



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:23 AM UTC

PDB ID : 9Q6X / pdb_00009q6x
Title : Human prolyl endopeptidase (PREP) - complex with KT-2-186
Authors : Fucci, I.J.; Thakur, K.; Pandian, J.; Yoo, E.; Monteiro, D.C.F.
Deposited on : 2025-08-22
Resolution : 1.66 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

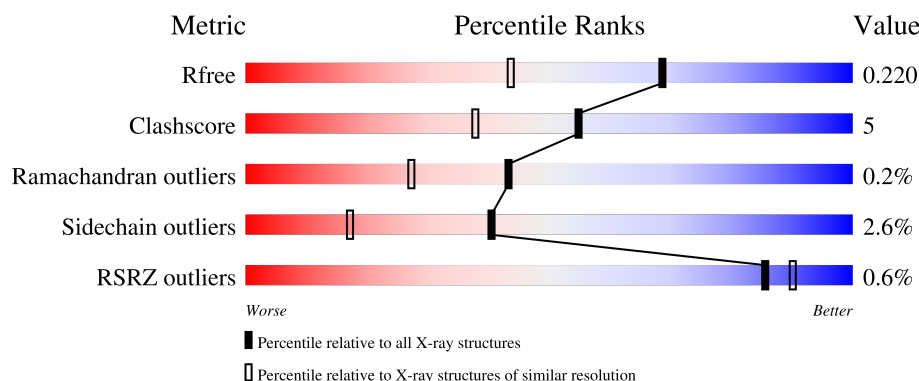
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.66 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	% 87% 10% ..
1	B	711	% 87% 11% ..
1	C	711	 86% 11% ..

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
2	SCN	C	822	-	-	X	-
2	SCN	C	824	-	-	X	-
2	SCN	C	828	-	-	X	-
3	PEG	B	807	-	-	X	-
3	PEG	C	802	-	-	X	-
3	PEG	C	814	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 19158 atoms, of which 69 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.

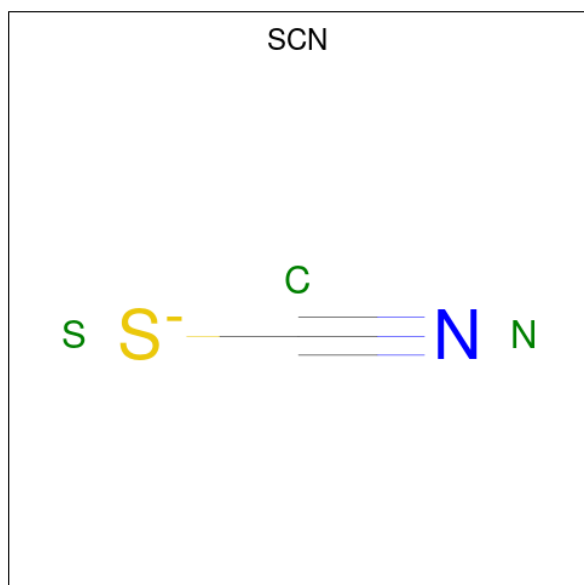
- Molecule 1 is a protein called Prolyl endopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	707	Total	C	N	O	S	0	4	0
			5696	3654	944	1070	28			
1	A	707	Total	C	N	O	S	0	5	0
			5699	3658	942	1071	28			
1	B	707	Total	C	N	O	S	0	3	0
			5688	3649	941	1070	28			

There are 3 discrepancies between the modelled and reference sequences:

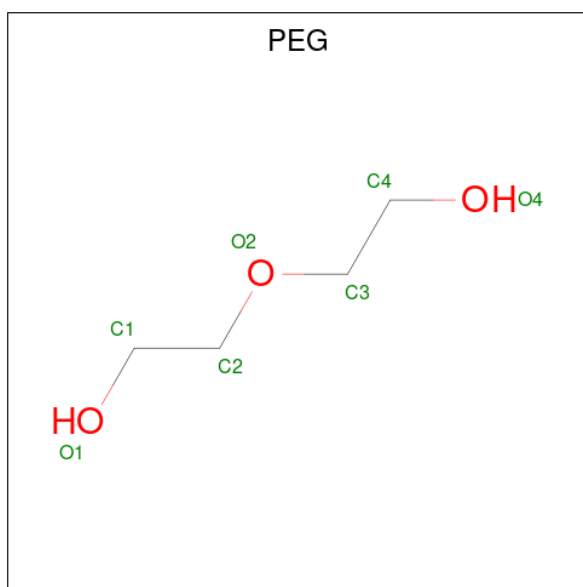
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	GLY	-	expression tag	UNP P48147
A	0	GLY	-	expression tag	UNP P48147
B	0	GLY	-	expression tag	UNP P48147

- Molecule 2 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



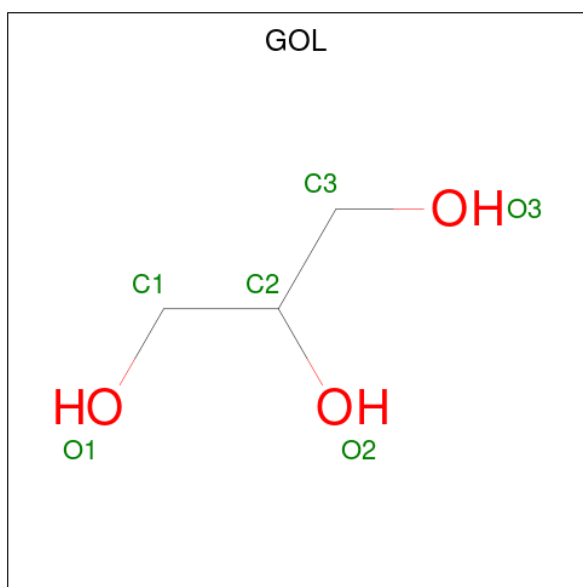
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C N S 3 1 1 1	0	0
2	C	1	Total C N S 3 1 1 1	0	0
2	C	1	Total C N S 3 1 1 1	0	0
2	C	1	Total C N S 3 1 1 1	0	0
2	C	1	Total C N S 3 1 1 1	0	0
2	C	1	Total C N S 3 1 1 1	0	0
2	C	1	Total C N S 3 1 1 1	0	0
2	C	1	Total C N S 3 1 1 1	0	0
2	C	1	Total C N S 3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

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

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



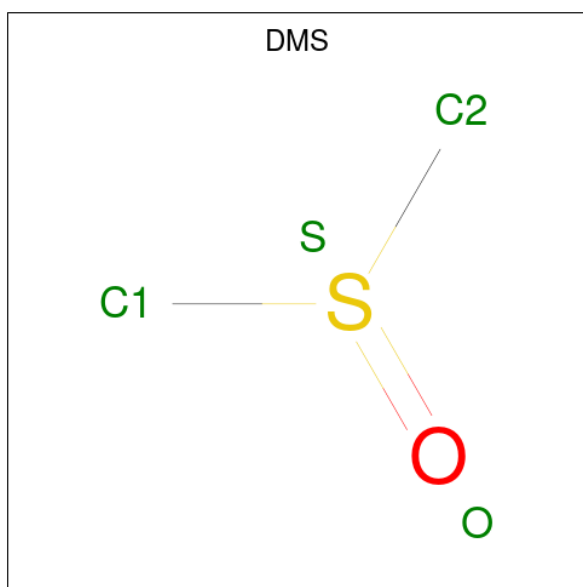
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total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

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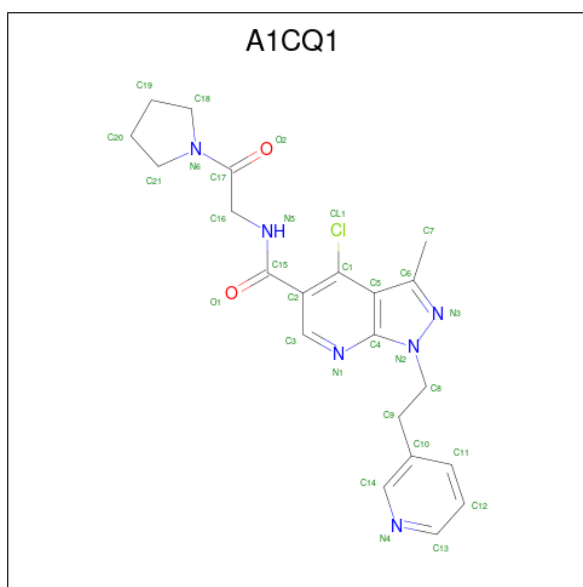
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 6	C 3	O 3	0	0
4	A	1	Total 6	C 3	O 3	0	0
4	A	1	Total 6	C 3	O 3	0	0
4	A	1	Total 6	C 3	O 3	0	0
4	A	1	Total 6	C 3	O 3	0	0
4	A	1	Total 6	C 3	O 3	0	0
4	A	1	Total 6	C 3	O 3	0	0
4	A	1	Total 6	C 3	O 3	0	0
4	A	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0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

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



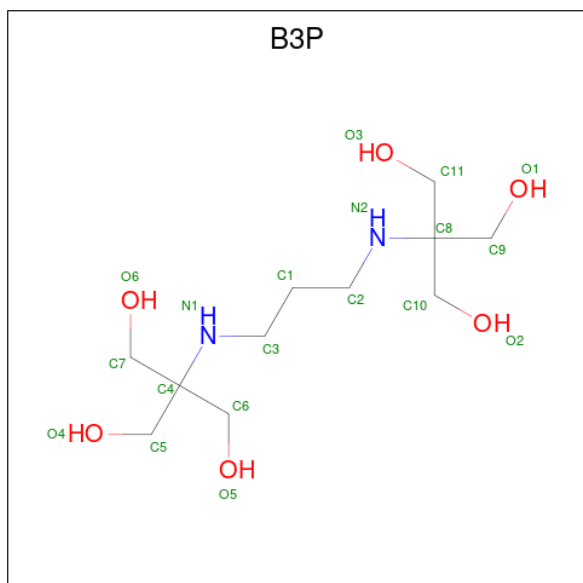
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 6 is 4-chloro-3-methyl-N-[2-oxo-2-(pyrrolidin-1-yl)ethyl]-1-[2-(pyridin-3-yl)ethyl]-1H-pyrazolo[3,4-b]pyridine-5-carboxamide (CCD ID: A1CQ1) (formula: $C_{21}H_{23}ClN_6O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	H	N	O	0	0
			52	21	23	6	2		
6	A	1	Total	C	H	N	O	0	0
			52	21	23	6	2		
6	B	1	Total	C	H	N	O	0	0
			52	21	23	6	2		

- Molecule 7 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
7	A	1	Total	C	N	O	0	0
			19	11	2	6		
7	B	1	Total	C	N	O	0	0
			19	11	2	6		

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Na	0	0
			1	1		

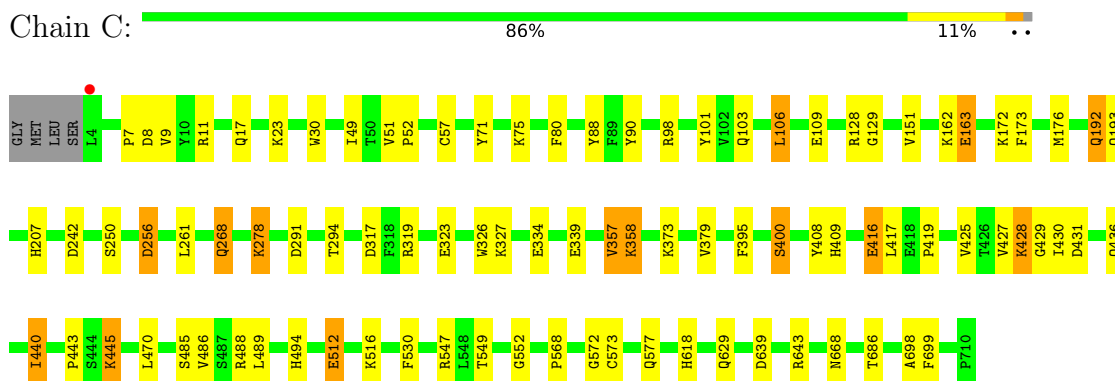
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	579	Total	O	0	0
			579	579		
9	A	534	Total	O	0	0
			534	534		
9	B	456	Total	O	0	1
			457	457		

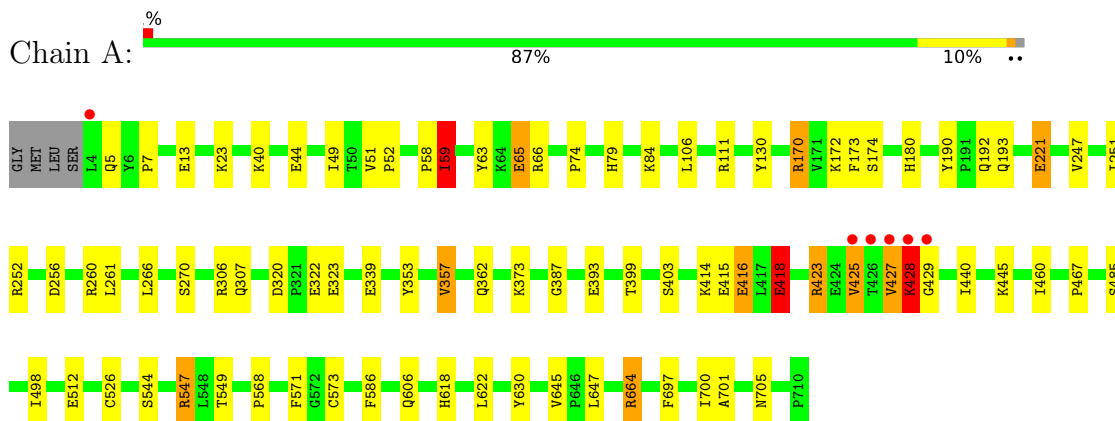
3 Residue-property plots [i](#)

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.

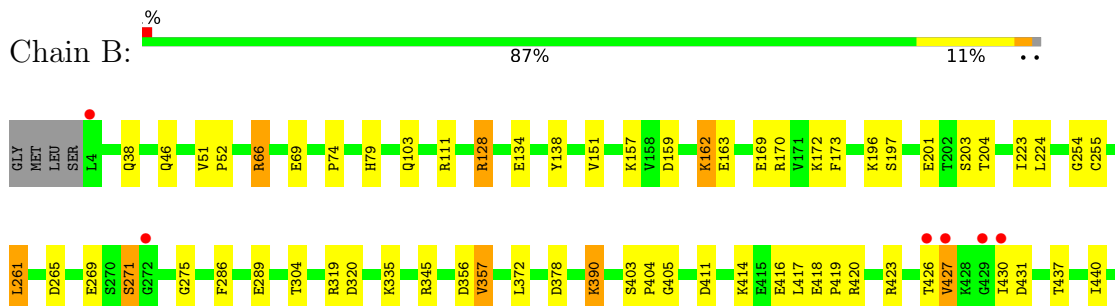
• Molecule 1: Prolyl endopeptidase



• 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	103.74Å 66.35Å 156.30Å 90.00° 101.87° 90.00°	Depositor
Resolution (Å)	34.60 – 1.66 34.60 – 1.66	Depositor EDS
% Data completeness (in resolution range)	74.1 (34.60-1.66) 74.3 (34.60-1.66)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 1.66Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.159 , 0.214 0.170 , 0.220	Depositor DCC
R_{free} test set	12213 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	16.2	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	19158	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.66% 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, A1CQ1, GOL, B3P, NA, DMS, PEG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.93	2/5866 (0.0%)	1.37	33/7952 (0.4%)
1	B	0.90	3/5849 (0.1%)	1.38	33/7929 (0.4%)
1	C	0.94	2/5860 (0.0%)	1.35	28/7943 (0.4%)
All	All	0.92	7/17575 (0.0%)	1.37	94/23824 (0.4%)

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	2
1	B	0	3
1	C	0	1
All	All	0	6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	ILE	CB-CG1	-7.12	1.39	1.53
1	C	250	SER	CA-CB	-6.37	1.45	1.53
1	B	663	SER	CA-CB	-5.92	1.44	1.53
1	B	512	GLU	CD-OE1	5.58	1.35	1.25
1	C	400	SER	CA-CB	-5.39	1.46	1.53
1	A	618	HIS	CD2-NE2	5.29	1.43	1.37
1	B	46	GLN	C-O	-5.09	1.18	1.24

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	512	GLU	CB-CG-CD	10.90	131.12	112.60
1	A	427	VAL	N-CA-CB	-8.95	103.33	112.28
1	A	705	ASN	CA-CB-CG	-8.83	103.77	112.60
1	B	66	ARG	CG-CD-NE	-7.92	94.58	112.00
1	A	339	GLU	CB-CA-C	-7.80	96.43	110.70
1	C	618	HIS	CA-CB-CG	-7.09	106.71	113.80
1	C	109	GLU	CB-CG-CD	7.04	124.56	112.60
1	A	66	ARG	CG-CD-NE	-7.04	96.52	112.00
1	A	705	ASN	CB-CA-C	-6.72	101.74	112.09
1	A	44	GLU	CB-CG-CD	6.70	123.98	112.60
1	B	624	GLU	CB-CG-CD	-6.70	101.22	112.60
1	C	686	THR	CA-CB-OG1	-6.64	99.64	109.60
1	A	221	GLU	CG-CD-OE2	-6.59	103.24	118.40
1	B	419	PRO	CB-CA-C	6.50	119.50	110.98
1	B	697	PHE	CA-CB-CG	-6.48	107.32	113.80
1	A	428	LYS	CB-CA-C	-6.48	97.53	110.42
1	A	65	GLU	CB-CG-CD	6.41	123.50	112.60
1	A	320	ASP	CA-CB-CG	6.39	118.99	112.60
1	C	431	ASP	CB-CA-C	6.38	121.09	110.88
1	B	134	GLU	CB-CA-C	6.38	121.38	110.79
1	B	134	GLU	N-CA-CB	-6.37	100.76	110.12
1	B	345	ARG	NE-CZ-NH2	6.35	124.92	119.20
1	B	265	ASP	CA-CB-CG	6.35	118.95	112.60
1	B	159	ASP	CA-CB-CG	6.34	118.94	112.60
1	A	526[A]	CYS	CB-CA-C	-6.20	101.15	110.88
1	A	526[B]	CYS	CB-CA-C	-6.20	101.15	110.88
1	A	512	GLU	N-CA-CB	6.18	119.86	110.28
1	C	429	GLY	CA-C-N	-6.00	117.26	122.96
1	C	429	GLY	C-N-CA	-6.00	117.26	122.96
1	C	339	GLU	CB-CA-C	-6.00	99.72	110.70
1	C	552	GLY	CA-C-N	5.99	125.73	121.65
1	C	552	GLY	C-N-CA	5.99	125.73	121.65
1	C	699	PHE	CA-CB-CG	5.97	119.77	113.80
1	B	547	ARG	CB-CA-C	-5.90	100.49	110.64
1	B	501	VAL	N-CA-CB	5.86	119.61	112.10
1	C	427	VAL	N-CA-CB	-5.84	104.38	111.21
1	B	588	LYS	N-CA-CB	5.80	119.49	110.44
1	C	173	PHE	CA-CB-CG	-5.78	108.02	113.80
1	A	697	PHE	CA-CB-CG	-5.77	108.03	113.80
1	A	13	GLU	CB-CG-CD	5.76	122.39	112.60
1	C	639	ASP	CA-CB-CG	5.71	118.31	112.60
1	B	372	LEU	N-CA-C	-5.68	106.02	113.12
1	A	418	GLU	CB-CA-C	5.66	115.77	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	172	LYS	CG-CD-CE	5.64	124.28	111.30
1	B	423	ARG	CB-CA-C	-5.64	97.92	109.94
1	B	437	THR	CA-CB-OG1	-5.63	101.15	109.60
1	B	162	LYS	N-CA-CB	-5.63	101.73	110.57
1	C	90	TYR	N-CA-CB	-5.60	101.42	110.71
1	A	393	GLU	CB-CG-CD	5.60	122.11	112.60
1	B	269	GLU	N-CA-CB	5.59	118.12	110.57
1	A	40	LYS	CB-CG-CD	-5.57	98.49	111.30
1	C	172	LYS	CB-CA-C	5.55	120.68	109.68
1	C	278	LYS	CB-CG-CD	5.51	123.97	111.30
1	A	221	GLU	CB-CA-C	-5.49	100.13	110.01
1	C	98	ARG	CG-CD-NE	-5.46	100.00	112.00
1	C	494	HIS	CB-CG-CD2	5.45	138.29	131.20
1	A	66	ARG	N-CA-CB	-5.43	102.12	110.16
1	A	111	ARG	CB-CA-C	-5.42	98.04	109.38
1	C	512	GLU	CB-CG-CD	5.41	121.79	112.60
1	C	256	ASP	CA-CB-CG	5.39	117.99	112.60
1	B	688	LYS	N-CA-CB	5.39	118.23	110.20
1	C	80	PHE	CA-CB-CG	5.35	119.15	113.80
1	B	204	THR	OG1-CB-CG2	-5.34	98.61	109.30
1	C	494	HIS	CB-CG-ND1	-5.31	114.74	122.70
1	C	334	GLU	N-CA-CB	5.28	118.47	110.28
1	A	418	GLU	CB-CG-CD	5.26	121.55	112.60
1	A	252	ARG	CD-NE-CZ	5.25	131.75	124.40
1	B	69	GLU	CB-CG-CD	5.25	121.53	112.60
1	B	320	ASP	CA-CB-CG	5.24	117.84	112.60
1	B	431	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	622	LEU	O-C-N	-5.23	116.76	121.31
1	A	571	PHE	CA-CB-CG	-5.20	108.60	113.80
1	C	192	GLN	CB-CA-C	5.19	118.34	109.72
1	A	58	PRO	CA-C-N	-5.19	112.53	121.09
1	A	58	PRO	C-N-CA	-5.19	112.53	121.09
1	A	415	GLU	CG-CD-OE1	-5.18	106.49	118.40
1	B	587	HIS	N-CA-C	-5.17	106.93	113.18
1	B	128	ARG	NE-CZ-NH1	-5.16	116.34	121.50
1	B	66	ARG	CD-NE-CZ	5.14	131.59	124.40
1	B	269	GLU	CB-CG-CD	5.12	121.30	112.60
1	C	106	LEU	N-CA-CB	5.11	118.22	110.14
1	A	63	TYR	N-CA-C	-5.11	105.62	111.14
1	C	11	ARG	NE-CZ-NH1	5.11	126.61	121.50
1	B	286	PHE	CA-CB-CG	5.09	118.89	113.80
1	C	512	GLU	CB-CA-C	-5.08	102.90	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	428	LYS	N-CA-CB	5.08	119.07	110.49
1	B	526[A]	CYS	CB-CA-C	-5.03	102.98	110.88
1	B	526[B]	CYS	CB-CA-C	-5.03	102.98	110.88
1	B	254	GLY	CA-C-O	-5.03	117.94	122.57
1	A	180	HIS	N-CA-C	-5.02	107.10	113.18
1	B	416	GLU	N-CA-C	5.02	116.45	110.97
1	B	390	LYS	CB-CG-CD	5.01	122.83	111.30
1	B	74	PRO	CB-CA-C	5.01	117.53	111.46
1	A	630	TYR	N-CA-CB	5.00	117.42	110.11

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	423	ARG	Sidechain
1	A	547	ARG	Sidechain
1	B	111	ARG	Sidechain
1	B	170	ARG	Sidechain
1	B	664	ARG	Sidechain
1	C	643	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	5699	0	5526	51	0
1	B	5688	0	5508	39	0
1	C	5696	0	5520	63	0
2	A	12	0	0	2	0
2	B	9	0	0	0	0
2	C	30	0	0	10	0
3	A	21	0	30	3	0
3	B	14	0	20	5	0
3	C	42	0	60	13	0
4	A	54	0	72	6	0
4	B	24	0	32	2	0
4	C	84	0	112	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	4	0	6	0	0
5	B	4	0	6	0	0
5	C	12	0	18	3	0
6	A	29	23	0	0	0
6	B	29	23	0	1	0
6	C	29	23	0	0	0
7	A	19	0	26	4	0
7	B	19	0	26	0	0
8	A	1	0	0	0	0
9	A	534	0	0	20	0
9	B	457	0	0	10	0
9	C	579	0	0	14	0
All	All	19089	69	16962	164	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 5.

All (164) 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:221:GLU:CD	9:A:901:HOH:O	2.03	1.00
1:C:88:TYR:N	9:C:901:HOH:O	1.63	0.99
1:A:270:SER:HB3	9:A:1322:HOH:O	1.66	0.96
1:C:425:VAL:HG22	5:C:823:DMS:H13	1.49	0.91
3:C:814:PEG:H12	9:C:1027:HOH:O	1.73	0.89
1:C:101:TYR:O	9:C:901:HOH:O	1.91	0.86
1:B:255:CYS:SG	6:B:812:A1CQ1:C1	2.64	0.84
7:A:801:B3P:H51	9:A:1116:HOH:O	1.80	0.82
1:C:425:VAL:HG13	5:C:823:DMS:H11	1.60	0.81
1:C:443:PRO:HD2	2:C:824:SCN:S	2.23	0.78
1:C:9:VAL:HA	3:C:814:PEG:H22	1.70	0.73
1:B:163:GLU:HG2	9:B:941:HOH:O	1.86	0.73
1:A:221:GLU:OE1	9:A:901:HOH:O	2.04	0.73
1:C:428:LYS:HD2	1:C:428:LYS:H	1.54	0.72
7:A:801:B3P:H61	9:A:1092:HOH:O	1.90	0.70
1:B:196:LYS:H	1:B:201[A]:GLU:CD	2.00	0.70
1:C:568:PRO:O	3:C:802:PEG:H22	1.91	0.70
4:A:811:GOL:H11	9:A:1279:HOH:O	1.91	0.69
1:A:247:VAL:HG23	1:A:266:LEU:HG	1.74	0.69
1:C:428:LYS:HD2	1:C:428:LYS:N	2.07	0.69
2:C:822:SCN:N	9:C:903:HOH:O	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:GLU:OE2	9:A:902:HOH:O	2.10	0.68
1:C:268:GLN:HE21	1:C:268:GLN:HA	1.59	0.68
1:C:17:GLN:NE2	2:C:827:SCN:S	2.67	0.68
1:C:572:GLY:HA2	3:C:802:PEG:H42	1.77	0.66
1:B:411:ASP:OD2	1:B:414:LYS:HE2	1.96	0.66
2:C:828:SCN:N	9:C:905:HOH:O	2.30	0.65
4:A:812:GOL:H2	9:A:947:HOH:O	1.97	0.64
1:C:7:PRO:HD3	1:C:49:ILE:HD11	1.79	0.63
7:A:801:B3P:O4	7:A:801:B3P:O5	2.06	0.63
1:A:568:PRO:O	4:A:808:GOL:H2	1.99	0.63
1:A:192:GLN:HE21	1:A:193:GLN:H	1.47	0.63
1:C:192:GLN:HE21	1:C:193:GLN:H	1.47	0.62
1:A:221:GLU:CG	9:A:901:HOH:O	2.43	0.62
1:A:190:TYR:HB3	4:A:803:GOL:H12	1.81	0.62
1:B:275:GLY:CA	3:B:807:PEG:H21	2.28	0.62
1:A:170:ARG:HD3	9:A:915:HOH:O	2.00	0.62
1:B:440:ILE:HD12	1:B:440:ILE:C	2.26	0.61
1:C:207:HIS:CD2	4:C:818:GOL:H2	2.35	0.61
1:A:221:GLU:HG3	9:A:901:HOH:O	2.01	0.61
1:A:387:GLY:H	2:A:815:SCN:C	2.15	0.60
1:A:65:GLU:HG3	9:A:1409:HOH:O	2.02	0.59
1:C:327:LYS:HD3	3:C:826:PEG:C2	2.33	0.59
1:C:416:GLU:HB3	9:C:1436:HOH:O	2.02	0.58
1:A:416:GLU:HB2	9:A:1373:HOH:O	2.04	0.58
1:A:664:ARG:HB3	1:A:664:ARG:NH1	2.19	0.58
1:C:379:VAL:HG12	2:C:822:SCN:S	2.44	0.58
1:A:65:GLU:CG	9:A:1409:HOH:O	2.52	0.57
1:C:129:GLY:HA2	4:C:810:GOL:H11	1.85	0.57
1:C:629:GLN:O	3:C:802:PEG:H21	2.04	0.57
1:B:79:HIS:NE2	1:B:103:GLN:NE2	2.52	0.56
1:C:425:VAL:HG13	5:C:823:DMS:C1	2.34	0.56
1:C:436:GLN:NE2	3:C:809:PEG:O4	2.38	0.56
1:C:416:GLU:H	1:C:416:GLU:CD	2.15	0.55
1:C:291:ASP:OD1	4:C:805:GOL:H2	2.07	0.55
1:C:242:ASP:OD2	1:C:294:THR:OG1	2.20	0.54
1:C:317:ASP:OD2	2:C:815:SCN:S	2.66	0.53
1:C:512:GLU:OE1	1:C:516:LYS:HE2	2.08	0.53
1:C:327:LYS:HD3	3:C:826:PEG:C1	2.38	0.53
3:C:814:PEG:H32	9:C:1027:HOH:O	2.08	0.53
1:A:130:TYR:CE2	4:A:817:GOL:H12	2.44	0.53
1:C:268:GLN:HA	1:C:268:GLN:NE2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:LYS:NZ	9:C:918:HOH:O	2.42	0.52
1:C:17:GLN:HB2	2:C:828:SCN:N	2.25	0.52
7:A:801:B3P:C6	9:A:1092:HOH:O	2.50	0.52
1:A:174:SER:O	3:A:802:PEG:H21	2.09	0.51
1:A:251:ILE:HB	1:A:260:ARG:HB2	1.91	0.51
1:B:404:PRO:HD3	1:B:427:VAL:HG22	1.92	0.51
1:B:628:ILE:HA	4:B:805:GOL:O3	2.10	0.51
1:A:423:ARG:HH21	1:A:423:ARG:HG3	1.76	0.50
1:A:544:SER:HB3	2:A:810:SCN:N	2.26	0.50
1:C:30:TRP:CH2	3:C:814:PEG:H31	2.46	0.50
1:C:71:TYR:CZ	1:C:75:LYS:HE2	2.46	0.50
1:A:362:GLN:HE22	3:A:804[B]:PEG:H31	1.76	0.50
1:B:271:SER:HA	9:B:990:HOH:O	2.10	0.50
1:B:692:GLU:O	1:B:696:MET:HG3	2.12	0.50
1:A:79:HIS:HE1	1:A:423:ARG:NH1	2.10	0.50
1:B:197:SER:N	1:B:201[A]:GLU:OE1	2.32	0.50
1:B:275:GLY:HA2	3:B:807:PEG:H21	1.91	0.50
1:C:443:PRO:O	2:C:824:SCN:S	2.70	0.50
1:B:196:LYS:N	1:B:201[A]:GLU:OE2	2.33	0.50
1:B:138:TYR:OH	1:B:157:LYS:HE2	2.11	0.50
1:C:207:HIS:NE2	4:C:818:GOL:H2	2.27	0.49
1:C:7:PRO:HD3	1:C:49:ILE:CD1	2.42	0.49
1:B:224:LEU:HB3	3:B:807:PEG:O2	2.13	0.48
1:C:51:VAL:HB	1:C:52:PRO:HD3	1.95	0.48
1:B:486:VAL:HG23	9:B:1162:HOH:O	2.14	0.48
1:B:196:LYS:N	1:B:201[A]:GLU:CD	2.69	0.48
9:C:1043:HOH:O	1:A:322:GLU:HG3	2.14	0.48
1:A:256:ASP:HB2	9:A:1080:HOH:O	2.14	0.47
1:A:460:ILE:HD13	1:A:498:ILE:HD11	1.94	0.47
1:A:549:THR:HG21	1:A:700:ILE:HD11	1.96	0.47
1:C:443:PRO:CD	2:C:824:SCN:S	3.01	0.47
1:B:390:LYS:HE2	9:B:1124:HOH:O	2.15	0.47
1:A:460:ILE:CD1	1:A:498:ILE:HD11	2.45	0.47
1:B:128:ARG:HD2	1:B:151:VAL:CG2	2.45	0.46
1:B:378:ASP:HB3	9:B:1224:HOH:O	2.14	0.46
1:C:440:ILE:C	1:C:440:ILE:HD12	2.40	0.46
1:B:289:GLU:O	1:B:304:THR:HA	2.15	0.46
1:A:172:LYS:HD3	1:A:173:PHE:CE2	2.51	0.46
1:C:547:ARG:NE	3:C:806:PEG:O4	2.47	0.46
1:A:399:THR:HG21	9:A:1314:HOH:O	2.16	0.46
1:A:323:GLU:OE1	9:A:903:HOH:O	2.21	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:LEU:H	3:B:807:PEG:H41	1.81	0.46
1:C:470:LEU:HG	1:C:530:PHE:CZ	2.50	0.46
1:A:467:PRO:HA	1:A:547:ARG:HB2	1.98	0.45
1:B:665:LYS:O	9:B:901:HOH:O	2.21	0.45
1:C:176:MET:HE3	4:C:810:GOL:H32	1.98	0.45
1:A:51:VAL:HB	1:A:52:PRO:HD3	1.98	0.45
1:C:445:LYS:HE2	1:C:445:LYS:HB2	1.37	0.45
1:B:335:LYS:HE3	9:B:1160:HOH:O	2.16	0.45
1:A:353:TYR:OH	3:A:804[B]:PEG:H11	2.17	0.44
1:B:172:LYS:HD3	1:B:173:PHE:CE2	2.52	0.44
1:A:586:PHE:C	1:A:586:PHE:CD1	2.95	0.44
1:B:51:VAL:HB	1:B:52:PRO:HD3	1.98	0.44
1:A:425:VAL:HG22	9:A:1336:HOH:O	2.18	0.44
1:C:256:ASP:HB2	9:C:1111:HOH:O	2.17	0.44
1:A:106:LEU:HD23	1:A:106:LEU:HA	1.72	0.44
1:C:163:GLU:HB3	9:C:963:HOH:O	2.18	0.43
1:C:577:GLN:NE2	9:C:943:HOH:O	2.51	0.43
1:C:400:SER:HB2	2:C:822:SCN:N	2.33	0.43
1:A:440:ILE:C	1:A:440:ILE:HD12	2.44	0.43
1:A:266:LEU:HD23	1:A:266:LEU:HA	1.91	0.43
1:A:606[A]:GLN:H	1:A:606[A]:GLN:CD	2.27	0.43
1:A:423:ARG:HH21	1:A:423:ARG:CG	2.31	0.43
1:C:358:LYS:HG2	1:C:379:VAL:CG1	2.49	0.42
1:C:128:ARG:HD2	1:C:151:VAL:CG2	2.49	0.42
1:A:428:LYS:HB2	1:A:429:GLY:H	1.65	0.42
1:C:549:THR:HA	1:C:573:CYS:O	2.20	0.42
1:A:7:PRO:HD3	1:A:49:ILE:CD1	2.49	0.42
1:C:106:LEU:HD23	1:C:106:LEU:HA	1.82	0.42
1:A:74:PRO:HG3	9:A:953:HOH:O	2.19	0.42
1:B:405:GLY:HA3	4:B:806:GOL:H32	2.01	0.42
1:A:645:VAL:HG23	1:A:647:LEU:HG	2.02	0.42
1:C:358:LYS:HE2	1:C:358:LYS:HB2	1.83	0.42
1:B:356:ASP:C	1:B:357:VAL:HG23	2.45	0.42
1:C:327:LYS:HD3	3:C:826:PEG:H11	2.01	0.41
1:C:323:GLU:HA	1:C:326:TRP:CE2	2.55	0.41
1:B:491:PHE:CE2	1:B:497:GLY:HA3	2.55	0.41
1:C:57:CYS:CB	1:C:698:ALA:HB1	2.50	0.41
1:A:416:GLU:HB3	1:A:418:GLU:HB2	2.01	0.41
1:B:169:GLU:HG2	9:B:1195:HOH:O	2.19	0.41
1:B:261:LEU:C	1:B:261:LEU:HD13	2.46	0.41
1:B:223:ILE:HG23	3:B:807:PEG:H32	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:546:LYS:HG2	9:B:1230:HOH:O	2.20	0.41
1:B:583:MET:HE1	1:B:599:TYR:CD2	2.55	0.41
1:C:291:ASP:OD1	4:C:805:GOL:C2	2.68	0.41
1:C:668:ASN:ND2	3:C:802:PEG:H41	2.36	0.41
1:B:642:ASP:HB2	9:B:910:HOH:O	2.20	0.41
1:C:395:PHE:HA	1:C:408:TYR:O	2.20	0.41
1:C:485:SER:CB	1:C:488[A]:ARG:HD2	2.51	0.41
1:A:485:SER:HA	4:A:809:GOL:H32	2.02	0.41
1:C:409:HIS:O	1:C:419:PRO:HA	2.21	0.41
1:A:59:ILE:HG12	1:A:701:ALA:CB	2.51	0.41
1:B:420:ARG:HG3	1:B:420:ARG:HH11	1.86	0.41
1:C:373:LYS:HE3	1:C:417:LEU:O	2.20	0.40
1:B:38:GLN:N	1:B:38:GLN:CD	2.79	0.40
1:A:306:ARG:HG3	1:A:307:GLN:HG3	2.04	0.40
1:B:430:ILE:HD13	1:B:489:LEU:HB3	2.02	0.40
1:C:430:ILE:HG21	1:C:489:LEU:HD13	2.03	0.40
1:A:549:THR:HA	1:A:573:CYS:O	2.21	0.40
1:C:278:LYS:HE3	9:C:1312:HOH:O	2.21	0.40
4:C:804:GOL:H31	9:C:950:HOH:O	2.20	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	710/711 (100%)	686 (97%)	22 (3%)	2 (0%)	36	21
1	B	708/711 (100%)	687 (97%)	19 (3%)	2 (0%)	36	21
1	C	709/711 (100%)	688 (97%)	20 (3%)	1 (0%)	48	30
All	All	2127/2133 (100%)	2061 (97%)	61 (3%)	5 (0%)	43	27

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	428	LYS
1	C	357	VAL
1	A	357	VAL
1	B	417	LEU
1	B	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	619/617 (100%)	603 (97%)	16 (3%)	40	17
1	B	617/617 (100%)	600 (97%)	17 (3%)	38	15
1	C	618/617 (100%)	604 (98%)	14 (2%)	44	21
All	All	1854/1851 (100%)	1807 (98%)	47 (2%)	40	18

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	8	ASP
1	C	23	LYS
1	C	103	GLN
1	C	163	GLU
1	C	261	LEU
1	C	268	GLN
1	C	319	ARG
1	C	357	VAL
1	C	358	LYS
1	C	416	GLU
1	C	428	LYS
1	C	440	ILE
1	C	445	LYS
1	C	486	VAL
1	A	5	GLN
1	A	23	LYS
1	A	59	ILE
1	A	84	LYS

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Mol	Chain	Res	Type
1	A	170	ARG
1	A	261	LEU
1	A	357	VAL
1	A	373	LYS
1	A	403	SER
1	A	414	LYS
1	A	416	GLU
1	A	418	GLU
1	A	425	VAL
1	A	427	VAL
1	A	445	LYS
1	A	664	ARG
1	B	66	ARG
1	B	162	LYS
1	B	203	SER
1	B	261	LEU
1	B	271	SER
1	B	319	ARG
1	B	403	SER
1	B	418	GLU
1	B	426	THR
1	B	427	VAL
1	B	512	GLU
1	B	546	LYS
1	B	547	ARG
1	B	598	ASP
1	B	604	SER
1	B	624	GLU
1	B	664	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	103	GLN
1	C	192	GLN
1	C	205	ASN
1	C	268	GLN
1	C	436	GLN
1	C	483	ASN
1	C	524	GLN
1	C	531	GLN
1	C	566	GLN

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Mol	Chain	Res	Type
1	C	577	GLN
1	A	192	GLN
1	A	205	ASN
1	A	267	GLN
1	A	268	GLN
1	A	362	GLN
1	A	439	GLN
1	A	483	ASN
1	A	524	GLN
1	A	531	GLN
1	A	551	ASN
1	A	566	GLN
1	A	577	GLN
1	B	103	GLN
1	B	267	GLN
1	B	362	GLN
1	B	524	GLN
1	B	531	GLN
1	B	566	GLN
1	B	577	GLN
1	B	606	GLN

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 66 ligands modelled in this entry, 1 is monoatomic - leaving 65 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
4	GOL	A	803	-	5,5,5	0.36	0	5,5,5	1.45	1 (20%)
2	SCN	C	819	-	1,2,2	0.01	0	0,1,1	-	-
5	DMS	B	809	-	3,3,3	0.38	0	3,3,3	0.05	0
4	GOL	C	832	-	5,5,5	0.13	0	5,5,5	0.33	0
4	GOL	A	808	-	5,5,5	0.22	0	5,5,5	0.83	0
5	DMS	C	821	-	3,3,3	0.60	0	3,3,3	0.32	0
4	GOL	A	805	-	5,5,5	0.22	0	5,5,5	0.35	0
2	SCN	C	816	-	1,2,2	0.40	0	0,1,1	-	-
2	SCN	A	814	-	1,2,2	0.05	0	0,1,1	-	-
7	B3P	B	801	-	18,18,18	0.67	0	23,23,23	1.01	0
4	GOL	C	834	-	5,5,5	0.33	0	5,5,5	0.63	0
2	SCN	C	824	-	1,2,2	0.20	0	0,1,1	-	-
3	PEG	C	814	-	6,6,6	1.10	0	5,5,5	1.07	0
3	PEG	B	808	-	6,6,6	0.38	0	5,5,5	0.24	0
4	GOL	A	817	-	5,5,5	0.10	0	5,5,5	0.36	0
3	PEG	C	806	-	6,6,6	0.67	0	5,5,5	0.41	0
2	SCN	C	827	-	1,2,2	1.14	0	0,1,1	-	-
4	GOL	C	810	-	5,5,5	0.56	0	5,5,5	1.52	1 (20%)
3	PEG	C	802	-	6,6,6	0.74	0	5,5,5	0.69	0
3	PEG	C	809	-	6,6,6	0.15	0	5,5,5	0.30	0
4	GOL	C	818	-	5,5,5	0.62	0	5,5,5	1.12	0
4	GOL	A	809	-	5,5,5	0.60	0	5,5,5	1.57	1 (20%)
5	DMS	A	813	-	3,3,3	0.56	0	3,3,3	0.33	0
2	SCN	A	807	-	1,2,2	0.55	0	0,1,1	-	-
2	SCN	B	810	-	1,2,2	0.51	0	0,1,1	-	-
4	GOL	C	803	-	5,5,5	0.17	0	5,5,5	0.50	0
4	GOL	C	807	-	5,5,5	0.33	0	5,5,5	0.88	0
3	PEG	B	807	-	6,6,6	0.21	0	5,5,5	0.21	0
2	SCN	C	828	-	1,2,2	0.43	0	0,1,1	-	-
2	SCN	B	811	-	1,2,2	1.47	0	0,1,1	-	-
3	PEG	A	804[B]	-	6,6,6	0.99	0	5,5,5	0.82	0
4	GOL	C	808	-	5,5,5	0.24	0	5,5,5	0.74	0
4	GOL	C	830	-	5,5,5	0.46	0	5,5,5	0.51	0
2	SCN	B	804	-	1,2,2	2.60	1 (100%)	0,1,1	-	-
2	SCN	A	815	-	1,2,2	0.34	0	0,1,1	-	-
5	DMS	C	823	-	3,3,3	0.46	0	3,3,3	0.37	0
4	GOL	C	811	-	5,5,5	0.17	0	5,5,5	0.53	0
4	GOL	C	813	-	5,5,5	0.33	0	5,5,5	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	B	803	-	5,5,5	0.13	0	5,5,5	0.34	0
6	A1CQ1	A	816	1	32,32,33	1.34	3 (9%)	44,44,46	2.59	11 (25%)
4	GOL	C	805	-	5,5,5	0.30	0	5,5,5	0.60	0
7	B3P	A	801	-	18,18,18	0.57	0	23,23,23	1.37	5 (21%)
2	SCN	C	822	-	1,2,2	0.00	0	0,1,1	-	-
3	PEG	C	817	-	6,6,6	0.51	0	5,5,5	0.22	0
5	DMS	C	825	-	3,3,3	0.43	0	3,3,3	0.43	0
4	GOL	A	811	-	5,5,5	0.52	0	5,5,5	1.18	0
6	A1CQ1	C	829	1	32,32,33	1.33	4 (12%)	44,44,46	2.50	12 (27%)
3	PEG	A	804[A]	-	6,6,6	0.66	0	5,5,5	0.37	0
4	GOL	C	833	-	5,5,5	0.21	0	5,5,5	0.28	0
2	SCN	A	810	-	1,2,2	2.54	1 (100%)	0,1,1	-	-
2	SCN	C	815	-	1,2,2	0.48	0	0,1,1	-	-
2	SCN	C	812	-	1,2,2	0.34	0	0,1,1	-	-
4	GOL	A	812	-	5,5,5	0.10	0	5,5,5	0.34	0
6	A1CQ1	B	812	-	32,32,33	1.45	4 (12%)	44,44,46	3.77	17 (38%)
4	GOL	A	806	-	5,5,5	0.17	0	5,5,5	0.29	0
4	GOL	C	804	-	5,5,5	0.18	0	5,5,5	0.57	0
4	GOL	B	806	-	5,5,5	0.25	0	5,5,5	0.65	0
4	GOL	B	805	-	5,5,5	0.36	0	5,5,5	0.57	0
4	GOL	B	802	-	5,5,5	0.24	0	5,5,5	0.38	0
3	PEG	A	802	-	6,6,6	0.95	0	5,5,5	0.94	0
4	GOL	C	831	-	5,5,5	0.19	0	5,5,5	0.60	0
2	SCN	C	801	-	1,2,2	0.42	0	0,1,1	-	-
3	PEG	C	826	-	6,6,6	0.98	0	5,5,5	0.71	0
2	SCN	C	820	-	1,2,2	0.19	0	0,1,1	-	-
4	GOL	A	818	-	5,5,5	0.25	0	5,5,5	0.57	0

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	803	-	-	1/4/4/4	-
4	GOL	C	832	-	-	0/4/4/4	-
4	GOL	A	808	-	-	4/4/4/4	-
4	GOL	A	805	-	-	2/4/4/4	-
7	B3P	B	801	-	-	2/28/28/28	-
4	GOL	C	834	-	-	1/4/4/4	-
3	PEG	B	808	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	C	814	-	-	2/4/4/4	-
4	GOL	A	817	-	-	2/4/4/4	-
3	PEG	C	806	-	-	3/4/4/4	-
4	GOL	C	810	-	-	2/4/4/4	-
3	PEG	C	802	-	-	2/4/4/4	-
3	PEG	C	809	-	-	0/4/4/4	-
4	GOL	C	818	-	-	2/4/4/4	-
4	GOL	A	809	-	-	1/4/4/4	-
4	GOL	C	803	-	-	4/4/4/4	-
4	GOL	C	807	-	-	3/4/4/4	-
3	PEG	B	807	-	-	1/4/4/4	-
3	PEG	A	804[B]	-	-	3/4/4/4	-
4	GOL	C	808	-	-	2/4/4/4	-
4	GOL	C	830	-	-	0/4/4/4	-
4	GOL	C	813	-	-	2/4/4/4	-
4	GOL	B	803	-	-	2/4/4/4	-
6	A1CQ1	A	816	1	-	4/18/25/25	0/4/4/4
4	GOL	C	805	-	-	4/4/4/4	-
7	B3P	A	801	-	-	12/28/28/28	-
6	A1CQ1	C	829	1	-	5/18/25/25	0/4/4/4
3	PEG	C	817	-	-	3/4/4/4	-
4	GOL	A	811	-	-	2/4/4/4	-
3	PEG	A	804[A]	-	-	3/4/4/4	-
4	GOL	C	833	-	-	2/4/4/4	-
4	GOL	A	812	-	-	4/4/4/4	-
6	A1CQ1	B	812	-	-	5/18/25/25	0/4/4/4
4	GOL	A	806	-	-	2/4/4/4	-
4	GOL	C	804	-	-	2/4/4/4	-
4	GOL	B	806	-	-	2/4/4/4	-
4	GOL	B	805	-	-	2/4/4/4	-
4	GOL	B	802	-	-	2/4/4/4	-
3	PEG	A	802	-	-	3/4/4/4	-
4	GOL	C	831	-	-	0/4/4/4	-
3	PEG	C	826	-	-	3/4/4/4	-
4	GOL	C	811	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	818	-	-	2/4/4/4	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	829	A1CQ1	C2-C15	-5.02	1.39	1.50
6	A	816	A1CQ1	C2-C15	-4.90	1.39	1.50
6	B	812	A1CQ1	C2-C15	-4.09	1.41	1.50
6	B	812	A1CQ1	C5-C4	-3.92	1.35	1.41
6	C	829	A1CQ1	C6-N3	2.83	1.35	1.32
6	A	816	A1CQ1	C6-N3	2.77	1.35	1.32
6	A	816	A1CQ1	C5-C6	-2.63	1.39	1.43
2	B	804	SCN	C-N	-2.60	1.06	1.15
2	A	810	SCN	C-N	-2.54	1.06	1.15
6	C	829	A1CQ1	C5-C6	-2.49	1.39	1.43
6	B	812	A1CQ1	C5-C6	-2.47	1.39	1.43
6	B	812	A1CQ1	C6-N3	2.14	1.34	1.32
6	C	829	A1CQ1	O2-C17	2.11	1.27	1.23

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	812	A1CQ1	C4-C5-C6	12.08	109.03	105.15
6	B	812	A1CQ1	C5-C6-N3	-11.80	106.14	110.76
6	B	812	A1CQ1	C9-C8-N2	-10.31	101.06	111.93
6	A	816	A1CQ1	C9-C8-N2	-8.70	102.76	111.93
6	C	829	A1CQ1	C9-C8-N2	-8.06	103.43	111.93
6	C	829	A1CQ1	C5-C6-N3	-6.89	108.06	110.76
6	A	816	A1CQ1	C5-C6-N3	-6.71	108.13	110.76
6	C	829	A1CQ1	C8-N2-N3	6.44	125.29	119.75
6	B	812	A1CQ1	C5-C4-N1	-6.22	119.63	127.01
6	A	816	A1CQ1	C8-N2-N3	6.02	124.93	119.75
6	B	812	A1CQ1	N1-C4-N2	5.76	134.33	125.34
6	B	812	A1CQ1	C8-N2-N3	5.35	124.35	119.75
6	A	816	A1CQ1	C5-C4-N1	-5.23	120.81	127.01
6	C	829	A1CQ1	C5-C4-N1	-5.00	121.08	127.01
6	B	812	A1CQ1	C5-C1-C2	4.80	128.61	120.70
6	A	816	A1CQ1	C4-N2-N3	-3.94	108.84	111.05
6	B	812	A1CQ1	C1-C2-C3	-3.77	114.05	117.92
6	C	829	A1CQ1	C4-N2-N3	-3.68	108.98	111.05
6	A	816	A1CQ1	N1-C4-N2	3.64	131.02	125.34
6	A	816	A1CQ1	C6-N3-N2	3.57	109.00	104.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	829	A1CQ1	C6-N3-N2	3.52	108.94	104.97
6	C	829	A1CQ1	N1-C4-N2	3.46	130.75	125.34
6	B	812	A1CQ1	C6-N3-N2	3.33	108.72	104.97
6	B	812	A1CQ1	C7-C6-N3	3.26	124.32	119.93
7	A	801	B3P	O5-C6-C4	-2.97	105.65	111.68
6	B	812	A1CQ1	C1-C5-C4	-2.97	114.68	117.67
6	A	816	A1CQ1	C7-C6-N3	2.96	123.92	119.93
6	B	812	A1CQ1	C2-C3-N1	-2.79	119.48	123.59
6	B	812	A1CQ1	C3-N1-C4	2.70	123.53	115.19
7	A	801	B3P	C5-C4-N1	-2.59	101.29	109.02
6	C	829	A1CQ1	C7-C6-N3	2.36	123.10	119.93
4	A	803	GOL	O1-C1-C2	2.36	120.98	110.38
7	A	801	B3P	C11-C8-C9	-2.34	104.90	110.02
6	B	812	A1CQ1	C16-C17-N6	2.23	121.04	117.29
7	A	801	B3P	C2-N2-C8	-2.23	112.90	116.17
4	C	810	GOL	O3-C3-C2	2.20	120.30	110.38
6	C	829	A1CQ1	C2-C3-N1	-2.19	120.37	123.59
6	B	812	A1CQ1	C11-C10-C14	2.18	120.30	117.10
6	A	816	A1CQ1	C2-C3-N1	-2.09	120.52	123.59
6	B	812	A1CQ1	C21-N6-C18	2.08	114.13	111.37
4	A	809	GOL	O2-C2-C3	2.07	117.76	109.18
6	C	829	A1CQ1	C13-N4-C14	2.07	120.47	116.85
6	A	816	A1CQ1	C4-C5-C6	2.05	105.81	105.15
6	C	829	A1CQ1	C21-N6-C18	2.04	114.07	111.37
6	C	829	A1CQ1	C4-C5-C6	2.02	105.80	105.15
7	A	801	B3P	O3-C11-C8	-2.02	107.58	111.68
6	A	816	A1CQ1	C1-C5-C6	-2.02	134.60	136.72
6	B	812	A1CQ1	O1-C15-N5	-2.02	118.67	122.59

There are no chirality outliers.

All (107) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	803	GOL	O1-C1-C2-O2
4	C	804	GOL	O1-C1-C2-C3
4	C	805	GOL	C1-C2-C3-O3
4	C	808	GOL	C1-C2-C3-O3
4	C	810	GOL	O1-C1-C2-C3
4	C	818	GOL	C1-C2-C3-O3
4	A	806	GOL	O1-C1-C2-C3
4	A	808	GOL	O1-C1-C2-C3
4	A	808	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	A	811	GOL	O1-C1-C2-C3
4	A	812	GOL	C1-C2-C3-O3
4	A	812	GOL	O2-C2-C3-O3
4	A	817	GOL	C1-C2-C3-O3
4	A	818	GOL	O1-C1-C2-C3
4	B	802	GOL	C1-C2-C3-O3
4	B	805	GOL	C1-C2-C3-O3
7	A	801	B3P	C7-C4-C5-O4
7	A	801	B3P	N1-C4-C6-O5
7	A	801	B3P	C5-C4-C6-O5
7	A	801	B3P	C7-C4-C6-O5
7	A	801	B3P	N1-C4-C7-O6
7	A	801	B3P	C5-C4-C7-O6
7	A	801	B3P	C6-C4-C7-O6
6	A	816	A1CQ1	O1-C15-C2-C3
6	A	816	A1CQ1	N5-C15-C2-C3
3	C	802	PEG	C1-C2-O2-C3
6	A	816	A1CQ1	N5-C15-C2-C1
6	A	816	A1CQ1	O1-C15-C2-C1
6	C	829	A1CQ1	N5-C15-C2-C1
6	C	829	A1CQ1	O1-C15-C2-C3
6	B	812	A1CQ1	O1-C15-C2-C3
6	C	829	A1CQ1	N5-C15-C2-C3
6	B	812	A1CQ1	N5-C15-C2-C1
6	B	812	A1CQ1	N5-C15-C2-C3
4	C	805	GOL	O1-C1-C2-O2
4	C	808	GOL	O2-C2-C3-O3
4	C	810	GOL	O1-C1-C2-O2
4	C	811	GOL	O1-C1-C2-O2
4	A	808	GOL	O2-C2-C3-O3
3	C	806	PEG	O2-C3-C4-O4
6	C	829	A1CQ1	O1-C15-C2-C1
6	B	812	A1CQ1	O1-C15-C2-C1
3	C	806	PEG	O1-C1-C2-O2
3	A	802	PEG	O2-C3-C4-O4
3	A	804[A]	PEG	O1-C1-C2-O2
3	B	808	PEG	O2-C3-C4-O4
4	C	803	GOL	O1-C1-C2-C3
4	C	803	GOL	C1-C2-C3-O3
4	C	805	GOL	O1-C1-C2-C3
4	C	807	GOL	C1-C2-C3-O3
4	C	811	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	C	813	GOL	C1-C2-C3-O3
4	A	805	GOL	C1-C2-C3-O3
4	A	812	GOL	O1-C1-C2-C3
4	B	806	GOL	C1-C2-C3-O3
3	C	814	PEG	O2-C3-C4-O4
3	C	826	PEG	O2-C3-C4-O4
3	C	814	PEG	C1-C2-O2-C3
4	C	804	GOL	O1-C1-C2-O2
4	C	805	GOL	O2-C2-C3-O3
4	C	807	GOL	O2-C2-C3-O3
4	C	813	GOL	O2-C2-C3-O3
4	C	818	GOL	O2-C2-C3-O3
4	A	806	GOL	O1-C1-C2-O2
4	A	808	GOL	O1-C1-C2-O2
4	A	811	GOL	O1-C1-C2-O2
4	A	818	GOL	O1-C1-C2-O2
4	B	805	GOL	O2-C2-C3-O3
7	A	801	B3P	N1-C4-C5-O4
3	C	802	PEG	O2-C3-C4-O4
3	C	826	PEG	O1-C1-C2-O2
3	A	804[B]	PEG	O2-C3-C4-O4
3	B	807	PEG	O2-C3-C4-O4
7	A	801	B3P	C1-C3-N1-C4
3	C	806	PEG	C1-C2-O2-C3
3	C	826	PEG	C4-C3-O2-C2
3	C	817	PEG	O1-C1-C2-O2
4	A	817	GOL	O2-C2-C3-O3
4	B	802	GOL	O2-C2-C3-O3
4	C	803	GOL	O2-C2-C3-O3
4	C	807	GOL	O1-C1-C2-O2
4	C	833	GOL	O1-C1-C2-O2
4	B	806	GOL	O2-C2-C3-O3
4	A	805	GOL	O2-C2-C3-O3
3	A	804[B]	PEG	C1-C2-O2-C3
4	C	833	GOL	O1-C1-C2-C3
3	B	808	PEG	O1-C1-C2-O2
7	B	801	B3P	C7-C4-C6-O5
3	A	802	PEG	C4-C3-O2-C2
3	A	802	PEG	O1-C1-C2-O2
7	A	801	B3P	O3-C11-C8-N2
4	C	834	GOL	C1-C2-C3-O3
4	A	803	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	A	812	GOL	O1-C1-C2-O2
3	A	804[A]	PEG	C1-C2-O2-C3
4	A	809	GOL	O1-C1-C2-O2
3	C	817	PEG	C4-C3-O2-C2
4	B	803	GOL	C1-C2-C3-O3
6	C	829	A1CQ1	C17-C16-N5-C15
3	A	804[B]	PEG	C4-C3-O2-C2
6	B	812	A1CQ1	C17-C16-N5-C15
3	C	817	PEG	C1-C2-O2-C3
7	B	801	B3P	N1-C4-C6-O5
4	B	803	GOL	O2-C2-C3-O3
7	A	801	B3P	C6-C4-C5-O4
3	A	804[A]	PEG	C4-C3-O2-C2
7	A	801	B3P	C2-C1-C3-N1

There are no ring outliers.

30 monomers are involved in 56 short contacts:

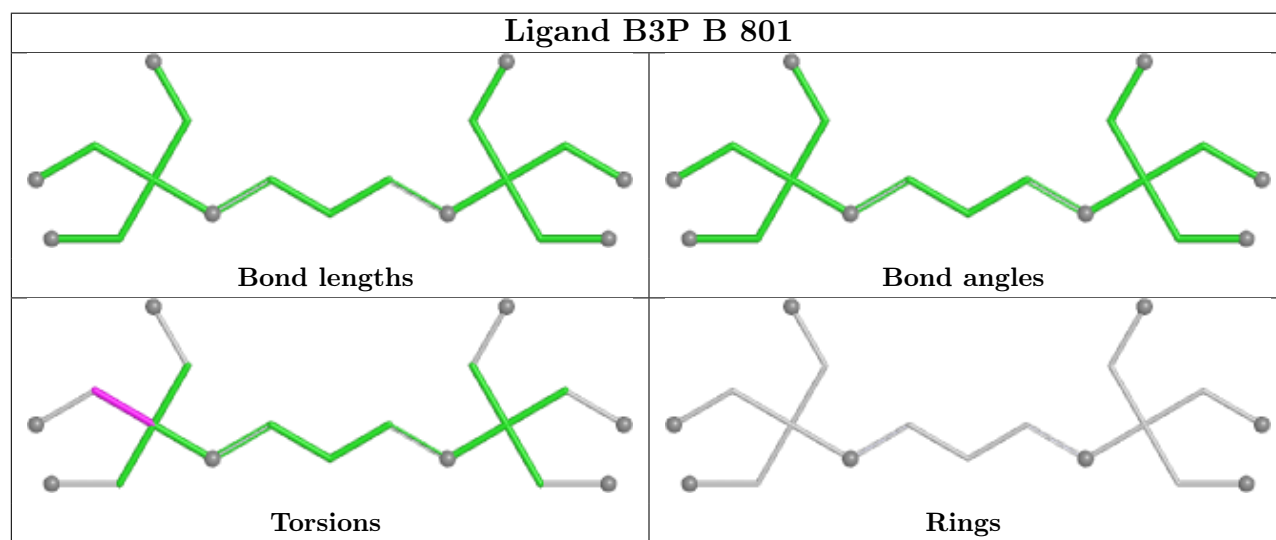
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	803	GOL	1	0
4	A	808	GOL	1	0
2	C	824	SCN	3	0
3	C	814	PEG	4	0
4	A	817	GOL	1	0
3	C	806	PEG	1	0
2	C	827	SCN	1	0
4	C	810	GOL	2	0
3	C	802	PEG	4	0
3	C	809	PEG	1	0
4	C	818	GOL	2	0
4	A	809	GOL	1	0
3	B	807	PEG	5	0
2	C	828	SCN	2	0
3	A	804[B]	PEG	2	0
2	A	815	SCN	1	0
5	C	823	DMS	3	0
4	C	805	GOL	2	0
7	A	801	B3P	4	0
2	C	822	SCN	3	0
4	A	811	GOL	1	0
2	A	810	SCN	1	0
2	C	815	SCN	1	0

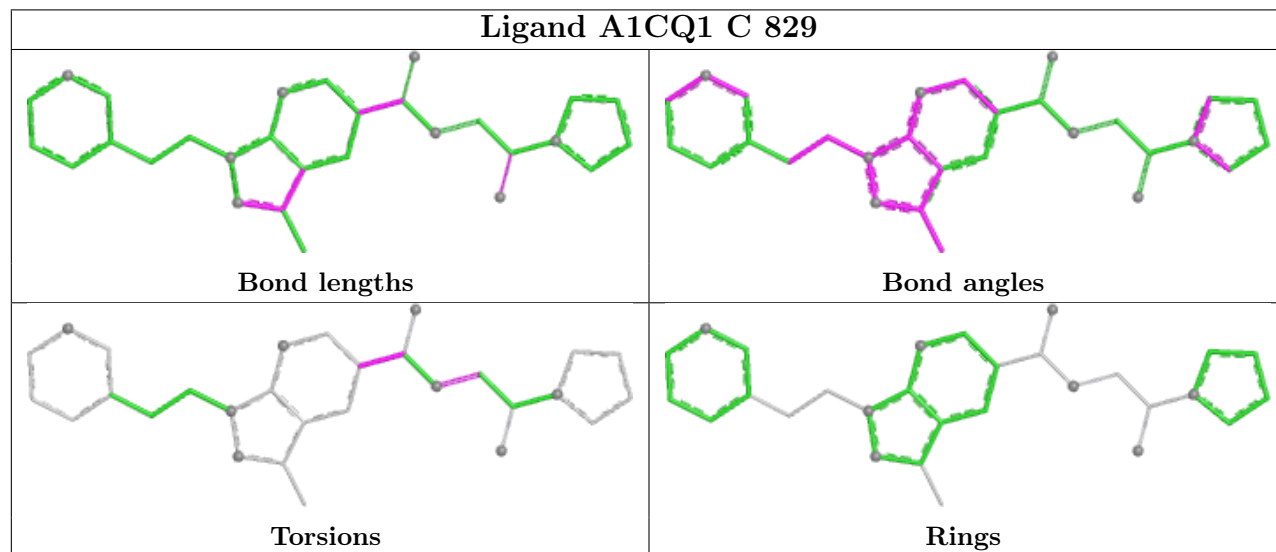
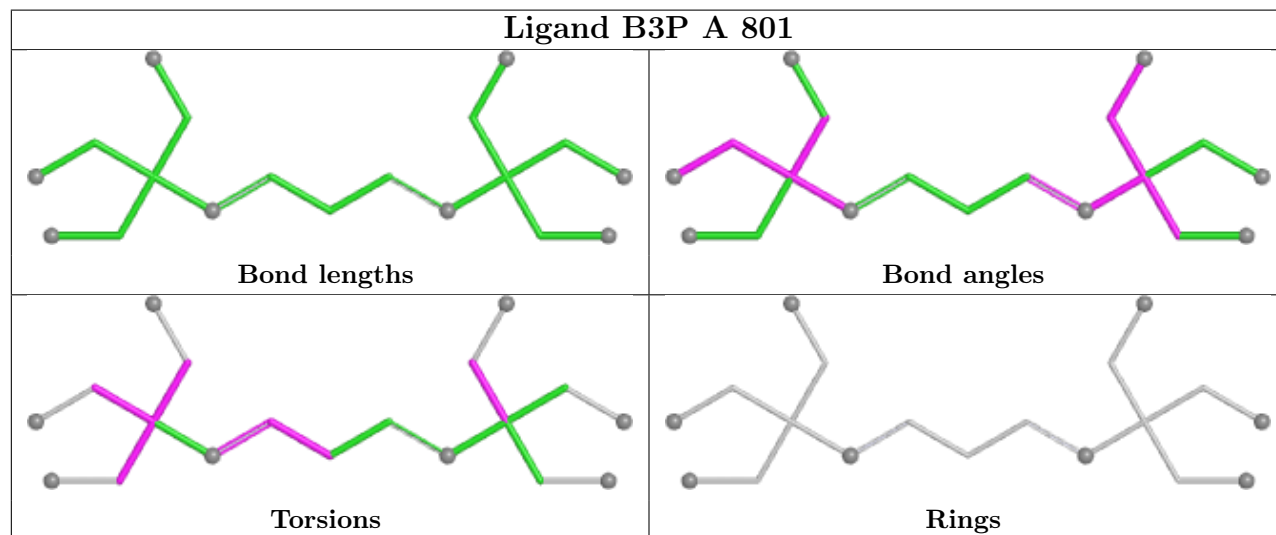
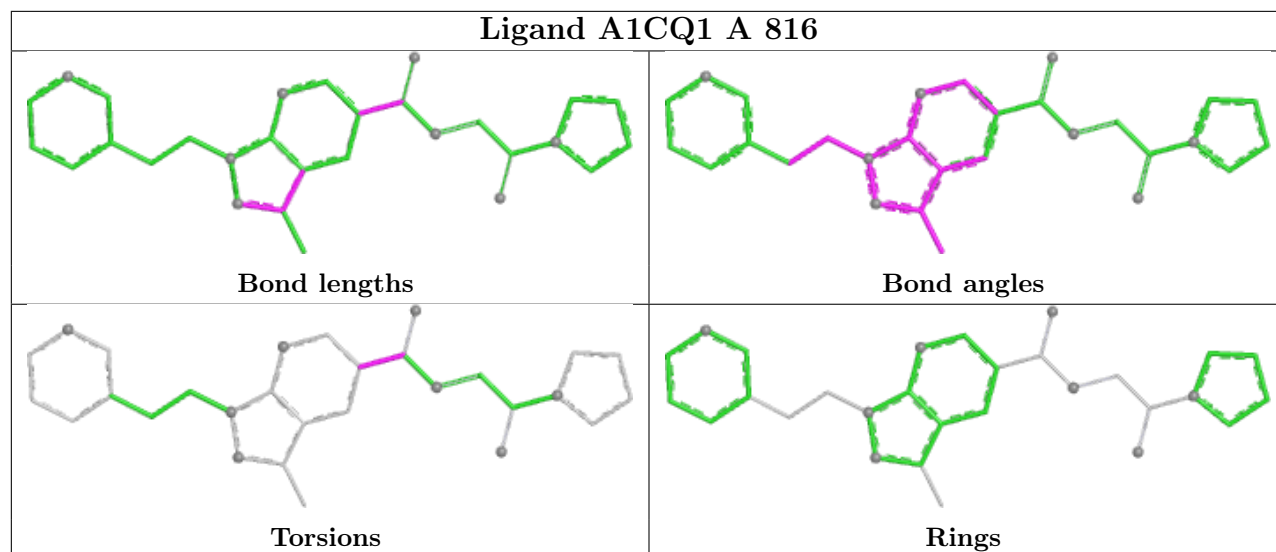
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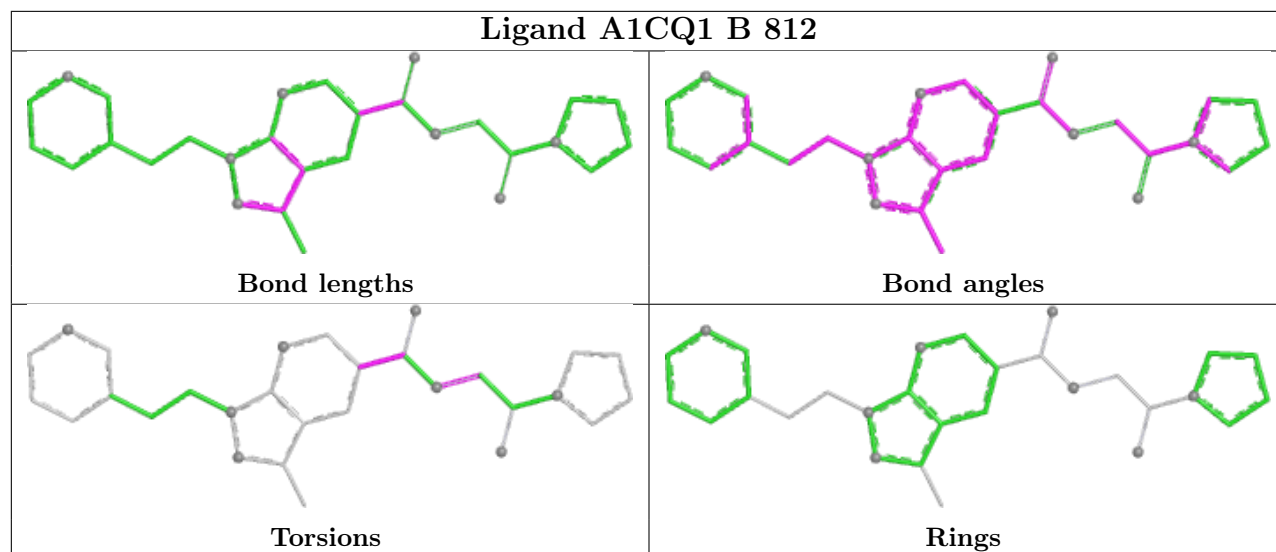
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	812	GOL	1	0
6	B	812	A1CQ1	1	0
4	C	804	GOL	1	0
4	B	806	GOL	1	0
4	B	805	GOL	1	0
3	A	802	PEG	1	0
3	C	826	PEG	3	0

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%)	-0.47	6 (0%) 82 87	9, 17, 35, 59	5 (0%)
1	B	707/711 (99%)	-0.29	6 (0%) 82 87	10, 21, 41, 70	3 (0%)
1	C	707/711 (99%)	-0.55	1 (0%) 92 94	8, 16, 33, 61	4 (0%)
All	All	2121/2133 (99%)	-0.43	13 (0%) 85 90	8, 18, 37, 70	12 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	427	VAL	5.0
1	B	4	LEU	3.5
1	B	427	VAL	3.5
1	B	426	THR	3.2
1	A	4	LEU	3.1
1	A	426	THR	3.1
1	B	272	GLY	2.8
1	B	429	GLY	2.5
1	B	430	ILE	2.5
1	C	4	LEU	2.3
1	A	429	GLY	2.3
1	A	428	LYS	2.2
1	A	425	VAL	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PEG	B	807	7/7	0.59	0.31	24,25,26,26	7
4	GOL	C	831	6/6	0.72	0.14	47,50,53,54	0
4	GOL	C	805	6/6	0.73	0.15	36,38,41,41	0
3	PEG	A	804[B]	7/7	0.75	0.23	19,21,22,24	7
3	PEG	A	804[A]	7/7	0.75	0.23	26,34,49,49	7
4	GOL	C	807	6/6	0.76	0.17	35,38,49,52	0
2	SCN	C	812	3/3	0.79	0.14	44,44,48,64	0
3	PEG	B	808	7/7	0.81	0.16	51,56,58,59	0
2	SCN	C	828	3/3	0.83	0.13	48,48,54,72	0
3	PEG	C	826	7/7	0.83	0.15	36,43,54,57	0
2	SCN	C	822	3/3	0.83	0.25	34,34,38,64	0
3	PEG	C	809	7/7	0.84	0.13	41,52,54,57	0
2	SCN	C	815	3/3	0.84	0.11	42,42,61,65	0
4	GOL	C	803	6/6	0.84	0.13	34,47,49,51	0
4	GOL	A	818	6/6	0.84	0.15	46,51,53,54	0
3	PEG	A	802	7/7	0.85	0.14	28,28,46,47	0
2	SCN	C	824	3/3	0.85	0.23	31,31,40,48	0
3	PEG	C	814	7/7	0.85	0.14	31,33,47,48	0
4	GOL	C	813	6/6	0.85	0.12	36,51,55,56	0
3	PEG	C	817	7/7	0.85	0.12	34,36,43,49	0
4	GOL	A	809	6/6	0.85	0.14	25,31,34,44	0
4	GOL	A	812	6/6	0.85	0.11	46,48,51,51	0
4	GOL	A	817	6/6	0.85	0.13	40,57,63,68	0
2	SCN	A	815	3/3	0.85	0.20	37,37,40,57	0
5	DMS	C	823	4/4	0.85	0.17	42,45,56,72	0
4	GOL	C	834	6/6	0.86	0.14	24,37,43,46	0
4	GOL	B	803	6/6	0.86	0.12	37,44,47,50	0
2	SCN	A	810	3/3	0.86	0.15	33,33,33,61	0
4	GOL	C	818	6/6	0.87	0.12	28,36,39,40	0
4	GOL	B	806	6/6	0.87	0.13	39,43,52,55	0
4	GOL	A	806	6/6	0.87	0.11	34,43,48,50	0
6	A1CQ1	B	812	29/30	0.87	0.08	20,20,20,20	0
2	SCN	C	827	3/3	0.88	0.11	45,45,52,64	0
3	PEG	C	806	7/7	0.88	0.12	35,39,46,47	0
4	GOL	C	808	6/6	0.88	0.12	20,40,44,46	0
2	SCN	A	814	3/3	0.88	0.13	47,47,50,53	0
4	GOL	B	802	6/6	0.89	0.12	31,43,48,48	0

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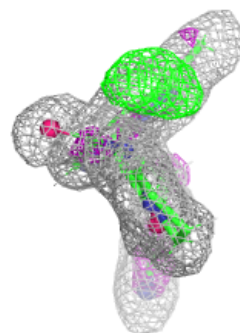
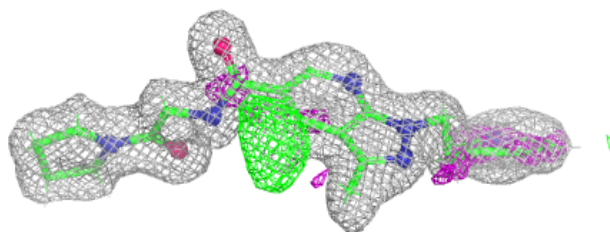
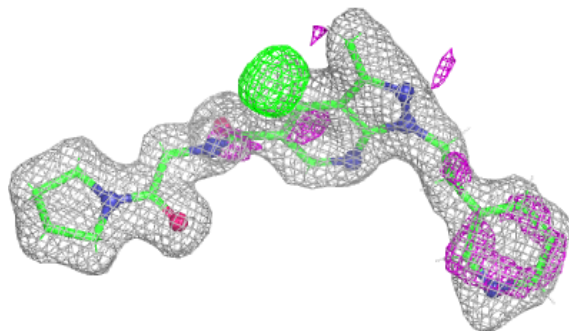
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	A	811	6/6	0.89	0.12	24,30,33,34	0
4	GOL	A	805	6/6	0.89	0.11	33,44,45,46	0
4	GOL	C	810	6/6	0.89	0.13	25,40,42,51	0
4	GOL	C	811	6/6	0.89	0.11	34,46,48,49	0
3	PEG	C	802	7/7	0.90	0.10	27,29,38,42	0
2	SCN	A	807	3/3	0.90	0.09	25,25,37,57	0
2	SCN	C	816	3/3	0.90	0.11	27,27,28,45	0
4	GOL	A	808	6/6	0.90	0.09	31,33,35,37	0
2	SCN	B	811	3/3	0.90	0.12	48,48,55,73	0
4	GOL	C	832	6/6	0.90	0.10	39,45,48,56	0
4	GOL	C	833	6/6	0.90	0.10	32,34,35,44	0
2	SCN	B	804	3/3	0.91	0.10	29,29,31,55	0
2	SCN	B	810	3/3	0.91	0.11	39,39,46,68	0
6	A1CQ1	A	816	29/30	0.91	0.08	20,20,20,20	0
4	GOL	B	805	6/6	0.91	0.11	29,37,40,49	0
6	A1CQ1	C	829	29/30	0.92	0.08	20,20,20,20	0
2	SCN	C	820	3/3	0.92	0.09	37,37,45,62	0
2	SCN	C	819	3/3	0.92	0.13	38,38,40,55	0
4	GOL	C	804	6/6	0.94	0.08	19,28,31,31	0
4	GOL	C	830	6/6	0.94	0.09	17,21,26,28	0
7	B3P	A	801	19/19	0.94	0.08	15,20,41,45	0
2	SCN	C	801	3/3	0.95	0.11	24,24,33,35	0
5	DMS	C	825	4/4	0.95	0.11	30,44,47,47	0
4	GOL	A	803	6/6	0.95	0.07	20,29,36,39	0
7	B3P	B	801	19/19	0.96	0.05	14,18,21,23	0
5	DMS	B	809	4/4	0.97	0.08	19,20,21,22	0
5	DMS	C	821	4/4	0.98	0.06	16,16,16,18	0
5	DMS	A	813	4/4	0.99	0.06	15,19,20,21	0
8	NA	A	819	1/1	0.99	0.04	13,13,13,13	0

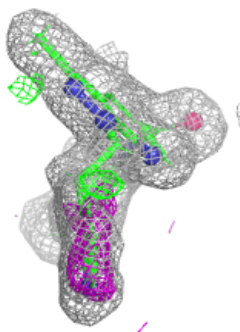
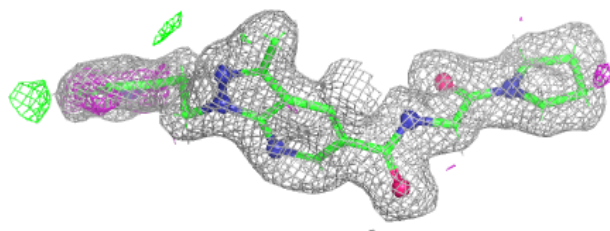
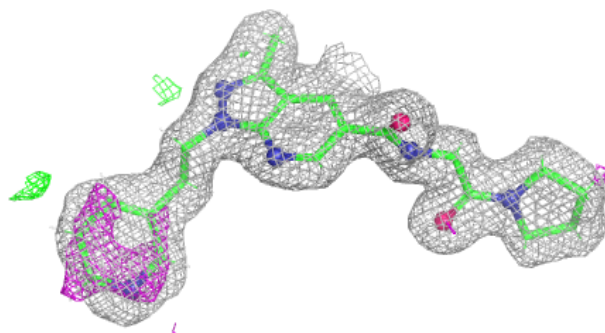
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1CQ1 B 812:

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

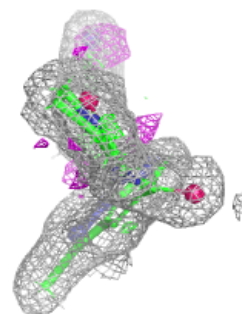
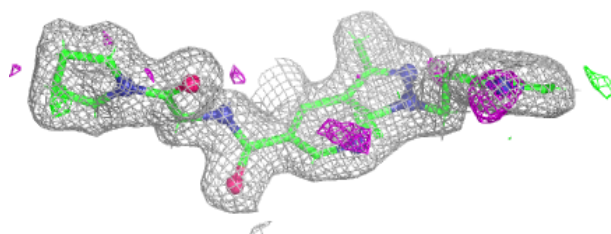
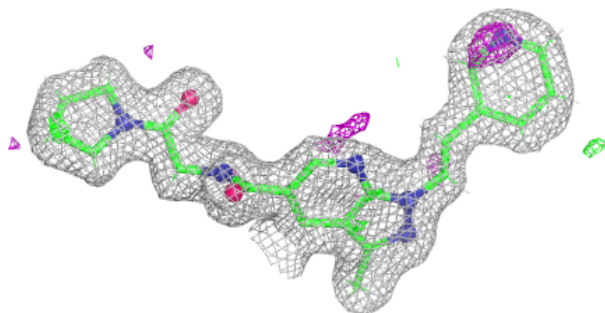
**Electron density around A1CQ1 A 816:**

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

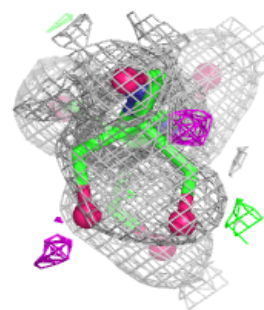
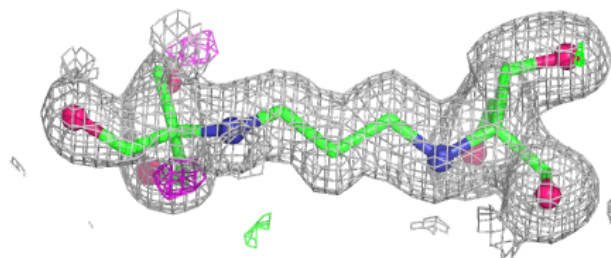
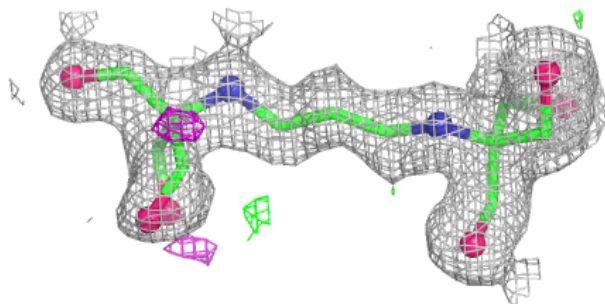


Electron density around A1CQ1 C 829:

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

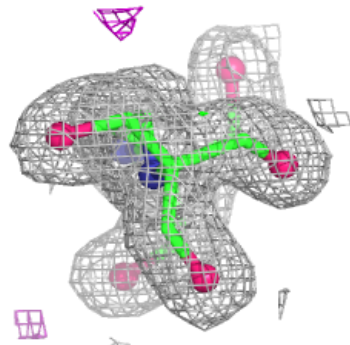
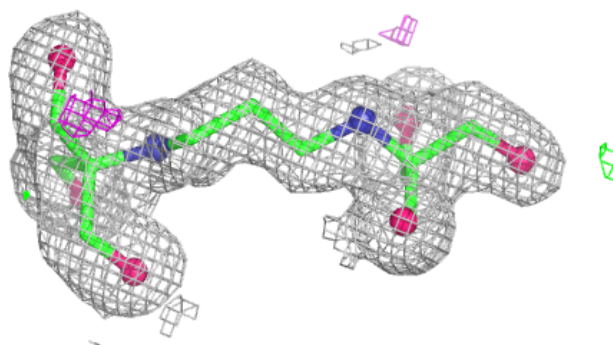
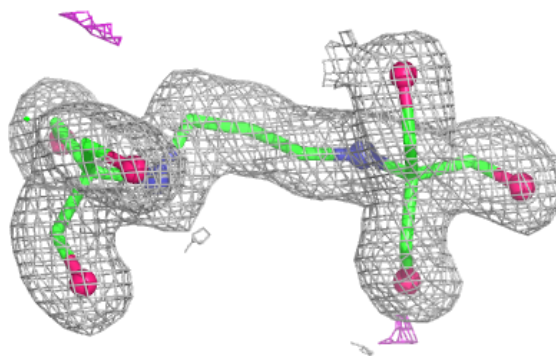
**Electron density around B3P A 801:**

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



Electron density around B3P B 801:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.