



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:17 AM UTC

PDB ID : 9Q62 / pdb_00009q62
Title : Human prolyl endopeptidase (PREP) - complex with KT-2-108
Authors : Fucci, I.J.; Thakur, K.; Pandian, J.; Yoo, E.; Monteiro, D.C.F.
Deposited on : 2025-08-21
Resolution : 1.83 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

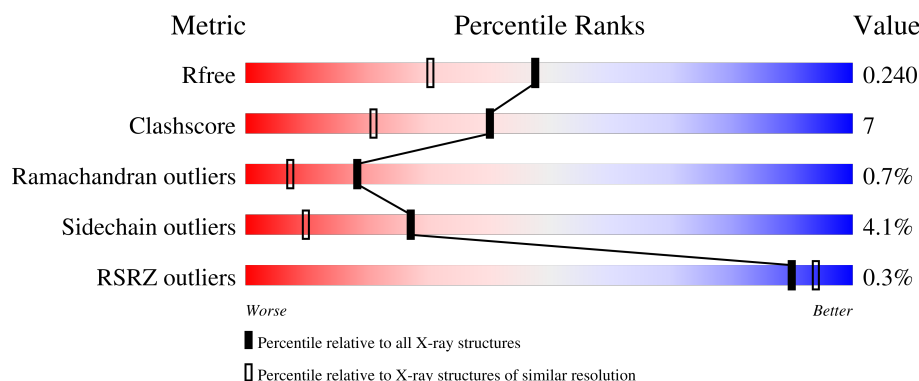
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.83 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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	 82% 15% ..
1	B	711	 77% 19% . ..
1	C	711	 74% 20% 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
5	SCN	A	806	-	-	X	-
5	SCN	A	815	-	-	X	-
5	SCN	B	808	-	-	X	-
6	GOL	A	809	-	X	-	-
6	GOL	B	804	-	-	X	-
6	GOL	C	806	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 35500 atoms, of which 16813 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	2	0
			11215	3648	5531	941	1068	27			
1	B	707	Total	C	H	N	O	S	177	0	0
			11187	3639	5514	941	1066	27			
1	C	707	Total	C	H	N	O	S	177	0	0
			11187	3639	5514	941	1066	27			

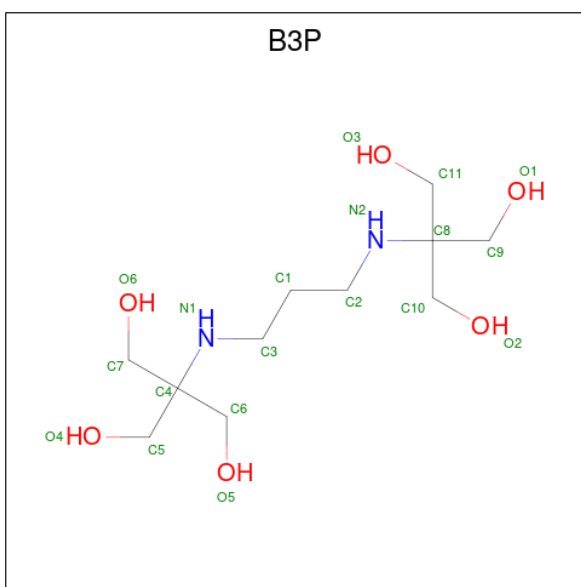
There are 3 discrepancies between the modelled and reference sequences:

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 POTASSIUM ION (CCD ID: K) (formula: K).

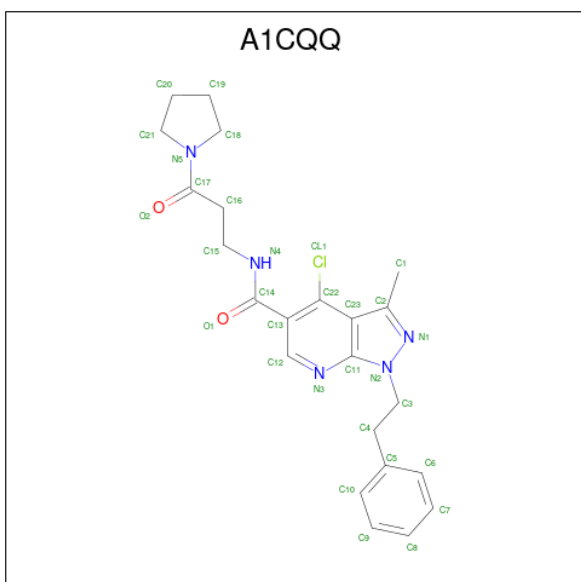
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		
2	B	1	Total	K	0	0
			1	1		
2	C	1	Total	K	0	0
			1	1		

- Molecule 3 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYLAMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: B3P) (formula: C₁₁H₂₆N₂O₆).



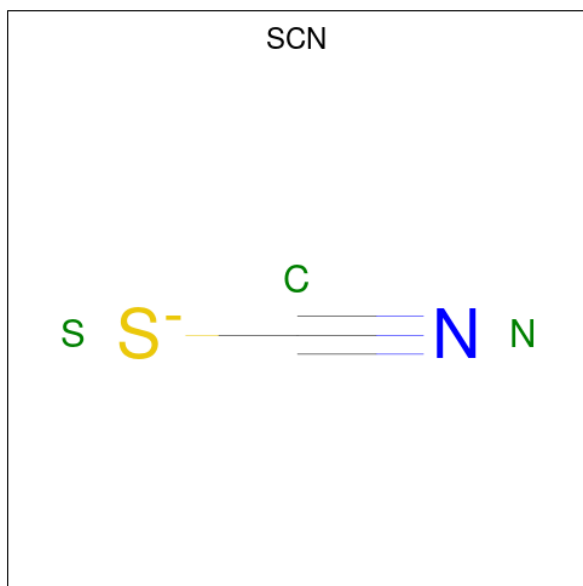
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 45	C 11	H 26	N 2	O 6	8	0
3	A	1	Total 45	C 11	H 26	N 2	O 6	8	0
3	B	1	Total 45	C 11	H 26	N 2	O 6	8	0
3	C	1	Total 45	C 11	H 26	N 2	O 6	8	0

- Molecule 4 is 4-chloro-3-methyl-N-[3-oxo-3-(pyrrolidin-1-yl)propyl]-1-(2-phenylethyl)-1H-pyrazolo[3,4-b]pyridine-5-carboxamide (CCD ID: A1CQQ) (formula: $C_{23}H_{26}ClN_5O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	3	0
			56	23	26	5	2		
4	B	1	Total	C	H	N	O	3	0
			56	23	26	5	2		
4	C	1	Total	C	H	N	O	3	0
			56	23	26	5	2		

- Molecule 5 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



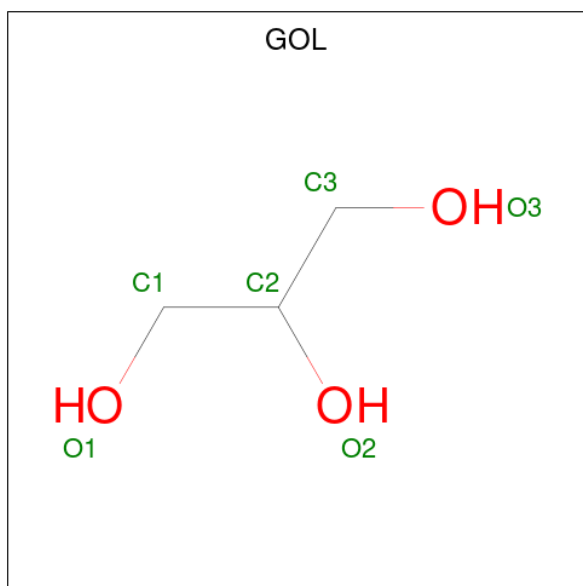
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	S	0	0
			3	1	1	1		
5	A	1	Total	C	N	S	0	0
			3	1	1	1		
5	A	1	Total	C	N	S	0	0
			3	1	1	1		
5	A	1	Total	C	N	S	0	0
			3	1	1	1		
5	A	1	Total	C	N	S	0	0
			3	1	1	1		
5	A	1	Total	C	N	S	0	0
			3	1	1	1		
5	B	1	Total	C	N	S	0	0
			3	1	1	1		

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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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

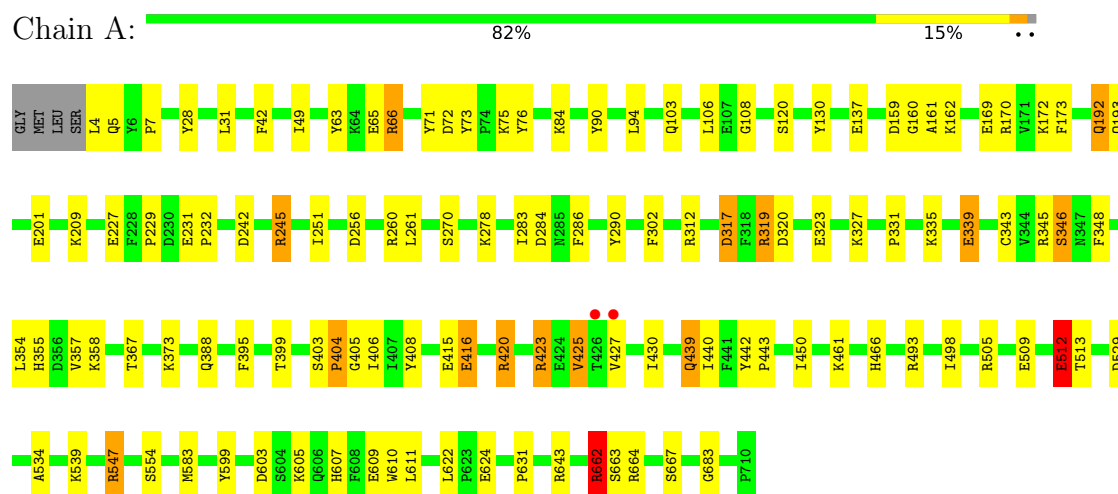
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	631	Total	O	0	0
			631	631		
7	B	370	Total	O	0	0
			370	370		
7	C	388	Total	O	0	0
			388	388		

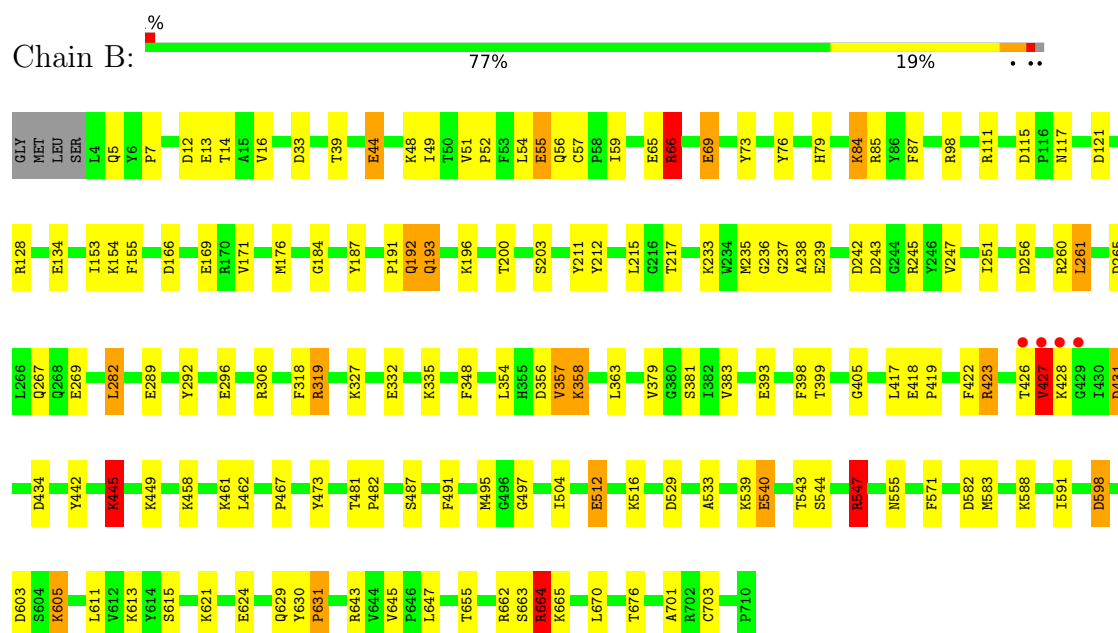
3 Residue-property plots

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

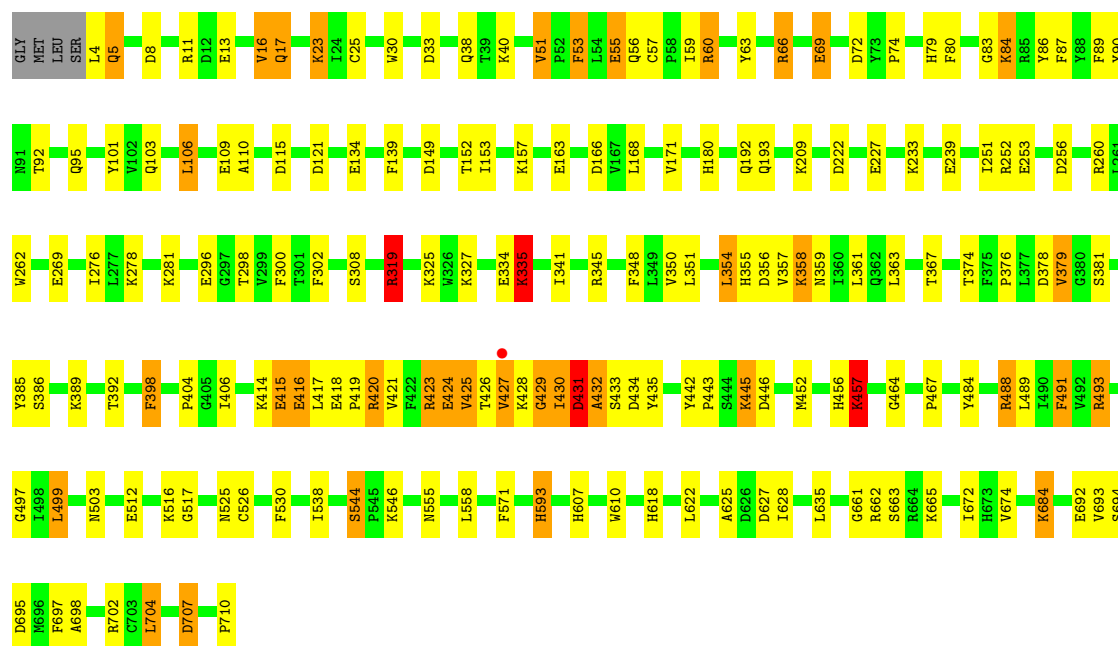


• Molecule 1: Prolyl endopeptidase



• Molecule 1: Prolyl endopeptidase

Chain C:  74% 20% 5% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.19Å 67.08Å 157.16Å 90.00° 99.20° 90.00°	Depositor
Resolution (Å)	43.90 – 1.83 43.90 – 1.83	Depositor EDS
% Data completeness (in resolution range)	74.4 (43.90-1.83) 74.9 (43.90-1.83)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 1.83Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.100)	Depositor
R, R_{free}	0.173 , 0.239 0.173 , 0.240	Depositor DCC
R_{free} test set	9652 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	19.0	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 33.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	35500	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SCN, A1CQQ, K, GOL, B3P

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	1.07	8/5842 (0.1%)	1.56	47/7920 (0.6%)
1	B	0.95	1/5825 (0.0%)	1.59	71/7897 (0.9%)
1	C	0.98	1/5825 (0.0%)	1.57	74/7897 (0.9%)
All	All	1.00	10/17492 (0.1%)	1.58	192/23714 (0.8%)

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	8
1	B	0	9
1	C	0	6
All	All	0	23

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	663	SER	CA-CB	-6.26	1.43	1.53
1	A	420	ARG	NE-CZ	5.80	1.39	1.33
1	A	512	GLU	CD-OE1	5.78	1.36	1.25
1	A	631	PRO	CA-CB	-5.62	1.45	1.53
1	C	593	HIS	ND1-CE1	5.50	1.38	1.32
1	B	319	ARG	NE-CZ	5.34	1.39	1.33
1	A	534	ALA	CA-CB	-5.29	1.45	1.53
1	A	603	ASP	C-O	-5.12	1.17	1.24
1	A	72	ASP	C-O	-5.12	1.18	1.23
1	A	439	GLN	C-O	-5.01	1.18	1.24

All (192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	445	LYS	CB-CA-C	-12.27	90.37	110.74
1	A	339	GLU	CB-CA-C	-10.29	91.88	110.70
1	B	335	LYS	CB-CA-C	10.22	125.08	109.13
1	C	445	LYS	N-CA-CB	-9.91	95.43	110.20
1	B	603	ASP	CA-CB-CG	9.54	122.14	112.60
1	C	25	CYS	CB-CA-C	9.37	125.11	109.84
1	C	296	GLU	CB-CG-CD	9.20	128.24	112.60
1	C	327	LYS	CB-CA-C	-9.16	92.89	109.38
1	C	423	ARG	CB-CA-C	-8.41	94.98	110.62
1	C	427	VAL	N-CA-CB	8.32	120.06	110.82
1	A	66	ARG	CG-CD-NE	-8.24	93.87	112.00
1	C	253	GLU	CB-CG-CD	7.93	126.09	112.60
1	A	403	SER	CB-CA-C	-7.76	99.73	110.13
1	B	327	LYS	CB-CA-C	-7.61	95.68	109.38
1	B	399	THR	CA-CB-OG1	-7.57	98.24	109.60
1	C	526	CYS	CB-CA-C	-7.57	98.95	110.90
1	B	66	ARG	NE-CZ-NH1	-7.48	114.02	121.50
1	C	499	LEU	N-CA-CB	-7.37	99.00	110.57
1	C	335	LYS	N-CA-CB	-7.36	98.05	110.49
1	C	367	THR	CA-CB-OG1	-7.32	98.61	109.60
1	A	137	GLU	CG-CD-OE1	7.32	135.23	118.40
1	C	166	ASP	CA-CB-CG	7.19	119.79	112.60
1	A	169	GLU	N-CA-CB	-7.19	99.86	111.22
1	B	55	GLU	CG-CD-OE2	-7.18	101.88	118.40
1	B	655	THR	OG1-CB-CG2	-7.12	95.06	109.30
1	B	332	GLU	CB-CA-C	-7.07	99.24	109.84
1	C	69	GLU	CB-CG-CD	6.97	124.46	112.60
1	B	379	VAL	N-CA-CB	6.95	118.11	110.53
1	A	663	SER	CA-CB-OG	-6.92	97.26	111.10
1	B	84	LYS	CB-CA-C	-6.92	98.86	110.56
1	B	422	PHE	N-CA-CB	-6.85	100.05	110.26
1	C	80	PHE	CA-CB-CG	6.83	120.63	113.80
1	B	419	PRO	CB-CA-C	-6.81	102.91	111.56
1	B	676	THR	CA-CB-OG1	-6.80	99.41	109.60
1	C	149	ASP	CA-CB-CG	6.80	119.40	112.60
1	C	452	MET	CG-SD-CE	6.79	115.84	100.90
1	B	383	VAL	N-CA-C	-6.67	106.63	113.10
1	B	613	LYS	CG-CD-CE	-6.66	95.98	111.30
1	C	13	GLU	CB-CG-CD	6.66	123.92	112.60
1	C	457	LYS	CB-CA-C	6.56	120.87	109.65
1	C	379	VAL	N-CA-CB	-6.55	103.62	110.95
1	C	252	ARG	NE-CZ-NH2	6.52	125.07	119.20
1	C	446	ASP	CA-CB-CG	6.50	119.10	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	13	GLU	CB-CG-CD	6.49	123.63	112.60
1	A	201	GLU	CB-CG-CD	6.49	123.63	112.60
1	A	327	LYS	CB-CG-CD	6.43	126.09	111.30
1	C	121	ASP	CB-CA-C	-6.41	97.42	109.72
1	C	421	VAL	N-CA-CB	6.39	118.10	110.95
1	B	56	GLN	N-CA-C	-6.37	105.61	113.19
1	C	84	LYS	CB-CA-C	-6.35	100.21	110.74
1	B	217	THR	OG1-CB-CG2	6.25	121.79	109.30
1	A	509	GLU	CB-CG-CD	6.24	123.21	112.60
1	B	193	GLN	OE1-CD-NE2	-6.24	116.36	122.60
1	B	66	ARG	CG-CD-NE	-6.23	98.29	112.00
1	A	512	GLU	CB-CG-CD	6.21	123.16	112.60
1	C	662	ARG	CD-NE-CZ	6.19	133.06	124.40
1	A	320	ASP	CA-CB-CG	6.17	118.77	112.60
1	C	53	PHE	N-CA-C	-6.15	104.68	111.82
1	B	282	LEU	N-CA-CB	-6.12	101.14	110.01
1	C	60	ARG	NE-CZ-NH1	-6.07	115.43	121.50
1	C	374	THR	CA-CB-OG1	-6.06	100.50	109.60
1	B	243	ASP	CA-CB-CG	6.04	118.64	112.60
1	C	416	GLU	CB-CG-CD	-6.04	102.33	112.60
1	A	664	ARG	CA-CB-CG	-6.03	102.05	114.10
1	B	598	ASP	CA-CB-CG	6.02	118.62	112.60
1	B	358	LYS	CB-CG-CD	6.01	125.13	111.30
1	C	424	GLU	N-CA-CB	-6.01	100.35	110.99
1	A	622	LEU	CB-CA-C	6.01	119.06	109.62
1	A	622	LEU	N-CA-CB	-6.01	98.98	109.73
1	B	265	ASP	CA-CB-CG	6.01	118.61	112.60
1	A	547	ARG	CB-CA-C	-5.98	99.59	109.99
1	B	169	GLU	CA-CB-CG	-5.96	102.19	114.10
1	A	339	GLU	N-CA-CB	5.95	119.07	110.20
1	B	84	LYS	N-CA-CB	5.95	119.25	110.56
1	C	423	ARG	N-CA-CB	5.94	120.76	111.56
1	A	159	ASP	CA-CB-CG	5.93	118.53	112.60
1	A	547	ARG	CG-CD-NE	-5.93	98.95	112.00
1	A	367	THR	CA-CB-OG1	-5.91	100.74	109.60
1	B	327	LYS	N-CA-CB	5.90	120.19	110.69
1	A	493	ARG	N-CA-CB	-5.90	101.42	110.20
1	C	171	VAL	N-CA-CB	-5.88	104.32	110.72
1	B	296	GLU	CB-CG-CD	5.84	122.53	112.60
1	A	137	GLU	CG-CD-OE2	-5.84	104.98	118.40
1	C	134	GLU	CB-CG-CD	5.82	122.50	112.60
1	B	154	LYS	CG-CD-CE	-5.81	97.93	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	269	GLU	N-CA-CB	5.80	118.58	109.83
1	C	139	PHE	CB-CA-C	5.79	120.19	109.70
1	C	157	LYS	CB-CA-C	5.77	119.17	109.48
1	B	481	THR	CA-CB-OG1	-5.77	100.95	109.60
1	C	152	THR	CA-CB-OG1	-5.76	100.96	109.60
1	C	23	LYS	CG-CD-CE	5.73	124.49	111.30
1	C	51	VAL	N-CA-CB	-5.73	106.89	110.50
1	B	664	ARG	CG-CD-NE	5.72	124.58	112.00
1	C	618	HIS	CA-CB-CG	-5.68	108.11	113.80
1	C	209	LYS	CB-CA-C	-5.67	99.58	110.24
1	B	247	VAL	N-CA-CB	5.65	117.82	111.21
1	B	14	THR	CA-CB-OG1	5.65	118.07	109.60
1	B	591	ILE	CA-C-N	5.63	127.18	120.14
1	B	591	ILE	C-N-CA	5.63	127.18	120.14
1	B	65	GLU	CB-CG-CD	5.59	122.11	112.60
1	B	191	PRO	CB-CA-C	-5.59	104.25	111.46
1	A	331	PRO	CB-CA-C	5.58	118.26	110.95
1	C	139	PHE	N-CA-CB	-5.56	101.18	110.80
1	C	40	LYS	CB-CG-CD	-5.55	98.53	111.30
1	B	39	THR	CA-CB-OG1	-5.54	101.29	109.60
1	B	512	GLU	CB-CG-CD	5.54	122.01	112.60
1	B	434	ASP	CB-CA-C	-5.53	100.86	110.09
1	A	245	ARG	NE-CZ-NH2	5.51	124.16	119.20
1	C	442	TYR	CB-CA-C	5.51	116.30	108.76
1	C	72	ASP	CA-CB-CG	5.50	118.10	112.60
1	B	543	THR	CA-CB-OG1	5.49	117.84	109.60
1	A	192	GLN	N-CA-CB	5.49	118.08	109.69
1	A	348	PHE	CA-CB-CG	5.48	119.28	113.80
1	B	318	PHE	CA-CB-CG	5.48	119.28	113.80
1	B	12	ASP	CA-CB-CG	5.47	118.07	112.60
1	A	65	GLU	CB-CG-CD	5.45	121.87	112.60
1	C	89	PHE	N-CA-CB	5.42	119.25	110.41
1	B	621	LYS	CB-CA-C	5.42	119.01	109.80
1	A	73	TYR	O-C-N	-5.41	117.15	121.80
1	C	491	PHE	CB-CA-C	5.41	119.76	110.79
1	C	704	LEU	N-CA-CB	-5.41	102.75	110.80
1	B	306	ARG	CB-CA-C	5.39	118.35	110.26
1	C	252	ARG	CD-NE-CZ	5.39	131.94	124.40
1	A	399	THR	CA-CB-OG1	-5.38	101.52	109.60
1	B	418	GLU	N-CA-CB	-5.37	100.81	110.37
1	A	319	ARG	CB-CA-C	-5.36	99.92	110.11
1	B	458	LYS	CG-CD-CE	-5.36	98.96	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	85	ARG	CD-NE-CZ	5.35	131.89	124.40
1	A	4	LEU	N-CA-CB	-5.34	101.41	110.50
1	B	155	PHE	N-CA-CB	-5.34	101.60	111.53
1	A	367	THR	OG1-CB-CG2	-5.34	98.62	109.30
1	C	222	ASP	CA-CB-CG	5.33	117.93	112.60
1	C	516	LYS	CG-CD-CE	5.33	123.56	111.30
1	C	239	GLU	CB-CG-CD	5.32	121.64	112.60
1	C	389	LYS	CB-CG-CD	-5.31	99.08	111.30
1	C	17	GLN	CB-CA-C	5.31	118.93	109.38
1	C	83	GLY	CA-C-N	5.31	128.78	120.82
1	C	83	GLY	C-N-CA	5.31	128.78	120.82
1	C	674	VAL	N-CA-CB	-5.30	105.00	111.21
1	C	95	GLN	O-C-N	-5.30	116.04	122.82
1	A	529	ASP	CA-CB-CG	5.29	117.89	112.60
1	B	356	ASP	CA-CB-CG	5.29	117.89	112.60
1	B	624	GLU	CB-CA-C	-5.29	101.85	110.85
1	B	540	GLU	CB-CA-C	5.28	119.51	110.01
1	C	55	GLU	CB-CA-C	-5.25	100.92	110.63
1	C	697	PHE	CA-CB-CG	-5.25	108.55	113.80
1	B	56	GLN	CB-CG-CD	5.25	121.52	112.60
1	B	134	GLU	N-CA-CB	-5.24	102.16	110.28
1	A	169	GLU	CB-CG-CD	-5.22	103.72	112.60
1	B	69	GLU	N-CA-CB	-5.21	102.42	109.98
1	B	256	ASP	CA-CB-CG	5.21	117.81	112.60
1	B	233	LYS	CD-CE-NZ	-5.20	95.25	111.90
1	B	461	LYS	N-CA-CB	5.20	118.66	110.23
1	B	703	CYS	CA-C-O	-5.19	114.00	119.97
1	C	398	PHE	CA-CB-CG	5.18	118.98	113.80
1	B	193	GLN	CB-CG-CD	5.18	121.41	112.60
1	B	87	PHE	N-CA-CB	-5.18	102.54	111.55
1	C	684	LYS	O-C-N	-5.18	115.96	121.30
1	A	662	ARG	CD-NE-CZ	-5.17	117.17	124.40
1	B	239	GLU	CB-CG-CD	5.16	121.37	112.60
1	C	180	HIS	N-CA-C	-5.16	106.95	113.20
1	C	269	GLU	CB-CG-CD	5.16	121.37	112.60
1	B	169	GLU	N-CA-CB	-5.16	103.32	111.05
1	C	538	ILE	N-CA-CB	-5.15	104.83	110.65
1	A	209	LYS	CB-CA-C	-5.15	100.45	109.71
1	C	319	ARG	CB-CA-C	-5.15	99.67	110.17
1	C	530	PHE	CA-CB-CG	5.13	118.93	113.80
1	A	42	PHE	CA-CB-CG	5.13	118.93	113.80
1	A	404	PRO	CA-C-N	-5.12	112.92	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	404	PRO	C-N-CA	-5.12	112.92	122.56
1	B	393	GLU	N-CA-CB	-5.11	103.48	111.56
1	A	66	ARG	N-CA-CB	-5.11	102.60	110.01
1	B	582	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	317	ASP	CA-CB-CG	5.10	117.70	112.60
1	C	92	THR	N-CA-C	-5.10	106.57	112.89
1	A	323	GLU	CB-CG-CD	5.09	121.26	112.60
1	C	503	ASN	CA-CB-CG	-5.08	107.52	112.60
1	C	327	LYS	N-CA-CB	5.07	118.86	110.69
1	A	547	ARG	CA-CB-CG	-5.06	103.98	114.10
1	A	667	SER	N-CA-C	-5.06	106.95	113.23
1	B	605	LYS	N-CA-CB	5.06	117.35	110.01
1	B	631	PRO	CB-CA-C	5.06	117.65	111.12
1	C	66	ARG	NE-CZ-NH2	5.05	123.75	119.20
1	C	55	GLU	N-CA-CB	5.05	118.00	110.22
1	C	33	ASP	CA-C-O	5.04	123.80	119.71
1	A	513	THR	N-CA-C	-5.03	105.89	112.23
1	A	94	LEU	N-CA-CB	-5.03	104.25	111.54
1	A	120	SER	CA-C-O	-5.02	115.58	121.10
1	C	16	VAL	N-CA-CB	5.01	119.58	111.36
1	B	662	ARG	CB-CA-C	-5.01	103.50	111.17
1	A	662	ARG	CA-CB-CG	-5.00	104.09	114.10
1	C	63	TYR	N-CA-C	-5.00	105.72	111.07

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	170	ARG	Sidechain
1	A	245	ARG	Sidechain
1	A	302	PHE	Peptide
1	A	312	ARG	Sidechain
1	A	319	ARG	Sidechain
1	A	420	ARG	Sidechain
1	A	643	ARG	Sidechain
1	A	662	ARG	Sidechain
1	B	128	ARG	Sidechain
1	B	319	ARG	Sidechain
1	B	423	ARG	Sidechain
1	B	547	ARG	Sidechain
1	B	643	ARG	Sidechain
1	B	66	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	664	ARG	Sidechain
1	B	670	LEU	Peptide
1	B	98	ARG	Sidechain
1	C	319	ARG	Sidechain
1	C	415	GLU	Peptide
1	C	429	GLY	Peptide
1	C	488	ARG	Sidechain
1	C	493	ARG	Sidechain
1	C	66	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	5684	5531	5507	54	0
1	B	5673	5514	5490	69	0
1	C	5673	5514	5490	95	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	38	52	52	1	0
3	B	19	26	26	1	0
3	C	19	26	26	0	0
4	A	30	26	0	0	0
4	B	30	26	0	1	0
4	C	30	26	0	0	0
5	A	24	0	0	6	0
5	B	18	0	0	5	0
5	C	3	0	0	1	0
6	A	24	32	32	1	0
6	B	18	24	24	7	0
6	C	12	16	16	7	0
7	A	631	0	0	12	1
7	B	370	0	0	12	0
7	C	388	0	0	10	0
All	All	18687	16813	16663	224	1

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 7.

All (224) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:GLU:HG2	7:A:1385:HOH:O	1.54	1.07
1:A:339:GLU:HG3	1:A:354[B]:LEU:HG	1.59	0.85
1:C:376:PRO:O	7:C:901:HOH:O	1.96	0.84
1:C:192:GLN:HE21	1:C:193:GLN:H	1.27	0.83
1:A:192:GLN:HE21	1:A:193:GLN:H	1.27	0.82
1:B:237:GLY:N	6:B:804:GOL:H32	1.97	0.79
1:C:443:PRO:HB2	7:C:935:HOH:O	1.84	0.78
1:C:692:GLU:OE1	7:C:902:HOH:O	2.05	0.75
1:B:462:LEU:O	7:B:901:HOH:O	2.04	0.74
1:A:172:LYS:HD3	1:A:173:PHE:CE2	2.24	0.73
1:A:388:GLN:HB3	5:A:815:SCN:N	2.04	0.72
1:C:38:GLN:HG2	7:C:1217:HOH:O	1.90	0.71
1:B:192:GLN:HE21	1:B:192:GLN:HA	1.56	0.70
1:C:163:GLU:HG3	7:C:1135:HOH:O	1.90	0.70
1:C:404:PRO:HD3	1:C:427:VAL:HG22	1.70	0.70
5:B:805:SCN:S	7:B:1059:HOH:O	2.50	0.69
1:A:339:GLU:HG2	1:A:354[B]:LEU:HD11	1.72	0.69
1:B:33:ASP:OD1	7:B:902:HOH:O	2.09	0.69
4:B:803:A1CQQ:C6	6:B:804:GOL:H2	2.23	0.68
1:B:261:LEU:HD12	1:B:282:LEU:HD23	1.74	0.68
1:A:416:GLU:HA	7:A:1396:HOH:O	1.93	0.67
1:C:431:ASP:OD1	1:C:432:ALA:N	2.27	0.67
1:A:317:ASP:OD2	7:A:902:HOH:O	2.12	0.66
1:B:166:ASP:O	7:B:903:HOH:O	2.14	0.66
1:C:233:LYS:HE2	1:C:593:HIS:HB2	1.78	0.66
1:B:192:GLN:HA	1:B:192:GLN:NE2	2.10	0.65
1:C:428:LYS:O	1:C:430:ILE:N	2.23	0.65
1:B:237:GLY:HA3	6:B:804:GOL:H11	1.78	0.65
1:B:236:GLY:C	6:B:804:GOL:H32	2.22	0.64
1:C:431:ASP:OD1	1:C:433:SER:N	2.30	0.64
1:A:512:GLU:HB3	7:A:1386:HOH:O	1.98	0.64
1:B:495:MET:HE3	1:B:701:ALA:HB2	1.80	0.63
1:B:571:PHE:O	1:B:631:PRO:HB3	1.99	0.62
1:B:245:ARG:HD2	1:B:267:GLN:NE2	2.14	0.62
1:C:262:TRP:CH2	1:C:281:LYS:HE2	2.34	0.62
1:A:339:GLU:CG	1:A:354[B]:LEU:HD11	2.30	0.62
1:A:662:ARG:NH2	7:A:906:HOH:O	2.32	0.62
1:C:348:PHE:HB3	1:C:363:LEU:HD11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:MET:C	6:B:804:GOL:H31	2.25	0.61
1:C:5:GLN:HE21	1:C:5:GLN:CA	2.13	0.61
1:C:5:GLN:HE21	1:C:5:GLN:N	1.99	0.61
1:A:339:GLU:HG2	1:A:354[B]:LEU:CD1	2.31	0.60
1:C:625:ALA:HB1	1:C:627:ASP:OD1	2.01	0.60
1:B:76:TYR:CD1	1:B:423:ARG:HD3	2.36	0.59
1:A:443:PRO:HD2	7:A:1075:HOH:O	2.01	0.59
1:C:628:ILE:O	1:C:665:LYS:NZ	2.35	0.59
1:A:339:GLU:CG	1:A:354[B]:LEU:CD1	2.80	0.59
1:C:467:PRO:O	1:C:497:GLY:HA2	2.02	0.58
1:C:707:ASP:OD1	1:C:707:ASP:N	2.35	0.58
1:C:345:ARG:HG3	1:C:392:THR:HA	1.85	0.58
1:A:343:CYS:HB3	5:A:815:SCN:S	2.44	0.58
1:C:262:TRP:CZ2	1:C:281:LYS:HE2	2.38	0.58
1:C:298:THR:OG1	1:C:319:ARG:CZ	2.52	0.58
1:B:539:LYS:CE	7:B:1233:HOH:O	2.52	0.57
1:B:7:PRO:HD3	1:B:49:ILE:HD11	1.85	0.57
1:C:464:GLY:O	1:C:544:SER:OG	2.22	0.57
1:C:86:TYR:CZ	1:C:106:LEU:HD12	2.39	0.57
1:B:55:GLU:HG2	7:B:908:HOH:O	2.04	0.57
1:C:431:ASP:O	1:C:432:ALA:HB2	2.05	0.57
1:C:493:ARG:O	1:C:493:ARG:NH1	2.37	0.56
1:A:76:TYR:CD1	1:A:423:ARG:HD3	2.40	0.56
1:A:256:ASP:HB2	7:A:956:HOH:O	2.04	0.56
1:B:54:LEU:O	1:B:57:CYS:HB2	2.05	0.56
1:C:488:ARG:HD3	1:C:499:LEU:HD11	1.88	0.56
1:C:431:ASP:O	1:C:432:ALA:CB	2.54	0.56
1:B:473:TYR:CZ	1:B:555:ASN:HB3	2.41	0.56
1:C:51:VAL:O	1:C:55:GLU:HG3	2.06	0.56
1:C:488:ARG:HD3	1:C:499:LEU:CD1	2.37	0.55
1:C:5:GLN:N	1:C:5:GLN:NE2	2.55	0.55
1:A:103:GLN:OE1	1:A:108:GLY:O	2.24	0.55
1:B:242:ASP:OD2	5:B:811:SCN:N	2.40	0.55
1:C:517:GLY:O	1:C:525:ASN:ND2	2.37	0.54
1:C:404:PRO:CD	1:C:427:VAL:HG22	2.38	0.54
1:C:276:ILE:HD12	6:C:806:GOL:H32	1.89	0.53
1:C:256:ASP:HB2	7:C:1009:HOH:O	2.07	0.53
1:C:325:LYS:HD3	1:C:325:LYS:N	2.23	0.53
1:A:358:LYS:NZ	1:A:439:GLN:OE1	2.40	0.53
1:C:430:ILE:HD13	1:C:489:LEU:HB3	1.90	0.53
1:C:276:ILE:HG21	6:C:806:GOL:C3	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:HIS:HB2	1:A:498:ILE:HD12	1.91	0.52
1:B:49:ILE:O	1:B:52:PRO:HD2	2.09	0.52
3:A:803:B3P:H31	7:A:1376:HOH:O	2.09	0.52
1:C:427:VAL:HG13	1:C:484:TYR:OH	2.09	0.52
1:C:415:GLU:O	1:C:415:GLU:HG2	2.09	0.51
1:A:404:PRO:HG2	1:A:425:VAL:O	2.09	0.51
1:C:456:HIS:ND1	1:C:456:HIS:C	2.67	0.51
1:C:491:PHE:CZ	1:C:497:GLY:HA3	2.45	0.51
1:C:276:ILE:HG21	6:C:806:GOL:H31	1.93	0.51
1:C:414:LYS:O	1:C:417:LEU:HD23	2.11	0.51
1:C:456:HIS:C	1:C:456:HIS:HD1	2.19	0.50
6:B:812:GOL:H12	7:B:1112:HOH:O	2.11	0.50
1:A:106:LEU:HD21	1:A:395:PHE:HZ	1.76	0.50
1:C:276:ILE:CG2	6:C:806:GOL:H32	2.41	0.50
1:B:184:GLY:HA3	1:B:212:TYR:CZ	2.47	0.50
1:C:11:ARG:HB2	5:C:805:SCN:C	2.41	0.50
1:C:276:ILE:HG23	6:C:806:GOL:H32	1.94	0.50
1:B:7:PRO:HD3	1:B:49:ILE:CD1	2.42	0.50
1:A:7:PRO:HD3	1:A:49:ILE:CD1	2.42	0.49
1:B:583:MET:HB2	1:B:615:SER:HB2	1.93	0.49
1:B:663:SER:O	7:B:904:HOH:O	2.20	0.49
1:B:645:VAL:HG23	1:B:647:LEU:HG	1.93	0.49
1:C:86:TYR:OH	1:C:106:LEU:HD12	2.13	0.49
1:A:547:ARG:HG2	7:A:1155:HOH:O	2.13	0.49
1:C:87:PHE:HA	1:C:101:TYR:O	2.12	0.49
1:B:16:VAL:O	1:B:16:VAL:HG23	2.13	0.49
1:A:192:GLN:HE21	1:A:193:GLN:N	2.04	0.48
1:A:683:GLY:HA2	7:A:1016:HOH:O	2.13	0.48
1:A:339:GLU:CG	1:A:354[B]:LEU:HG	2.38	0.48
1:C:684:LYS:HE3	7:C:986:HOH:O	2.12	0.48
1:A:260:ARG:NH1	1:A:284:ASP:OD1	2.43	0.48
1:C:74:PRO:O	1:C:425:VAL:HG11	2.14	0.48
1:C:153:ILE:HB	1:C:168:LEU:HB2	1.96	0.48
1:B:427:VAL:O	1:B:428:LYS:C	2.56	0.48
1:B:539:LYS:HE2	7:B:1233:HOH:O	2.13	0.48
1:B:629:GLN:HG3	1:B:630:TYR:O	2.14	0.47
1:A:242:ASP:OD2	5:A:815:SCN:S	2.72	0.47
1:B:51:VAL:O	1:B:55:GLU:HG3	2.14	0.47
1:C:30:TRP:CZ3	1:C:38:GLN:HB3	2.50	0.47
1:C:546:LYS:HG2	7:C:1191:HOH:O	2.14	0.47
1:A:345:ARG:O	1:A:346:SER:HB2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:TRP:CE2	1:C:281:LYS:HG2	2.49	0.47
1:B:398:PHE:O	1:B:405:GLY:HA2	2.15	0.47
1:B:115:ASP:OD1	1:B:115:ASP:C	2.58	0.47
1:B:192:GLN:HE21	1:B:193:GLN:H	1.63	0.47
1:C:251:ILE:HB	1:C:260:ARG:HB2	1.96	0.47
1:C:607:HIS:CD2	1:C:610:TRP:CZ3	3.02	0.47
1:C:115:ASP:C	1:C:115:ASP:OD1	2.55	0.47
1:C:430:ILE:HG22	1:C:430:ILE:O	2.14	0.47
1:B:44:GLU:HG2	7:B:1204:HOH:O	2.15	0.46
1:B:66:ARG:HH22	1:B:69:GLU:HG2	1.80	0.46
1:B:539:LYS:HE3	7:B:1233:HOH:O	2.13	0.46
1:C:420:ARG:HG3	1:C:420:ARG:HH11	1.81	0.46
1:C:627:ASP:OD1	1:C:627:ASP:N	2.48	0.46
1:A:339:GLU:HG3	1:A:354[B]:LEU:CG	2.38	0.46
1:B:462:LEU:HD13	1:B:540:GLU:O	2.16	0.46
1:A:283:ILE:HG21	1:A:290:TYR:CE1	2.51	0.45
1:A:607:HIS:CD2	1:A:610:TRP:CH2	3.04	0.45
1:A:395:PHE:HA	1:A:408:TYR:O	2.17	0.45
1:C:109:GLU:HG2	1:C:110:ALA:N	2.32	0.45
1:C:546:LYS:O	1:C:704:LEU:HD22	2.16	0.45
1:B:547:ARG:NH1	1:B:547:ARG:CB	2.80	0.45
1:C:17:GLN:HB2	7:C:1216:HOH:O	2.17	0.45
6:A:816:GOL:C3	7:A:941:HOH:O	2.65	0.45
1:C:493:ARG:HH22	1:C:710:PRO:C	2.25	0.45
1:C:693:VAL:O	1:C:694:SER:C	2.60	0.45
1:C:635:LEU:HB2	1:C:672:ILE:HG13	1.99	0.44
1:C:335:LYS:HE3	7:C:1151:HOH:O	2.17	0.44
1:B:547:ARG:CB	1:B:547:ARG:HH11	2.30	0.44
1:B:176:MET:H	5:B:808:SCN:C	2.30	0.44
1:C:435:TYR:HA	1:C:457:LYS:HA	1.99	0.44
1:B:289:GLU:OE2	3:B:802:B3P:H61	2.17	0.44
1:C:5:GLN:HE21	1:C:5:GLN:HA	1.81	0.44
1:B:261:LEU:HD13	1:B:261:LEU:C	2.42	0.44
1:B:467:PRO:O	1:B:497:GLY:HA2	2.18	0.44
1:B:547:ARG:NH1	1:B:547:ARG:HB2	2.32	0.44
1:B:664:ARG:HG2	1:B:665:LYS:N	2.33	0.44
1:C:341:ILE:HD12	1:C:351:LEU:CD1	2.48	0.44
1:C:622:LEU:HD11	1:C:663:SER:HB2	1.99	0.44
1:B:504:ILE:HG22	1:B:529:ASP:HB3	2.00	0.44
1:C:79:HIS:NE2	1:C:103:GLN:OE1	2.44	0.44
1:C:445:LYS:HB2	1:C:445:LYS:HE3	1.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:GLU:HG3	1:A:229:PRO:HD3	2.00	0.43
1:B:381:SER:OG	1:B:482:PRO:HD2	2.18	0.43
1:B:73:TYR:HB3	1:B:428:LYS:HD2	2.00	0.43
1:B:348:PHE:HB3	1:B:363:LEU:HD11	2.00	0.43
1:C:341:ILE:HA	1:C:350:VAL:O	2.17	0.43
1:B:238:ALA:O	5:B:808:SCN:S	2.76	0.43
1:B:292:TYR:O	5:B:807:SCN:S	2.76	0.43
1:B:647:LEU:C	1:B:647:LEU:HD12	2.44	0.43
1:A:63:TYR:CD1	1:A:63:TYR:C	2.96	0.43
1:B:449:LYS:HD3	1:B:449:LYS:HA	1.86	0.43
1:C:5:GLN:CA	1:C:5:GLN:NE2	2.80	0.43
1:C:430:ILE:O	1:C:431:ASP:O	2.36	0.43
1:B:431:ASP:OD1	1:B:431:ASP:C	2.61	0.43
1:B:491:PHE:O	1:B:495:MET:HB2	2.19	0.43
1:C:491:PHE:CE2	1:C:497:GLY:HA3	2.53	0.43
1:A:335:LYS:HE3	5:A:806:SCN:S	2.59	0.43
1:B:445:LYS:HE3	1:B:445:LYS:HB2	1.71	0.43
1:A:583:MET:HE1	1:A:599:TYR:CD2	2.54	0.43
1:C:355:HIS:O	1:C:356:ASP:C	2.60	0.43
1:C:385:TYR:CG	1:C:386:SER:N	2.87	0.43
1:A:28:TYR:HB3	1:A:31:LEU:HD12	2.01	0.42
1:B:153:ILE:HG13	1:B:171:VAL:HG21	2.00	0.42
1:B:491:PHE:CE2	1:B:497:GLY:HA3	2.54	0.42
1:C:53:PHE:CE1	1:C:702:ARG:HD3	2.54	0.42
1:C:276:ILE:CG2	6:C:806:GOL:C3	2.97	0.42
1:B:187:TYR:CE1	1:B:211:TYR:HB2	2.54	0.42
1:C:555:ASN:O	1:C:558:LEU:HB3	2.20	0.42
1:B:251:ILE:HB	1:B:260:ARG:HB2	2.02	0.42
6:B:812:GOL:C1	7:B:1112:HOH:O	2.67	0.42
1:C:358:LYS:HD2	1:C:379:VAL:HG13	2.00	0.42
1:C:378:ASP:HB2	1:C:398:PHE:CZ	2.54	0.42
1:A:260:ARG:HG3	1:A:286:PHE:CE1	2.55	0.42
1:A:440:ILE:C	1:A:440:ILE:HD12	2.44	0.42
1:B:79:HIS:HE1	1:B:423:ARG:NH1	2.17	0.42
1:C:341:ILE:HD12	1:C:351:LEU:HD11	2.01	0.42
1:A:355:HIS:HA	5:A:806:SCN:S	2.60	0.42
1:C:74:PRO:HB3	1:C:90:TYR:HE1	1.85	0.42
1:B:215:LEU:HD12	1:B:215:LEU:HA	1.89	0.42
1:B:583:MET:HB3	1:B:611:LEU:HD22	2.02	0.42
1:C:60:ARG:NE	1:C:695:ASP:OD1	2.52	0.42
1:A:505:ARG:HD3	5:A:807:SCN:C	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:VAL:CG1	1:C:361:LEU:HD11	2.50	0.41
1:C:431:ASP:OD1	1:C:434:ASP:N	2.50	0.41
1:A:405:GLY:C	1:A:406:ILE:CG1	2.93	0.41
1:B:196:LYS:HE3	1:B:200:THR:OG1	2.20	0.41
1:C:57:CYS:HB2	1:C:698:ALA:HB1	2.03	0.41
1:A:345:ARG:O	1:A:346:SER:CB	2.68	0.41
1:A:251:ILE:HB	1:A:260:ARG:HB2	2.02	0.41
1:C:354:LEU:HD13	1:C:359:ASN:ND2	2.35	0.41
1:C:227:GLU:O	6:C:806:GOL:H2	2.20	0.41
1:A:75:LYS:O	1:A:90:TYR:HA	2.21	0.41
1:A:583:MET:HB3	1:A:611:LEU:HD22	2.01	0.41
1:C:300:PHE:HB3	1:C:302:PHE:CE2	2.56	0.41
1:B:442:TYR:OH	1:B:533:ALA:HB2	2.21	0.41
1:A:84:LYS:HB2	7:A:1488:HOH:O	2.21	0.40
1:B:51:VAL:N	1:B:52:PRO:CD	2.84	0.40
1:A:71:TYR:CZ	1:A:75:LYS:HE2	2.56	0.40
1:B:55:GLU:C	1:B:57:CYS:H	2.29	0.40
1:A:130:TYR:CD1	1:A:130:TYR:C	2.99	0.40
1:A:160:GLY:O	1:A:161:ALA:C	2.64	0.40
1:A:442:TYR:CZ	1:A:450:ILE:HB	2.55	0.40
1:B:115:ASP:OD1	1:B:117:ASN:HB2	2.21	0.40
1:A:231:GLU:N	1:A:232:PRO:HD3	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1129:HOH:O	7:A:1296:HOH:O[1_565]	2.08	0.12

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	707/711 (99%)	680 (96%)	24 (3%)	3 (0%)	30	18
1	B	705/711 (99%)	676 (96%)	26 (4%)	3 (0%)	30	18
1	C	705/711 (99%)	663 (94%)	34 (5%)	8 (1%)	11	3
All	All	2117/2133 (99%)	2019 (95%)	84 (4%)	14 (1%)	18	7

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	417	LEU
1	C	416	GLU
1	C	419	PRO
1	C	429	GLY
1	C	431	ASP
1	A	357	VAL
1	B	357	VAL
1	B	427	VAL
1	C	432	ALA
1	A	415	GLU
1	C	420	ARG
1	A	554	SER
1	C	661	GLY
1	C	357	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	616/617 (100%)	598 (97%)	18 (3%)	37	20
1	B	614/617 (100%)	587 (96%)	27 (4%)	25	8
1	C	614/617 (100%)	584 (95%)	30 (5%)	22	6
All	All	1844/1851 (100%)	1769 (96%)	75 (4%)	27	10

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	66	ARG
1	A	162	LYS
1	A	261	LEU
1	A	270	SER
1	A	278	LYS
1	A	346	SER
1	A	373	LYS
1	A	416	GLU
1	A	423	ARG
1	A	425	VAL
1	A	427	VAL
1	A	430	ILE
1	A	461	LYS
1	A	512	GLU
1	A	539	LYS
1	A	605	LYS
1	A	624	GLU
1	B	5	GLN
1	B	44	GLU
1	B	48	LYS
1	B	59	ILE
1	B	66	ARG
1	B	84	LYS
1	B	111	ARG
1	B	121	ASP
1	B	192	GLN
1	B	203	SER
1	B	261	LEU
1	B	354	LEU
1	B	357	VAL
1	B	358	LYS
1	B	426	THR
1	B	427	VAL
1	B	431	ASP
1	B	445	LYS
1	B	487	SER
1	B	512	GLU
1	B	516	LYS
1	B	544	SER
1	B	547	ARG
1	B	588	LYS
1	B	598	ASP

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Mol	Chain	Res	Type
1	B	605	LYS
1	B	664	ARG
1	C	4	LEU
1	C	5	GLN
1	C	8	ASP
1	C	16	VAL
1	C	23	LYS
1	C	56	GLN
1	C	59	ILE
1	C	69	GLU
1	C	84	LYS
1	C	106	LEU
1	C	278	LYS
1	C	308	SER
1	C	334	GLU
1	C	335	LYS
1	C	354	LEU
1	C	358	LYS
1	C	381	SER
1	C	406	ILE
1	C	418	GLU
1	C	423	ARG
1	C	424	GLU
1	C	425	VAL
1	C	426	THR
1	C	430	ILE
1	C	431	ASP
1	C	457	LYS
1	C	512	GLU
1	C	544	SER
1	C	571	PHE
1	C	707	ASP

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

Mol	Chain	Res	Type
1	A	103	GLN
1	A	192	GLN
1	A	205	ASN
1	A	436	GLN
1	A	477	ASN
1	B	103	GLN

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Mol	Chain	Res	Type
1	B	192	GLN
1	B	193	GLN
1	B	205	ASN
1	B	388	GLN
1	B	439	GLN
1	B	477	ASN
1	B	524	GLN
1	B	531	GLN
1	B	551	ASN
1	B	566	GLN
1	B	577	GLN
1	C	5	GLN
1	C	192	GLN
1	C	205	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 3 are monoatomic - leaving 31 for Mogul analysis.

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	GOL	C	804	-	5,5,5	0.32	0	5,5,5	1.19	0
3	B3P	A	802	-	18,18,18	0.75	1 (5%)	23,23,23	0.68	1 (4%)
5	SCN	B	810	-	1,2,2	1.27	0	0,1,1	-	-
5	SCN	A	805	-	1,2,2	0.06	0	0,1,1	-	-
5	SCN	A	810	-	1,2,2	3.24	1 (100%)	0,1,1	-	-
5	SCN	A	815	-	1,2,2	0.45	0	0,1,1	-	-
6	GOL	A	808	-	5,5,5	0.25	0	5,5,5	1.04	0
5	SCN	A	811	-	1,2,2	0.05	0	0,1,1	-	-
5	SCN	B	807	-	1,2,2	1.43	0	0,1,1	-	-
3	B3P	C	802	-	18,18,18	0.68	0	23,23,23	1.07	2 (8%)
5	SCN	A	814	-	1,2,2	1.00	0	0,1,1	-	-
5	SCN	B	811	-	1,2,2	0.34	0	0,1,1	-	-
5	SCN	B	808	-	1,2,2	0.50	0	0,1,1	-	-
5	SCN	A	813	-	1,2,2	0.23	0	0,1,1	-	-
3	B3P	B	802	-	18,18,18	0.83	1 (5%)	23,23,23	1.68	5 (21%)
5	SCN	C	805	-	1,2,2	0.02	0	0,1,1	-	-
6	GOL	A	809	-	5,5,5	0.51	0	5,5,5	1.46	2 (40%)
6	GOL	A	812	-	5,5,5	0.24	0	5,5,5	0.93	0
6	GOL	B	804	-	5,5,5	0.99	0	5,5,5	1.94	1 (20%)
6	GOL	B	812	-	5,5,5	0.48	0	5,5,5	0.92	0
6	GOL	C	806	-	5,5,5	0.48	0	5,5,5	0.94	0
4	A1CQQ	C	803	1	33,33,34	1.30	2 (6%)	44,45,47	1.84	7 (15%)
5	SCN	B	805	-	1,2,2	0.80	0	0,1,1	-	-
3	B3P	A	803	-	18,18,18	1.09	2 (11%)	23,23,23	2.87	6 (26%)
6	GOL	B	806	-	5,5,5	0.22	0	5,5,5	0.42	0
4	A1CQQ	B	803	1	33,33,34	0.91	1 (3%)	44,45,47	1.79	7 (15%)
5	SCN	B	809	-	1,2,2	1.81	0	0,1,1	-	-
6	GOL	A	816	-	5,5,5	0.36	0	5,5,5	0.76	0
4	A1CQQ	A	804	-	33,33,34	1.07	3 (9%)	44,45,47	1.33	7 (15%)
5	SCN	A	807	-	1,2,2	0.22	0	0,1,1	-	-
5	SCN	A	806	-	1,2,2	1.42	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
3	B3P	C	802	-	-	1/28/28/28	-
3	B3P	A	803	-	-	4/28/28/28	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	B	806	-	-	1/4/4/4	-
6	GOL	C	804	-	-	0/4/4/4	-
4	A1CQQ	B	803	1	-	4/19/26/26	0/4/4/4
3	B3P	A	802	-	-	1/28/28/28	-
6	GOL	A	816	-	-	2/4/4/4	-
3	B3P	B	802	-	-	8/28/28/28	-
6	GOL	A	809	-	-	4/4/4/4	-
4	A1CQQ	A	804	-	-	4/19/26/26	0/4/4/4
6	GOL	A	812	-	-	2/4/4/4	-
6	GOL	A	808	-	-	2/4/4/4	-
6	GOL	B	804	-	-	4/4/4/4	-
6	GOL	B	812	-	-	4/4/4/4	-
6	GOL	C	806	-	-	4/4/4/4	-
4	A1CQQ	C	803	1	-	4/19/26/26	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	803	A1CQQ	C23-C11	-3.44	1.36	1.41
5	A	810	SCN	C-N	3.24	1.26	1.15
4	A	804	A1CQQ	C12-C13	2.99	1.43	1.39
3	A	803	B3P	C3-N1	-2.98	1.43	1.46
4	C	803	A1CQQ	C12-N3	-2.88	1.28	1.34
3	B	802	B3P	C6-C4	2.67	1.56	1.53
3	A	803	B3P	C9-C8	2.61	1.56	1.53
4	A	804	A1CQQ	O2-C17	2.60	1.28	1.23
3	A	802	B3P	C11-C8	2.45	1.56	1.53
4	B	803	A1CQQ	O2-C17	2.21	1.27	1.23
4	A	804	A1CQQ	C22-C13	2.19	1.42	1.39

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	803	B3P	C6-C4-N1	7.87	132.49	109.02
4	B	803	A1CQQ	C23-C2-N1	-7.19	107.94	110.76
3	A	803	B3P	C3-N1-C4	6.25	125.31	116.17
4	C	803	A1CQQ	C23-C2-N1	-6.18	108.34	110.76
4	C	803	A1CQQ	C11-C23-C2	6.11	107.11	105.15
3	A	803	B3P	C2-N2-C8	6.06	125.03	116.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802	B3P	O6-C7-C4	-4.67	102.18	111.68
3	A	803	B3P	O6-C7-C4	-4.10	103.35	111.68
4	B	803	A1CQQ	C2-N1-N2	4.09	109.58	104.97
4	A	804	A1CQQ	C23-C2-N1	-3.75	109.29	110.76
4	C	803	A1CQQ	C4-C3-N2	3.70	115.83	111.93
4	A	804	A1CQQ	C22-C13-C12	-3.36	114.47	117.92
4	C	803	A1CQQ	C22-C23-C11	-3.31	114.33	117.67
6	B	804	GOL	O1-C1-C2	3.23	124.93	110.38
3	A	803	B3P	C7-C4-N1	-3.23	99.37	109.02
4	B	803	A1CQQ	C16-C17-N5	-3.02	113.51	118.09
4	C	803	A1CQQ	C3-N2-N1	2.85	122.20	119.75
4	B	803	A1CQQ	C15-N4-C14	-2.65	116.11	122.11
3	B	802	B3P	C3-N1-C4	2.63	120.02	116.17
4	A	804	A1CQQ	C3-C4-C5	-2.55	104.94	112.15
3	A	803	B3P	C6-C4-C5	-2.52	104.49	110.02
3	B	802	B3P	C7-C4-C6	-2.48	104.59	110.02
3	C	802	B3P	C11-C8-C9	-2.45	104.65	110.02
4	C	803	A1CQQ	C16-C17-N5	-2.41	114.44	118.09
3	B	802	B3P	C7-C4-N1	2.40	116.18	109.02
3	B	802	B3P	C7-C4-C5	-2.32	104.93	110.02
6	A	809	GOL	O3-C3-C2	-2.23	100.35	110.38
4	C	803	A1CQQ	C3-C4-C5	-2.21	105.92	112.15
6	A	809	GOL	O2-C2-C1	2.19	118.23	109.18
4	A	804	A1CQQ	C22-C13-C14	2.15	127.50	120.40
4	B	803	A1CQQ	C3-C4-C5	-2.12	106.18	112.15
4	A	804	A1CQQ	C1-C2-C23	2.10	131.19	127.56
4	A	804	A1CQQ	C3-N2-N1	2.08	121.54	119.75
3	A	802	B3P	C11-C8-C9	-2.04	105.54	110.02
3	C	802	B3P	O5-C6-C4	-2.03	107.56	111.68
4	A	804	A1CQQ	O1-C14-N4	-2.02	118.65	122.59
4	B	803	A1CQQ	C11-N2-N1	-2.01	109.92	111.05
4	B	803	A1CQQ	O2-C17-C16	2.01	126.69	121.26

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	803	B3P	C5-C4-N1-C3
3	A	803	B3P	C6-C4-N1-C3
3	A	803	B3P	C7-C4-N1-C3
3	B	802	B3P	N1-C4-C5-O4
3	B	802	B3P	C6-C4-C5-O4

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Mol	Chain	Res	Type	Atoms
3	B	802	B3P	C7-C4-C5-O4
3	B	802	B3P	N2-C8-C9-O1
3	B	802	B3P	C11-C8-C9-O1
6	A	808	GOL	C1-C2-C3-O3
6	A	808	GOL	O2-C2-C3-O3
6	A	809	GOL	C1-C2-C3-O3
6	A	816	GOL	O1-C1-C2-C3
6	B	804	GOL	O1-C1-C2-C3
6	B	812	GOL	C1-C2-C3-O3
6	C	806	GOL	O1-C1-C2-C3
6	C	806	GOL	O2-C2-C3-O3
4	A	804	A1CQQ	C22-C13-C14-O1
4	C	803	A1CQQ	C22-C13-C14-O1
4	B	803	A1CQQ	C12-C13-C14-O1
4	C	803	A1CQQ	C12-C13-C14-O1
4	A	804	A1CQQ	C22-C13-C14-N4
4	B	803	A1CQQ	C22-C13-C14-O1
4	B	803	A1CQQ	C22-C13-C14-N4
4	C	803	A1CQQ	C22-C13-C14-N4
4	A	804	A1CQQ	C12-C13-C14-O1
4	B	803	A1CQQ	C12-C13-C14-N4
4	C	803	A1CQQ	C12-C13-C14-N4
3	A	803	B3P	C3-C1-C2-N2
6	A	809	GOL	O2-C2-C3-O3
6	B	804	GOL	O1-C1-C2-O2
3	B	802	B3P	C10-C8-C9-O1
4	A	804	A1CQQ	C12-C13-C14-N4
6	A	809	GOL	O1-C1-C2-C3
6	A	812	GOL	C1-C2-C3-O3
6	B	804	GOL	C1-C2-C3-O3
6	B	812	GOL	O1-C1-C2-C3
6	C	806	GOL	C1-C2-C3-O3
6	A	816	GOL	O1-C1-C2-O2
6	B	804	GOL	O2-C2-C3-O3
6	B	812	GOL	O2-C2-C3-O3
6	C	806	GOL	O1-C1-C2-O2
6	B	806	GOL	O2-C2-C3-O3
6	A	812	GOL	O2-C2-C3-O3
3	A	802	B3P	O2-C10-C8-C9
3	C	802	B3P	O3-C11-C8-C10
6	A	809	GOL	O1-C1-C2-O2
6	B	812	GOL	O1-C1-C2-O2

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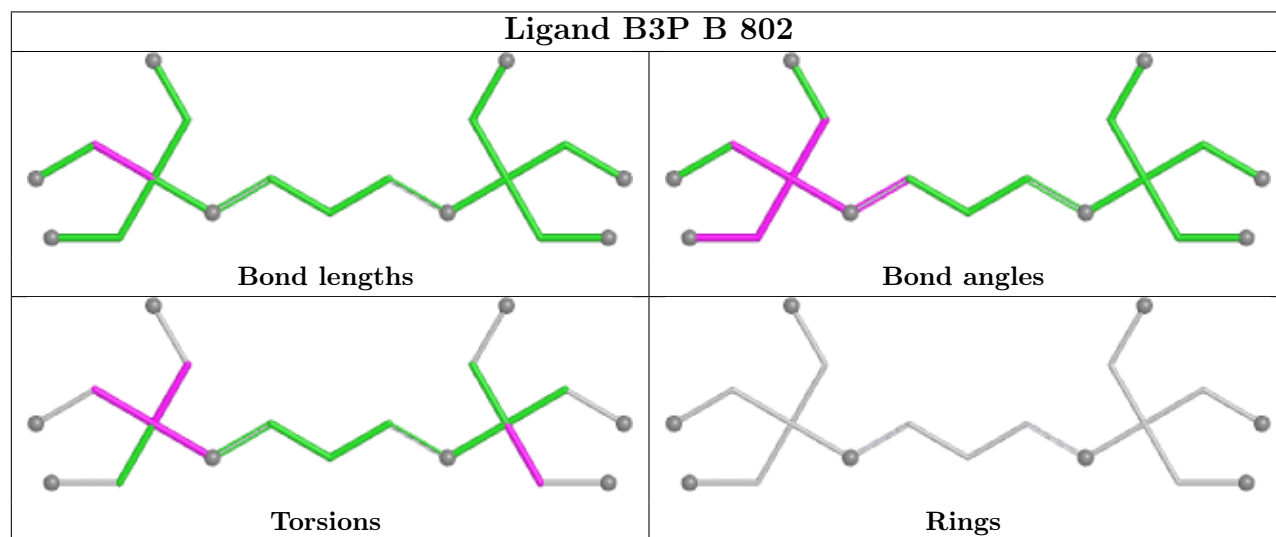
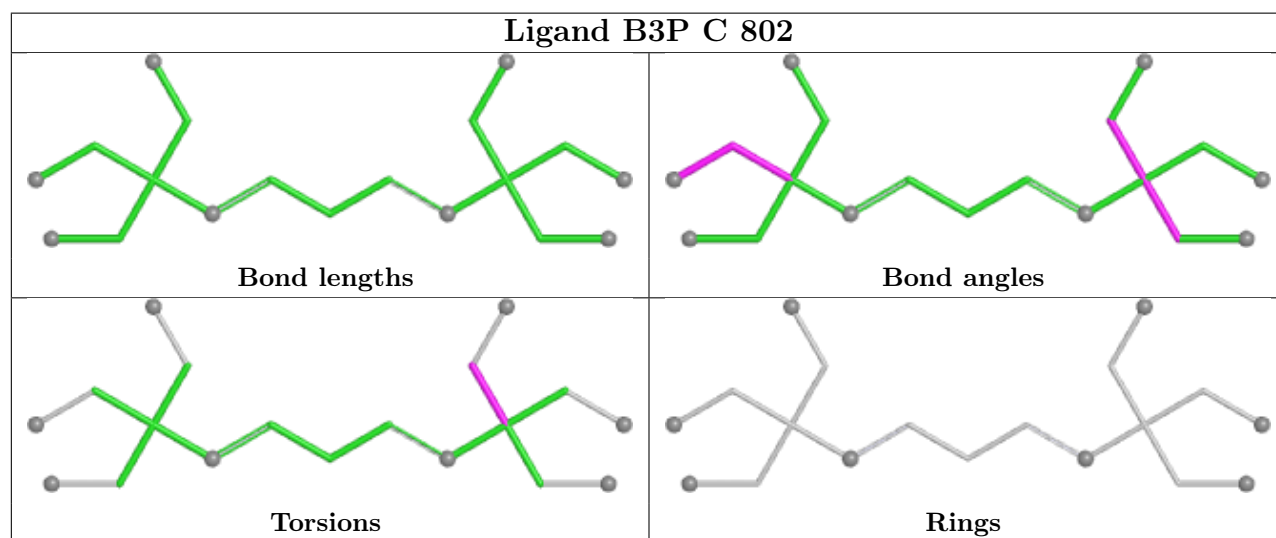
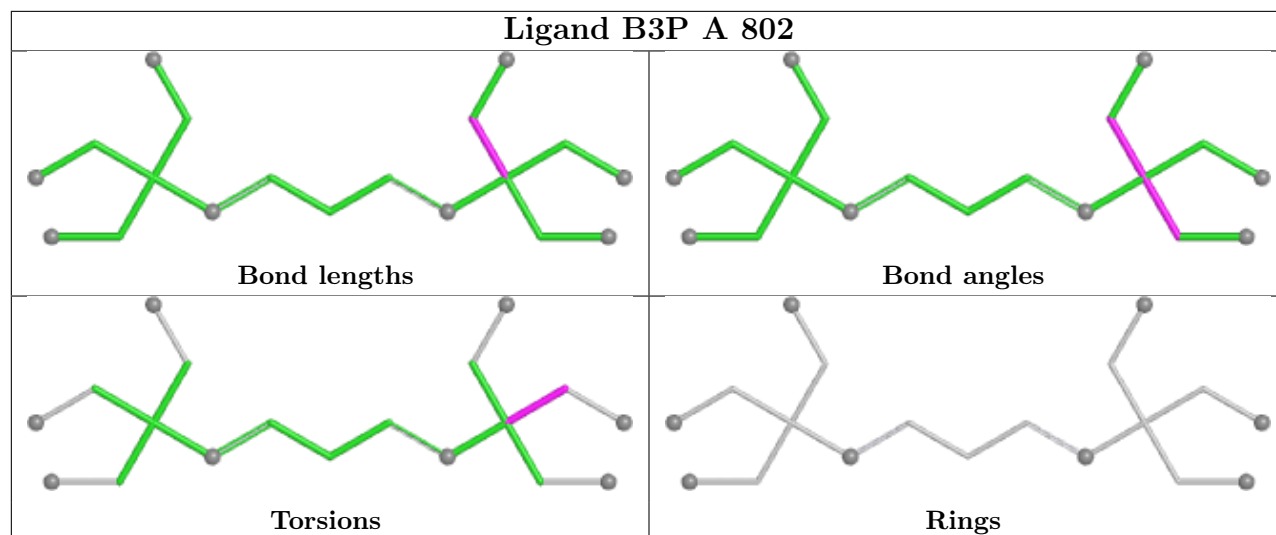
Mol	Chain	Res	Type	Atoms
3	B	802	B3P	C7-C4-N1-C3
3	B	802	B3P	C7-C4-C6-O5

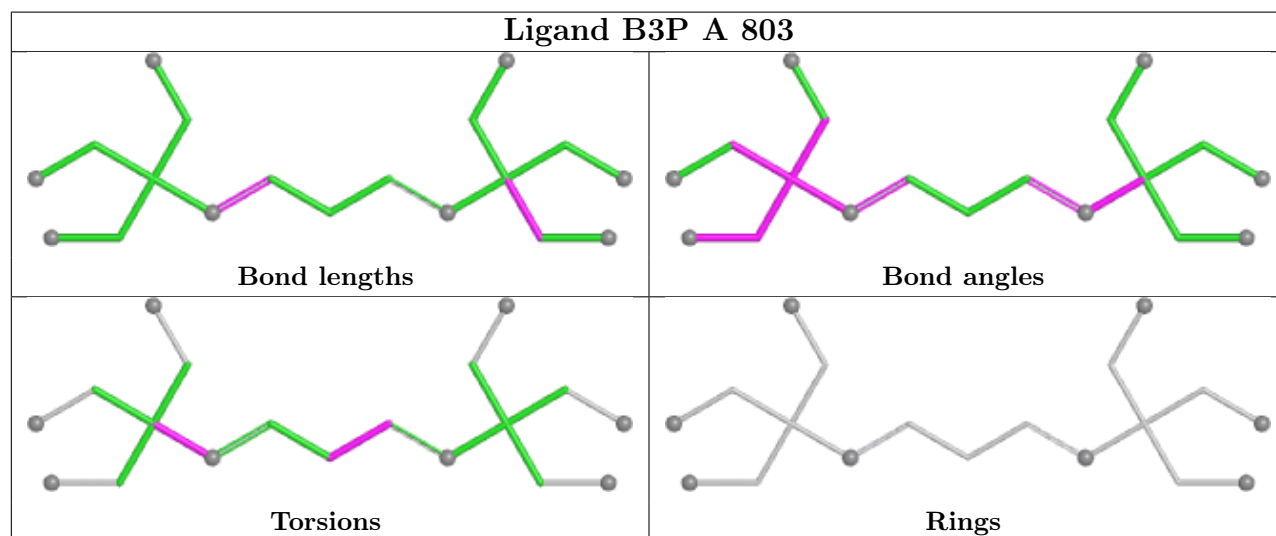
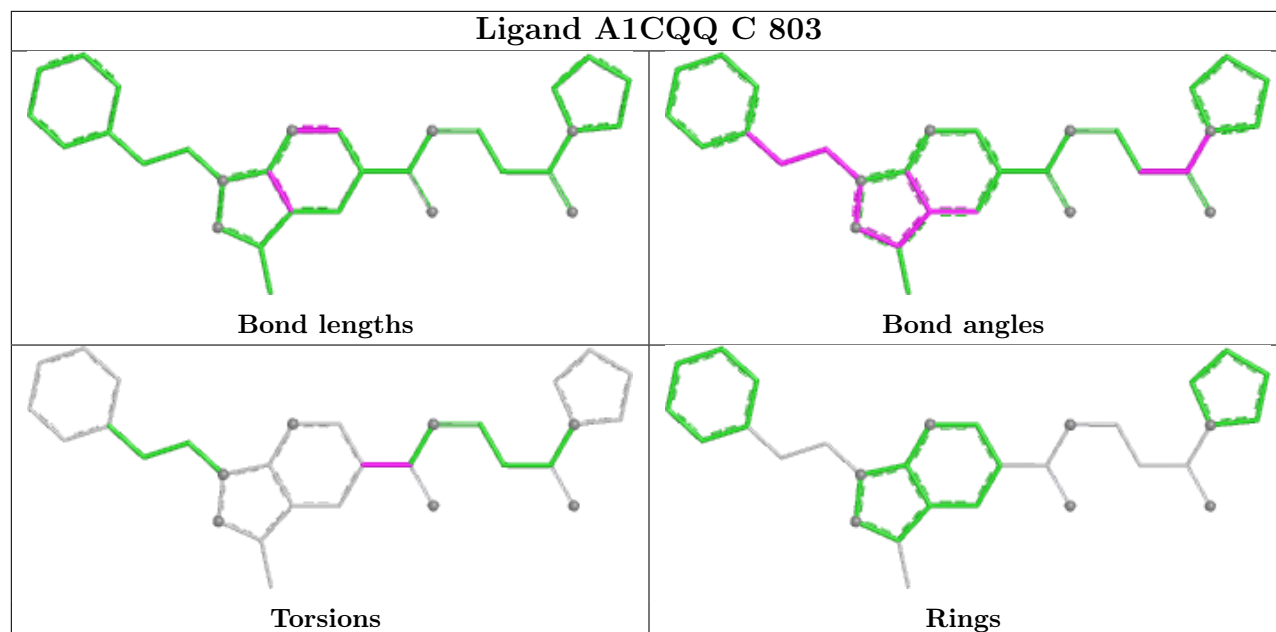
There are no ring outliers.

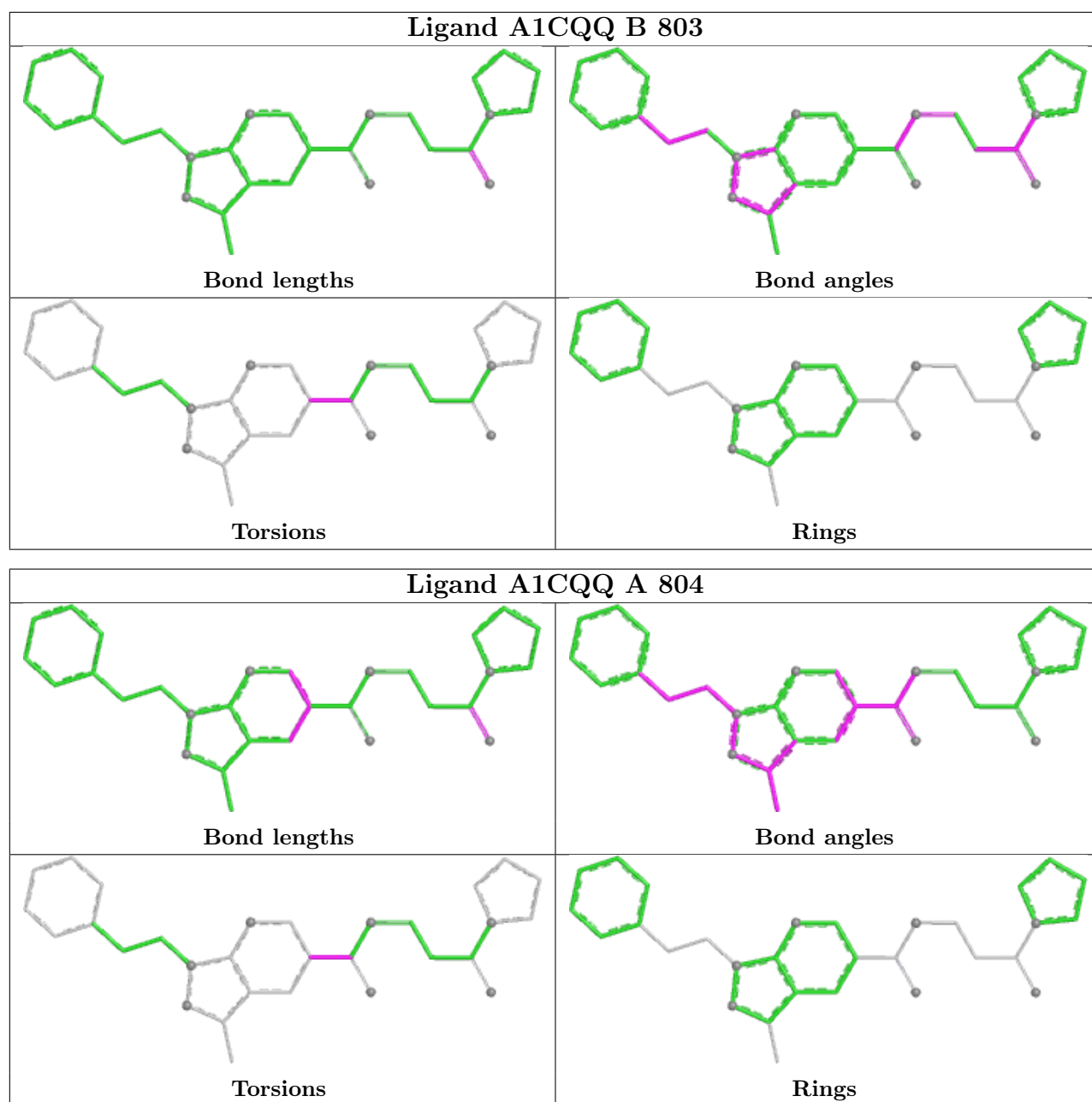
15 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	815	SCN	3	0
5	B	807	SCN	1	0
5	B	811	SCN	1	0
5	B	808	SCN	2	0
3	B	802	B3P	1	0
5	C	805	SCN	1	0
6	B	804	GOL	5	0
6	B	812	GOL	2	0
6	C	806	GOL	7	0
5	B	805	SCN	1	0
3	A	803	B3P	1	0
4	B	803	A1CQQ	1	0
6	A	816	GOL	1	0
5	A	807	SCN	1	0
5	A	806	SCN	2	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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%)	-0.93	2 (0%) 90 94	7, 17, 34, 70	2 (0%)
1	B	707/711 (99%)	-0.51	4 (0%) 85 90	13, 26, 47, 104	0
1	C	707/711 (99%)	-0.44	1 (0%) 92 95	8, 27, 51, 88	0
All	All	2121/2133 (99%)	-0.63	7 (0%) 90 94	7, 23, 47, 104	2 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	427	VAL	5.0
1	B	429	GLY	3.9
1	C	427	VAL	3.7
1	A	427	VAL	3.4
1	A	426	THR	2.9
1	B	426	THR	2.1
1	B	428	LYS	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,

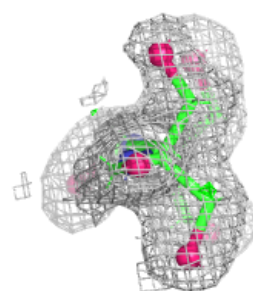
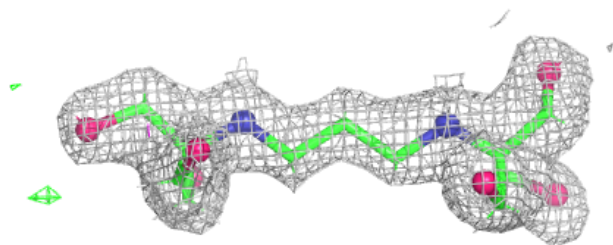
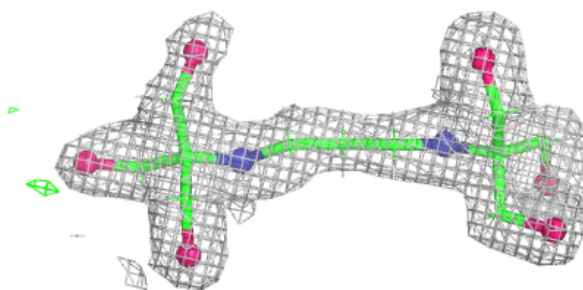
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SCN	B	810	3/3	0.85	0.23	17,17,18,26	3
6	GOL	C	806	6/6	0.87	0.11	27,38,45,46	3
6	GOL	B	812	6/6	0.88	0.10	33,36,41,41	3
5	SCN	B	809	3/3	0.88	0.11	26,26,33,51	0
5	SCN	C	805	3/3	0.89	0.12	40,40,41,48	0
5	SCN	B	808	3/3	0.90	0.13	29,29,31,45	0
5	SCN	B	811	3/3	0.91	0.11	38,38,44,55	0
5	SCN	B	805	3/3	0.91	0.13	17,17,35,35	0
6	GOL	B	804	6/6	0.92	0.15	19,29,41,41	3
6	GOL	A	812	6/6	0.92	0.09	30,36,41,41	3
6	GOL	A	816	6/6	0.92	0.09	34,43,45,47	3
5	SCN	A	813	3/3	0.93	0.11	34,34,42,51	0
5	SCN	A	811	3/3	0.93	0.10	31,31,37,50	0
2	K	B	801	1/1	0.94	0.08	54,54,54,54	0
5	SCN	B	807	3/3	0.94	0.11	32,32,38,42	0
2	K	C	801	1/1	0.94	0.07	45,45,45,45	0
5	SCN	A	815	3/3	0.94	0.11	29,29,38,42	0
6	GOL	A	808	6/6	0.95	0.06	27,30,41,41	3
3	B3P	C	802	19/19	0.95	0.06	21,25,41,41	8
3	B3P	B	802	19/19	0.96	0.06	18,24,41,41	8
3	B3P	A	803	19/19	0.96	0.06	11,20,41,41	8
4	A1CQQ	B	803	30/31	0.96	0.06	15,19,37,41	3
5	SCN	A	807	3/3	0.96	0.11	20,20,31,31	0
5	SCN	A	810	3/3	0.97	0.08	24,24,35,39	0
6	GOL	A	809	6/6	0.97	0.07	11,21,41,41	3
3	B3P	A	802	19/19	0.97	0.04	12,15,41,41	8
4	A1CQQ	C	803	30/31	0.97	0.05	15,20,36,41	3
5	SCN	A	814	3/3	0.97	0.07	30,30,33,40	0
6	GOL	B	806	6/6	0.97	0.07	16,24,41,44	3
5	SCN	A	805	3/3	0.97	0.10	23,23,29,32	0
6	GOL	C	804	6/6	0.97	0.05	13,19,41,41	3
4	A1CQQ	A	804	30/31	0.97	0.05	12,15,28,41	3
5	SCN	A	806	3/3	0.98	0.09	22,22,26,35	0
2	K	A	801	1/1	0.99	0.03	27,27,27,27	0

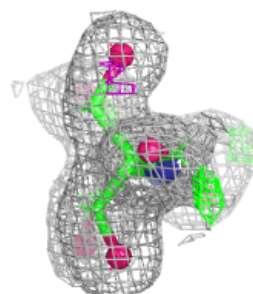
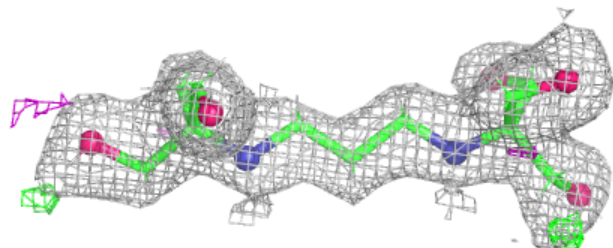
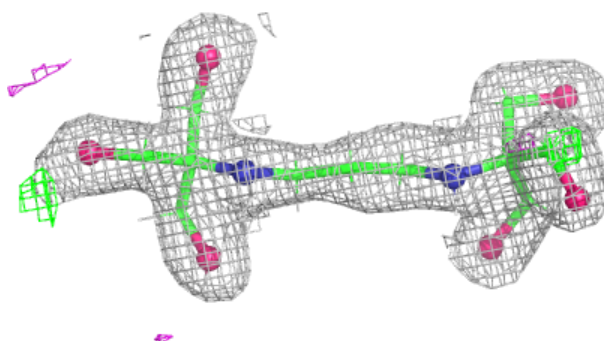
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around B3P C 802:

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

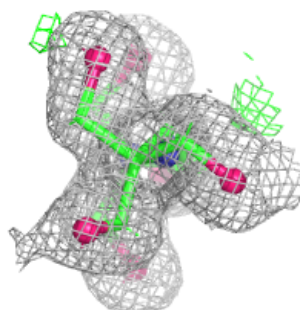
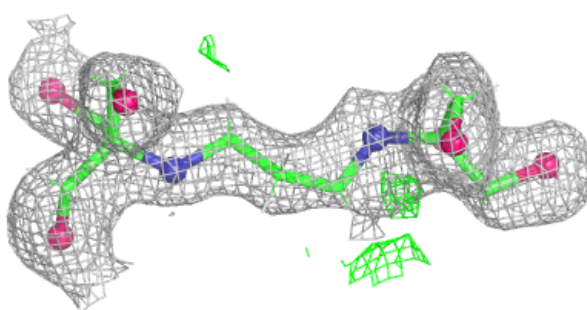
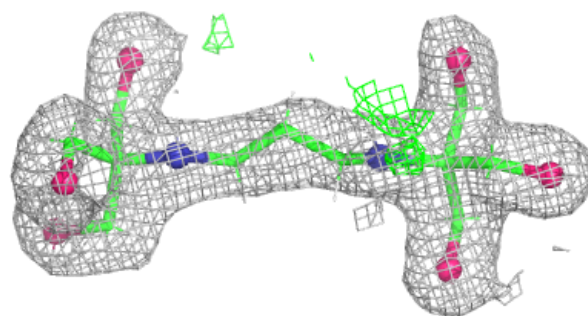
**Electron density around B3P B 802:**

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

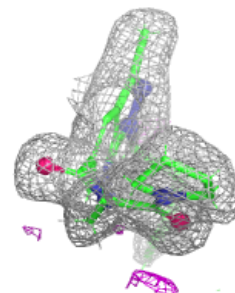
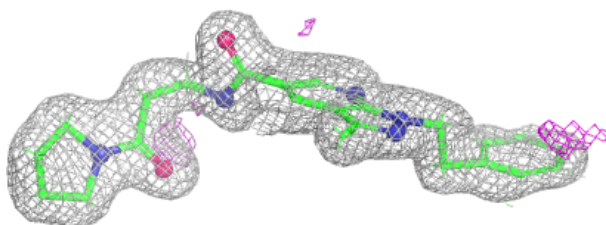
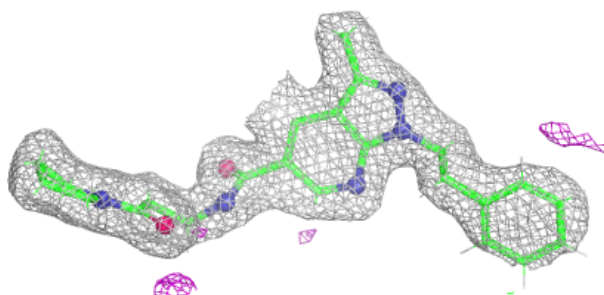


Electron density around B3P A 803:

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

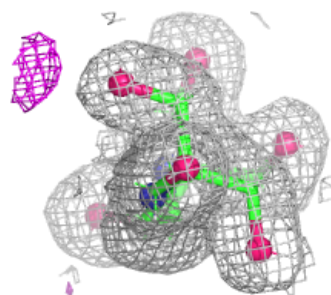
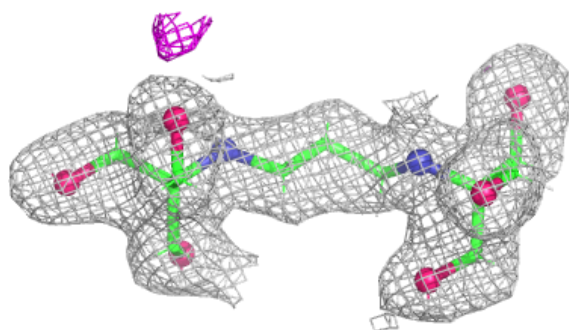
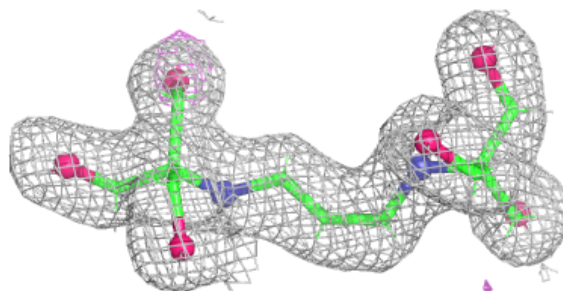
**Electron density around A1CQQ B 803:**

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

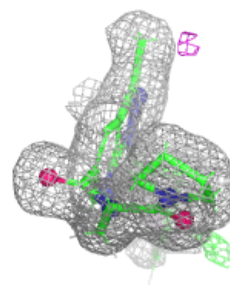
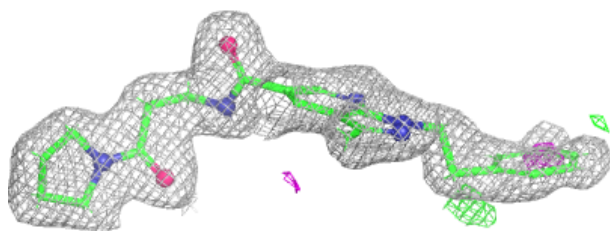
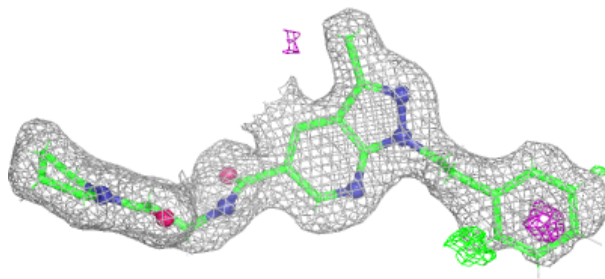


Electron density around B3P A 802:

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

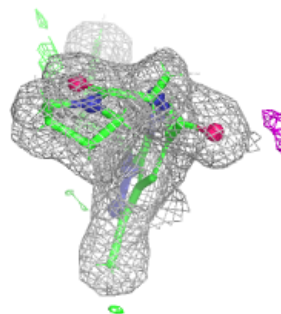
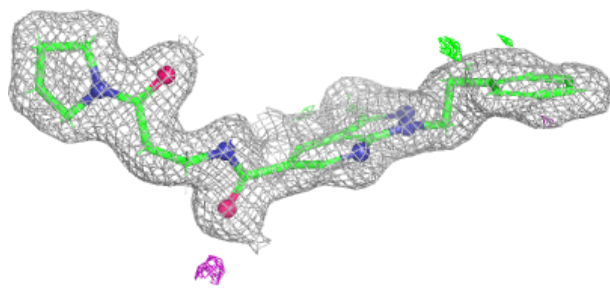
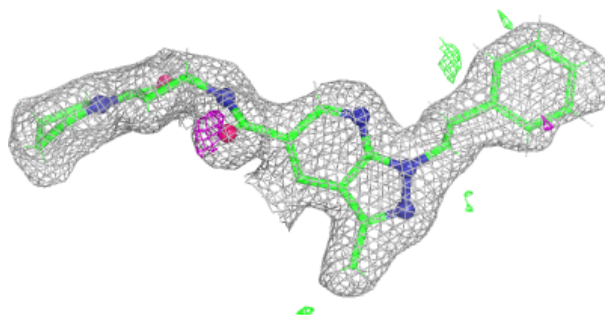
**Electron density around A1CQQ C 803:**

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



Electron density around A1CQQ A 804:

$2mF_o - DF_c$ (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.