:B:583:MET:HB2	1:B:615:SER:HB2	2.03	0.41
1:B:639:ASP:CG	1:B:676:THR:HA	2.46	0.41
1:C:113:PHE:HE2	1:C:139:PHE:CD2	2.39	0.41
1:C:302:PHE:CD2	1:C:316:ILE:HD12	2.55	0.41
1:C:305:ASN:O	1:C:306:ARG:C	2.64	0.41
1:C:346:SER:CB	1:C:389:LYS:HE3	2.51	0.41
1:C:430:ILE:HB	1:C:435:TYR:HE2	1.86	0.41
1:C:435:TYR:CE1	1:C:457:LYS:HG3	2.56	0.41
1:C:463:ASP:OD1	1:C:463:ASP:C	2.64	0.41
1:A:53:PHE:CZ	1:A:702:ARG:HD3	2.55	0.41
1:B:105:SER:O	1:B:106:LEU:C	2.64	0.41
1:C:37:GLU:CA	1:C:37:GLU:OE1	2.65	0.41
1:C:626:ASP:HA	7:C:941:HOH:O	2.19	0.40
1:C:692:GLU:O	1:C:695:ASP:HB2	2.21	0.40
1:A:96:ASN:HB3	1:A:685:PRO:CB	2.51	0.40
1:B:167:VAL:O	6:B:810:SCN:S	2.79	0.40
1:B:491:PHE:HD1	1:B:495:MET:HE2	1.86	0.40
1:A:146:SER:HB3	1:A:677:LYS:HA	2.03	0.40
1:B:70:LEU:HD22	1:B:430:ILE:CD1	2.51	0.40
1:B:172:LYS:NZ	7:B:963:HOH:O	2.53	0.40
1:C:629:GLN:HB2	1:C:666:GLN:OE1	2.22	0.40
1:A:335:LYS:CE	1:A:356:ASP:OD1	2.69	0.40
1:C:76:TYR:HB2	1:C:407:ILE:HD11	2.04	0.40
1:C:522:ASN:HB3	1:C:525:ASN:ND2	2.36	0.40
1:B:256:ASP:HB2	7:B:907:HOH:O	2.21	0.40
1:C:625:ALA:HB3	1:C:628:ILE:HG12	2.03	0.40
1:C:628:ILE:HA	7:C:948:HOH:O	2.21	0.40
1:C:643:ARG:HD3	1:C:643:ARG:HA	1.88	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%)	674 (96%)	28 (4%)	3 (0%)	30	17
1	B	707/711 (99%)	670 (95%)	33 (5%)	4 (1%)	21	10
1	C	706/711 (99%)	631 (89%)	60 (8%)	15 (2%)	5	1
All	All	2118/2133 (99%)	1975 (93%)	121 (6%)	22 (1%)	12	4

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	371	LEU
1	C	379	VAL
1	C	404	PRO
1	C	427	VAL
1	B	590	THR
1	C	159	ASP
1	B	432	ALA
1	C	72	ASP
1	C	432	ALA
1	C	445	LYS
1	C	446	ASP
1	B	357	VAL
1	C	215	LEU
1	A	270	SER
1	A	357	VAL
1	B	554	SER
1	C	417	LEU
1	C	428	LYS
1	C	421	VAL
1	C	357	VAL
1	C	167	VAL
1	A	578	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	614/617 (100%)	601 (98%)	13 (2%)	47	33
1	B	616/617 (100%)	599 (97%)	17 (3%)	38	23
1	C	615/617 (100%)	578 (94%)	37 (6%)	17	5
All	All	1845/1851 (100%)	1778 (96%)	67 (4%)	31	16

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	59	ILE
1	A	106	LEU
1	A	247	VAL
1	A	270	SER
1	A	271	SER
1	A	278	LYS
1	A	339	GLU
1	A	357	VAL
1	A	423	ARG
1	A	445	LYS
1	A	498	ILE
1	A	598	ASP
1	B	5	GLN
1	B	8	ASP
1	B	23	LYS
1	B	203	SER
1	B	261	LEU
1	B	319	ARG
1	B	334	GLU
1	B	357	VAL
1	B	373	LYS
1	B	374	THR
1	B	416	GLU
1	B	425	VAL
1	B	427	VAL

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Mol	Chain	Res	Type
1	B	445	LYS
1	B	486	VAL
1	B	604	SER
1	B	637	THR
1	C	38	GLN
1	C	65	GLU
1	C	69	GLU
1	C	85	ARG
1	C	119	LEU
1	C	124	THR
1	C	135	ASP
1	C	144	SER
1	C	152	THR
1	C	203	SER
1	C	214	VAL
1	C	219	GLN
1	C	228	PHE
1	C	230	ASP
1	C	240	LEU
1	C	261	LEU
1	C	303	LYS
1	C	308	SER
1	C	346	SER
1	C	359	ASN
1	C	363	LEU
1	C	373	LYS
1	C	377	LEU
1	C	378	ASP
1	C	390	LYS
1	C	393	GLU
1	C	403	SER
1	C	412	LEU
1	C	425	VAL
1	C	430	ILE
1	C	438	VAL
1	C	448	THR
1	C	591	ILE
1	C	598	ASP
1	C	604	SER
1	C	605	LYS
1	C	692	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	GLN
1	A	193	GLN
1	A	205	ASN
1	A	362	GLN
1	A	397	GLN
1	A	477	ASN
1	A	522	ASN
1	A	606	GLN
1	B	56	GLN
1	B	103	GLN
1	B	205	ASN
1	B	267	GLN
1	B	362	GLN
1	B	397	GLN
1	B	503	ASN
1	B	551	ASN
1	B	577	GLN
1	C	17	GLN
1	C	207	HIS
1	C	267	GLN
1	C	307	GLN
1	C	310	ASN
1	C	477	ASN
1	C	551	ASN
1	C	577	GLN
1	C	593	HIS
1	C	668	ASN

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

38 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	$\# Z > 2$
6	SCN	B	803	-	1,2,2	1.08	0	0,1,1	-	-
6	SCN	A	814	-	1,2,2	0.73	0	0,1,1	-	-
2	A1CQZ	B	801	1	32,32,33	1.17	3 (9%)	44,44,46	2.10	12 (27%)
4	GOL	C	804	-	5,5,5	0.21	0	5,5,5	0.44	0
5	PEG	A	805	-	6,6,6	0.84	0	5,5,5	0.58	0
4	GOL	C	802	-	5,5,5	0.18	0	5,5,5	0.41	0
4	GOL	B	804	-	5,5,5	0.23	0	5,5,5	0.44	0
6	SCN	B	811	-	1,2,2	0.42	0	0,1,1	-	-
4	GOL	B	805	-	5,5,5	0.36	0	5,5,5	0.70	0
2	A1CQZ	C	801	1	32,32,33	1.04	2 (6%)	44,44,46	1.59	6 (13%)
6	SCN	A	810	-	1,2,2	0.85	0	0,1,1	-	-
6	SCN	B	810	-	1,2,2	0.76	0	0,1,1	-	-
6	SCN	C	806	-	1,2,2	0.61	0	0,1,1	-	-
3	B3P	A	802	-	18,18,18	1.03	2 (11%)	23,23,23	0.99	2 (8%)
6	SCN	A	809	-	1,2,2	0.74	0	0,1,1	-	-
6	SCN	B	806	-	1,2,2	0.19	0	0,1,1	-	-
4	GOL	A	806	-	5,5,5	0.62	0	5,5,5	0.88	0
4	GOL	A	803	-	5,5,5	0.94	0	5,5,5	0.67	0
6	SCN	B	808	-	1,2,2	0.11	0	0,1,1	-	-
4	GOL	B	802	-	5,5,5	0.70	0	5,5,5	0.76	0
6	SCN	B	812	-	1,2,2	1.01	0	0,1,1	-	-
6	SCN	B	809	-	1,2,2	1.22	0	0,1,1	-	-
4	GOL	B	813	-	5,5,5	0.25	0	5,5,5	0.37	0
6	SCN	A	817	-	1,2,2	1.09	0	0,1,1	-	-
2	A1CQZ	A	801	1	32,32,33	1.22	2 (6%)	44,44,46	1.60	7 (15%)
6	SCN	C	807	-	1,2,2	1.04	0	0,1,1	-	-
6	SCN	A	811	-	1,2,2	0.48	0	0,1,1	-	-
4	GOL	C	803	-	5,5,5	0.18	0	5,5,5	0.43	0
4	GOL	A	804	-	5,5,5	0.25	0	5,5,5	0.90	0
6	SCN	B	807	-	1,2,2	0.32	0	0,1,1	-	-
4	GOL	A	807	-	5,5,5	0.36	0	5,5,5	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	818	-	5,5,5	0.15	0	5,5,5	0.43	0
3	B3P	A	812	-	18,18,18	0.93	2 (11%)	23,23,23	1.72	6 (26%)
6	SCN	A	808	-	1,2,2	1.03	0	0,1,1	-	-
6	SCN	A	815	-	1,2,2	0.13	0	0,1,1	-	-
6	SCN	A	813	-	1,2,2	0.65	0	0,1,1	-	-
6	SCN	C	805	-	1,2,2	0.39	0	0,1,1	-	-
6	SCN	A	816	-	1,2,2	0.67	0	0,1,1	-	-

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
4	GOL	A	806	-	-	2/4/4/4	-
4	GOL	A	818	-	-	1/4/4/4	-
2	A1CQZ	A	801	1	-	6/18/25/25	0/4/4/4
2	A1CQZ	B	801	1	-	4/18/25/25	0/4/4/4
4	GOL	A	803	-	-	0/4/4/4	-
4	GOL	B	802	-	-	2/4/4/4	-
3	B3P	A	812	-	-	11/28/28/28	-
4	GOL	C	804	-	-	2/4/4/4	-
4	GOL	C	802	-	-	4/4/4/4	-
5	PEG	A	805	-	-	3/4/4/4	-
4	GOL	B	804	-	-	4/4/4/4	-
4	GOL	C	803	-	-	2/4/4/4	-
4	GOL	A	804	-	-	2/4/4/4	-
4	GOL	B	805	-	-	0/4/4/4	-
2	A1CQZ	C	801	1	-	10/18/25/25	0/4/4/4
4	GOL	A	807	-	-	2/4/4/4	-
3	B3P	A	802	-	-	3/28/28/28	-
4	GOL	B	813	-	-	2/4/4/4	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	A1CQZ	C2-N1	5.56	1.37	1.32
2	B	801	A1CQZ	C11-N3	-3.03	1.28	1.34
2	B	801	A1CQZ	C11-N2	-2.83	1.33	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	A1CQZ	C12-N3	-2.67	1.28	1.34
2	A	801	A1CQZ	C12-C13	2.38	1.42	1.39
2	C	801	A1CQZ	C12-C13	2.35	1.42	1.39
3	A	802	B3P	C7-C4	2.33	1.56	1.53
2	C	801	A1CQZ	C11-N2	-2.27	1.33	1.35
3	A	812	B3P	C11-C8	2.12	1.55	1.53
3	A	802	B3P	C11-C8	2.06	1.55	1.53
3	A	812	B3P	C10-C8	2.05	1.55	1.53

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	A1CQZ	C22-C2-N1	-8.08	107.59	110.76
2	A	801	A1CQZ	C22-C2-N1	-5.88	108.45	110.76
2	C	801	A1CQZ	C22-C2-N1	-5.16	108.74	110.76
2	C	801	A1CQZ	C11-C22-C2	4.40	106.56	105.15
2	B	801	A1CQZ	C4-C3-N2	-4.25	107.45	111.93
3	A	812	B3P	O3-C11-C8	3.75	119.31	111.68
2	B	801	A1CQZ	C11-C22-C2	3.70	106.34	105.15
2	B	801	A1CQZ	C3-N2-N1	3.57	122.82	119.75
2	A	801	A1CQZ	C4-C3-N2	3.53	115.64	111.93
3	A	812	B3P	O2-C10-C8	3.32	118.44	111.68
2	C	801	A1CQZ	C4-C3-N2	-3.25	108.50	111.93
2	C	801	A1CQZ	C3-N2-N1	3.24	122.53	119.75
3	A	812	B3P	O5-C6-C4	3.20	118.20	111.68
3	A	812	B3P	C2-N2-C8	3.12	120.73	116.17
2	B	801	A1CQZ	C16-C15-N4	2.86	117.93	110.90
2	B	801	A1CQZ	C21-C13-C14	2.73	129.44	120.40
2	A	801	A1CQZ	O1-C14-C13	2.72	126.28	120.90
2	B	801	A1CQZ	C2-N1-N2	2.62	107.93	104.97
2	B	801	A1CQZ	C3-C4-C5	2.55	119.36	112.15
2	B	801	A1CQZ	C21-C22-C11	-2.47	115.18	117.67
2	A	801	A1CQZ	C3-N2-N1	2.45	121.86	119.75
3	A	802	B3P	O4-C5-C4	2.38	116.52	111.68
3	A	802	B3P	C5-C4-N1	-2.33	102.06	109.02
2	A	801	A1CQZ	C1-C2-C22	2.26	131.47	127.56
2	B	801	A1CQZ	O2-C16-N5	-2.20	118.20	122.12
2	B	801	A1CQZ	C13-C14-N4	-2.17	112.61	117.12
3	A	812	B3P	C3-N1-C4	2.17	119.34	116.17
2	B	801	A1CQZ	C12-C13-C14	-2.15	113.72	120.58
2	A	801	A1CQZ	C2-N1-N2	2.07	107.30	104.97
2	A	801	A1CQZ	C21-C22-C2	2.06	138.88	136.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	812	B3P	C5-C4-N1	-2.04	102.94	109.02
2	C	801	A1CQZ	C21-C13-C12	2.03	120.01	117.92
2	C	801	A1CQZ	C3-C4-C5	2.01	117.84	112.15

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	A1CQZ	N2-C3-C4-C5
2	B	801	A1CQZ	C12-C13-C14-O1
2	C	801	A1CQZ	O2-C16-N5-C17
2	C	801	A1CQZ	C15-C16-N5-C17
2	C	801	A1CQZ	O2-C16-N5-C20
2	C	801	A1CQZ	C15-C16-N5-C20
3	A	812	B3P	C1-C2-N2-C8
3	A	812	B3P	C6-C4-N1-C3
3	A	812	B3P	C7-C4-N1-C3
4	A	804	GOL	C1-C2-C3-O3
4	A	806	GOL	C1-C2-C3-O3
4	A	806	GOL	O2-C2-C3-O3
4	A	807	GOL	O1-C1-C2-C3
4	B	802	GOL	C1-C2-C3-O3
4	B	804	GOL	O1-C1-C2-C3
4	C	802	GOL	O1-C1-C2-C3
4	C	802	GOL	C1-C2-C3-O3
4	C	803	GOL	C1-C2-C3-O3
2	B	801	A1CQZ	C21-C13-C14-N4
2	A	801	A1CQZ	C12-C13-C14-O1
2	A	801	A1CQZ	C21-C13-C14-O1
2	A	801	A1CQZ	C12-C13-C14-N4
2	B	801	A1CQZ	C12-C13-C14-N4
2	C	801	A1CQZ	C12-C13-C14-N4
2	A	801	A1CQZ	C21-C13-C14-N4
2	B	801	A1CQZ	C21-C13-C14-O1
2	C	801	A1CQZ	C12-C13-C14-O1
2	C	801	A1CQZ	C21-C13-C14-N4
4	B	802	GOL	O2-C2-C3-O3
3	A	812	B3P	C1-C3-N1-C4
4	B	804	GOL	C1-C2-C3-O3
4	B	813	GOL	O1-C1-C2-C3
4	A	804	GOL	O2-C2-C3-O3
4	A	807	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	B	804	GOL	O1-C1-C2-O2
4	C	803	GOL	O2-C2-C3-O3
3	A	812	B3P	N1-C4-C6-O5
5	A	805	PEG	O2-C3-C4-O4
2	C	801	A1CQZ	C21-C13-C14-O1
5	A	805	PEG	O1-C1-C2-O2
4	C	802	GOL	O1-C1-C2-O2
4	C	802	GOL	O2-C2-C3-O3
3	A	812	B3P	C5-C4-N1-C3
4	A	818	GOL	O1-C1-C2-O2
4	B	804	GOL	O2-C2-C3-O3
2	C	801	A1CQZ	C3-C4-C5-C6
2	C	801	A1CQZ	C3-C4-C5-C10
4	B	813	GOL	O1-C1-C2-O2
3	A	802	B3P	N1-C4-C5-O4
3	A	802	B3P	C7-C4-C5-O4
3	A	812	B3P	C7-C4-C6-O5
3	A	812	B3P	C2-C1-C3-N1
5	A	805	PEG	C4-C3-O2-C2
3	A	812	B3P	O3-C11-C8-C10
2	A	801	A1CQZ	C4-C3-N2-N1
4	C	804	GOL	C1-C2-C3-O3
3	A	812	B3P	O3-C11-C8-N2
3	A	802	B3P	C1-C2-N2-C8
3	A	812	B3P	C11-C8-C9-O1
4	C	804	GOL	O2-C2-C3-O3

There are no ring outliers.

16 monomers are involved in 31 short contacts:

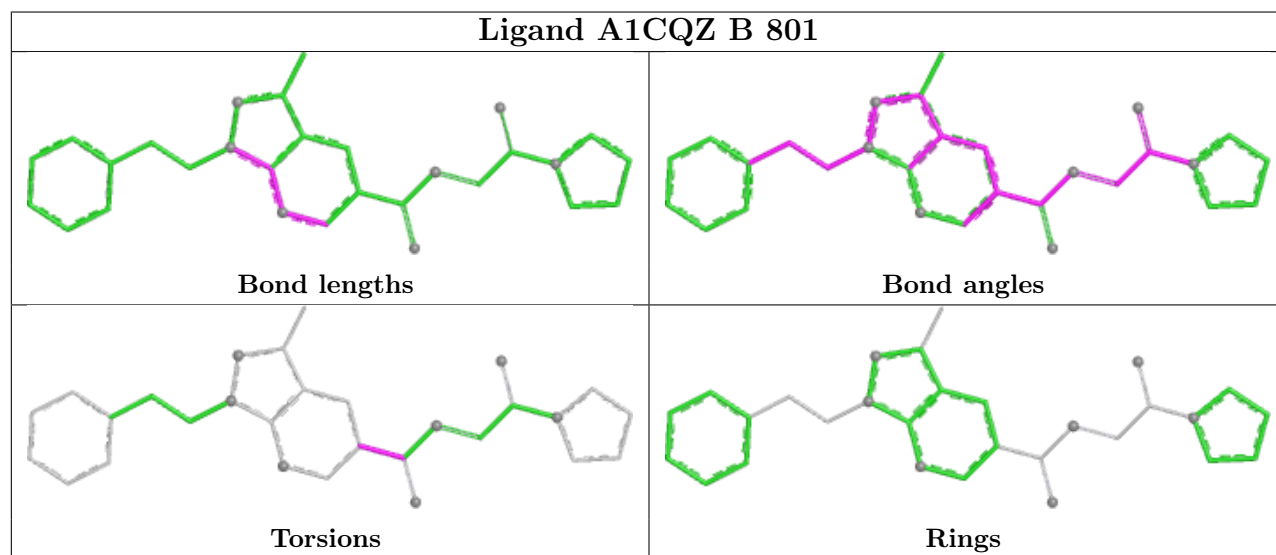
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	805	PEG	5	0
6	B	810	SCN	3	0
6	C	806	SCN	1	0
3	A	802	B3P	2	0
6	A	809	SCN	1	0
6	B	806	SCN	1	0
4	A	806	GOL	5	0
4	A	803	GOL	1	0
4	B	802	GOL	1	0
6	B	812	SCN	1	0
4	B	813	GOL	1	0

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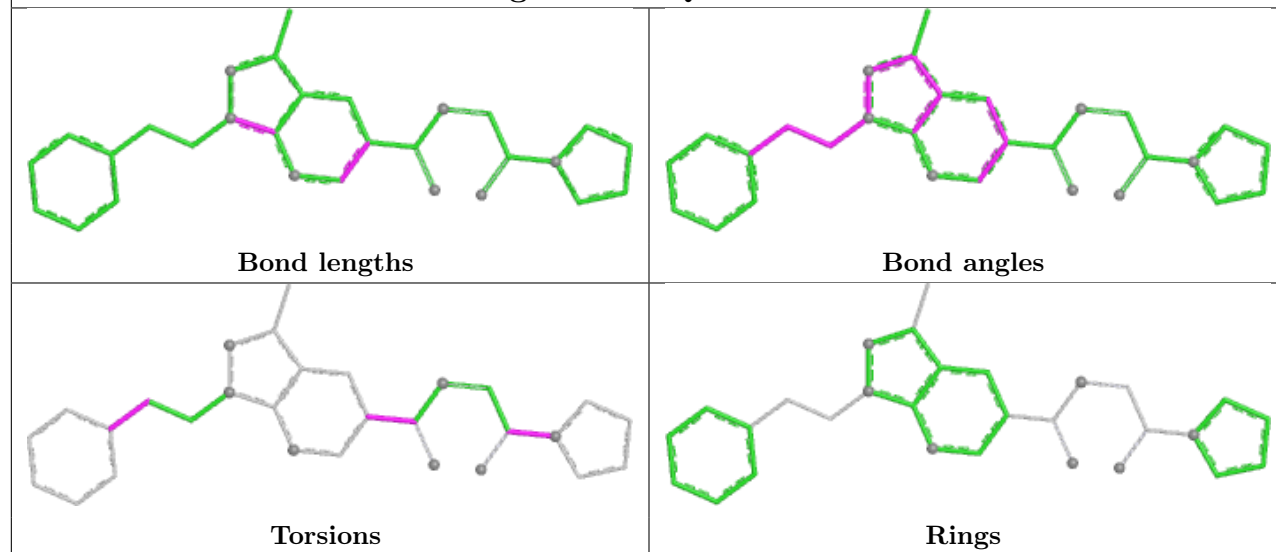
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	811	SCN	1	0
4	A	807	GOL	5	0
3	A	812	B3P	1	0
6	A	815	SCN	1	0
6	C	805	SCN	1	0

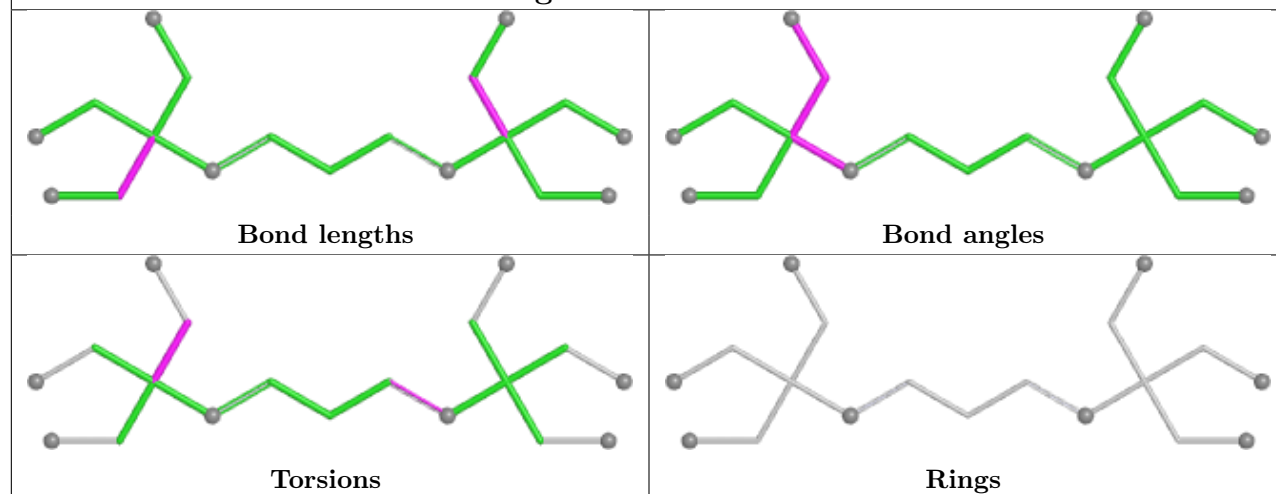
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



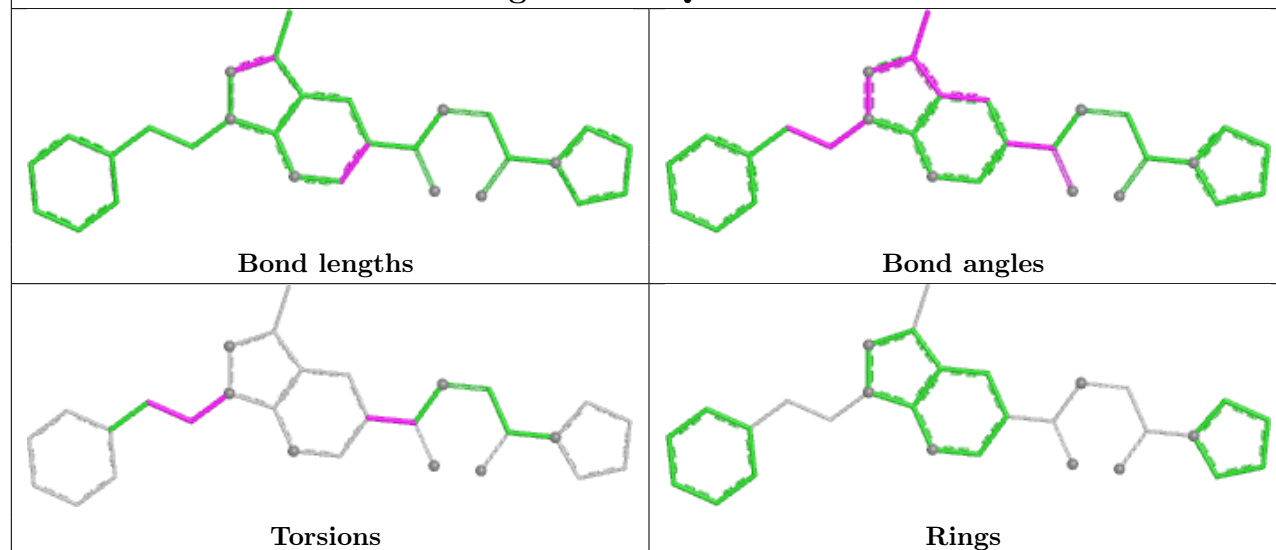
Ligand A1CQZ C 801

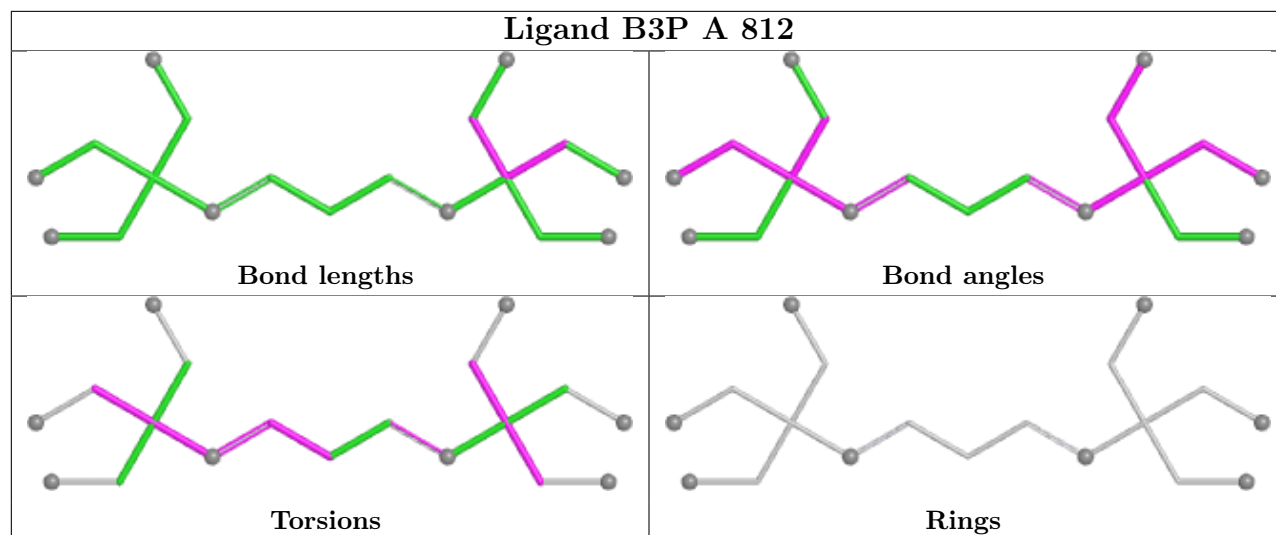


Ligand B3P A 802



Ligand A1CQZ A 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

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	707/711 (99%)	-0.72	0 100 100	9, 19, 38, 61	0
1	B	707/711 (99%)	-0.57	1 (0%) 92 93	10, 22, 41, 70	2 (0%)
1	C	707/711 (99%)	0.61	57 (8%) 18 19	19, 44, 72, 108	1 (0%)
All	All	2121/2133 (99%)	-0.23	58 (2%) 56 59	9, 25, 62, 108	3 (0%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	430	ILE	4.8
1	C	371	LEU	4.6
1	C	379	VAL	4.0
1	C	331	PRO	4.0
1	C	330	VAL	3.7
1	C	4	LEU	3.6
1	C	215	LEU	3.5
1	C	406	ILE	3.5
1	C	321	PRO	3.4
1	C	427	VAL	3.3
1	C	426	THR	3.2
1	C	405	GLY	3.1
1	C	277	LEU	3.1
1	C	408	TYR	3.1
1	C	226	ALA	3.0
1	C	246	TYR	3.0
1	C	229	PRO	3.0
1	C	425	VAL	2.9
1	C	350	VAL	2.8
1	C	302	PHE	2.8
1	C	223	ILE	2.8
1	C	396	TYR	2.7
1	C	428	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	293	VAL	2.7
1	C	326	TRP	2.6
1	C	228	PHE	2.6
1	C	368	THR	2.6
1	C	429	GLY	2.6
1	C	138	TYR	2.6
1	C	377	LEU	2.6
1	C	376	PRO	2.5
1	C	282	LEU	2.5
1	C	272	GLY	2.4
1	C	313	VAL	2.4
1	C	372	LEU	2.4
1	C	329	LEU	2.3
1	C	279	TRP	2.2
1	C	421	VAL	2.2
1	B	4	LEU	2.2
1	C	283	ILE	2.2
1	C	106	LEU	2.2
1	C	363	LEU	2.2
1	C	73	TYR	2.2
1	C	76	TYR	2.2
1	C	419	PRO	2.2
1	C	102	VAL	2.1
1	C	374	THR	2.1
1	C	333	HIS	2.1
1	C	432	ALA	2.1
1	C	118	ILE	2.1
1	C	351	LEU	2.1
1	C	301	THR	2.0
1	C	437	THR	2.0
1	C	191	PRO	2.0
1	C	357	VAL	2.0
1	C	422	PHE	2.0
1	C	367	THR	2.0
1	C	438	VAL	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(Å ²)	Q<0.9
4	GOL	B	813	6/6	0.80	0.23	18,25,43,43	14
4	GOL	A	806	6/6	0.82	0.14	38,41,45,47	3
3	B3P	A	812	19/19	0.84	0.13	38,58,73,79	8
4	GOL	C	804	6/6	0.85	0.11	43,52,57,57	3
6	SCN	C	806	3/3	0.85	0.11	33,33,56,69	0
4	GOL	B	805	6/6	0.86	0.12	36,39,44,51	3
4	GOL	A	818	6/6	0.88	0.11	42,43,54,58	3
5	PEG	A	805	7/7	0.89	0.09	31,38,43,43	2
4	GOL	C	803	6/6	0.89	0.10	37,43,49,51	3
6	SCN	A	808	3/3	0.90	0.13	29,29,40,50	0
6	SCN	A	813	3/3	0.90	0.10	30,30,37,55	0
6	SCN	A	815	3/3	0.90	0.14	60,60,63,68	0
6	SCN	B	811	3/3	0.90	0.14	54,54,61,64	0
4	GOL	A	804	6/6	0.90	0.09	29,37,43,46	3
6	SCN	B	810	3/3	0.91	0.11	39,39,48,54	0
6	SCN	A	814	3/3	0.91	0.14	44,44,44,50	0
6	SCN	A	817	3/3	0.91	0.11	20,20,26,63	0
6	SCN	C	805	3/3	0.92	0.11	48,48,49,51	0
6	SCN	B	806	3/3	0.92	0.08	39,39,45,54	0
4	GOL	B	804	6/6	0.93	0.07	28,33,43,43	3
4	GOL	A	807	6/6	0.93	0.10	27,37,43,43	3
6	SCN	B	807	3/3	0.94	0.10	33,33,46,50	0
6	SCN	A	809	3/3	0.94	0.11	42,42,49,50	0
6	SCN	A	810	3/3	0.94	0.10	48,48,54,56	0
6	SCN	A	811	3/3	0.94	0.12	36,36,40,44	0
4	GOL	B	802	6/6	0.94	0.10	19,26,43,43	3
6	SCN	C	807	3/3	0.94	0.07	33,33,44,57	0
3	B3P	A	802	19/19	0.95	0.06	17,30,43,43	8
2	A1CQZ	C	801	29/30	0.95	0.07	22,31,44,47	3
6	SCN	B	812	3/3	0.95	0.12	33,33,35,42	0
4	GOL	C	802	6/6	0.95	0.11	21,37,43,51	3
4	GOL	A	803	6/6	0.95	0.13	12,25,43,43	3

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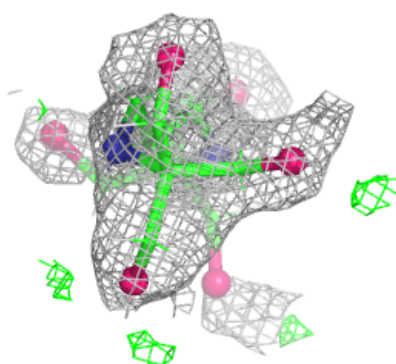
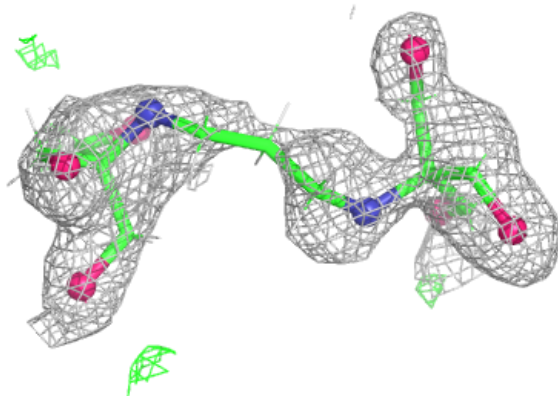
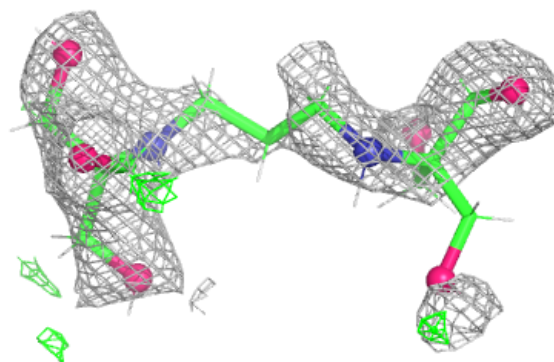
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SCN	B	808	3/3	0.95	0.08	37,37,46,49	0
2	A1CQZ	B	801	29/30	0.96	0.06	18,25,34,43	3
6	SCN	B	803	3/3	0.97	0.05	24,24,25,37	0
2	A1CQZ	A	801	29/30	0.97	0.06	15,20,38,43	3
6	SCN	B	809	3/3	0.97	0.08	30,30,36,38	0
6	SCN	A	816	3/3	0.98	0.11	31,31,34,46	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.

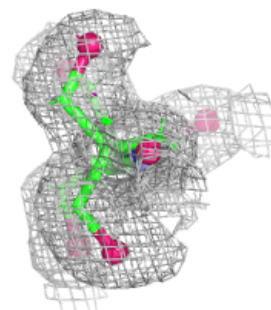
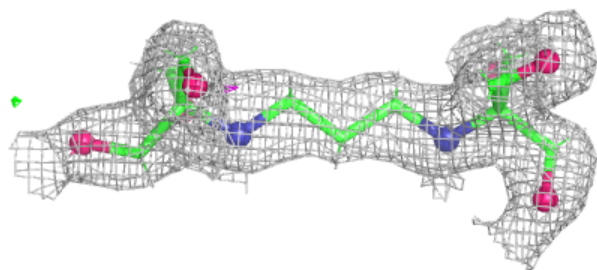
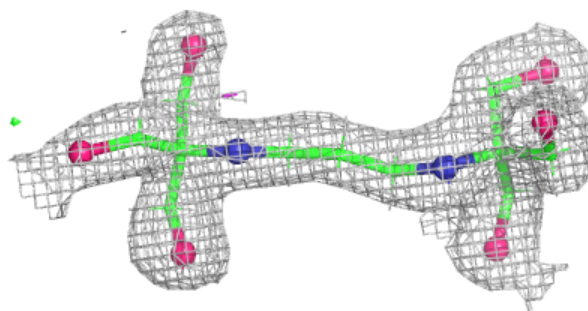
Electron density around B3P A 812:

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

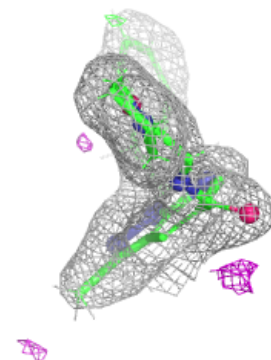
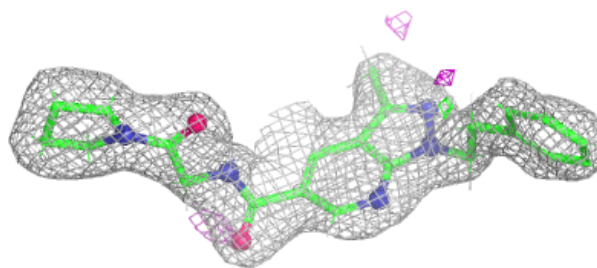
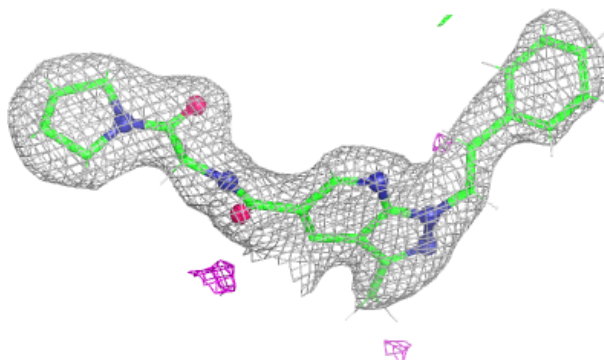


Electron density around B3P A 802:

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

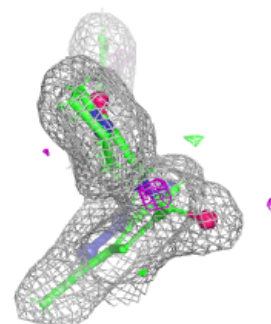
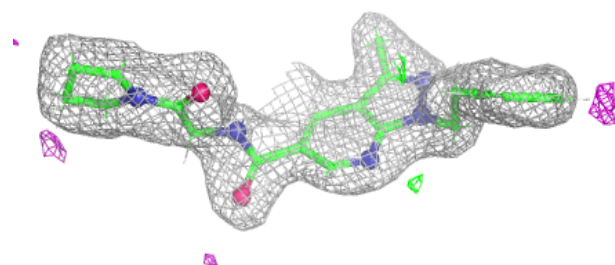
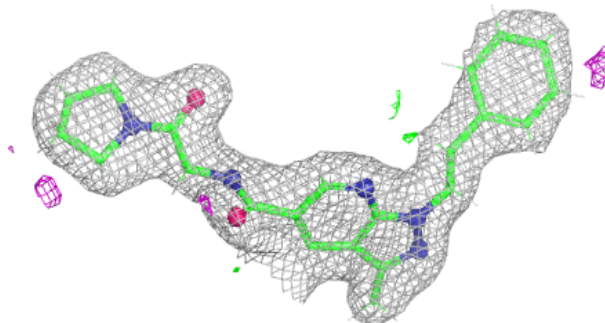
**Electron density around A1CQZ C 801:**

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

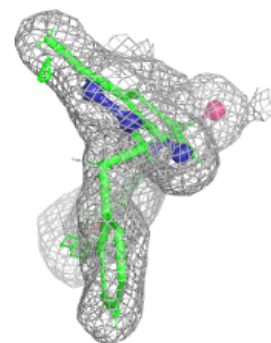
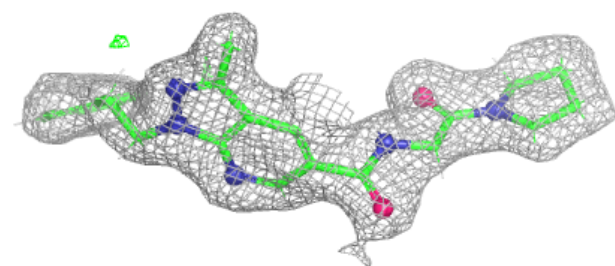
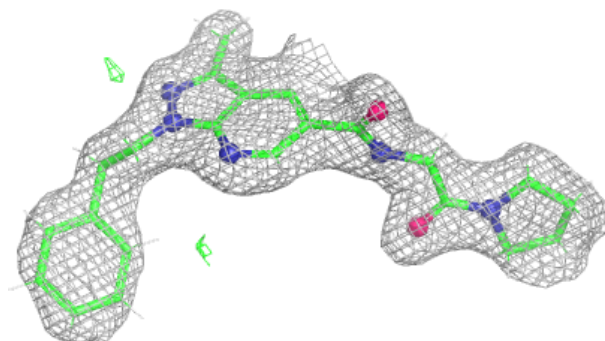


Electron density around A1CQZ B 801:

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

**Electron density around A1CQZ 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.