



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:32 AM UTC

PDB ID : 9Q6L / pdb_00009q6l
Title : Human prolyl endopeptidase (PREP) - complex with KT-2-197
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

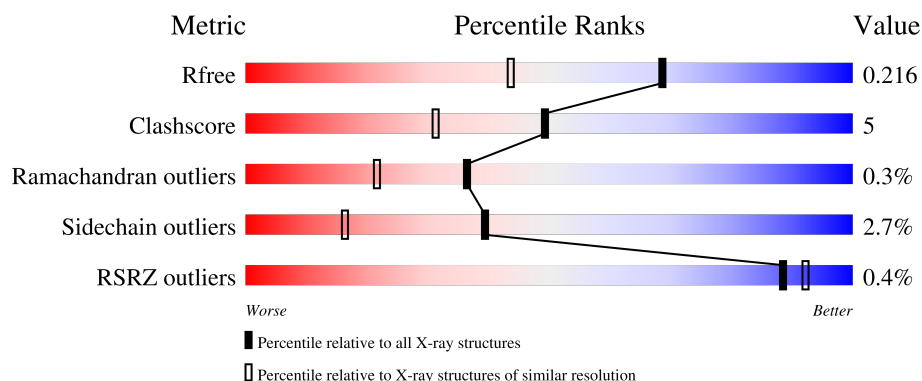
1 Overall quality at a glance

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	 85% 12% ..
1	C	711	 84% 13% ..

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	A	815	-	-	X	-
2	SCN	C	820	-	-	X	-
2	SCN	C	822	-	-	X	-
2	SCN	C	826	-	-	X	-
3	PEG	C	802	-	-	X	-
3	PEG	C	813	-	-	X	-
3	PEG	C	824	-	-	X	-
4	GOL	A	810	-	X	-	-
4	GOL	C	809	-	X	-	-
5	DMS	C	821	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 36338 atoms, of which 17137 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.

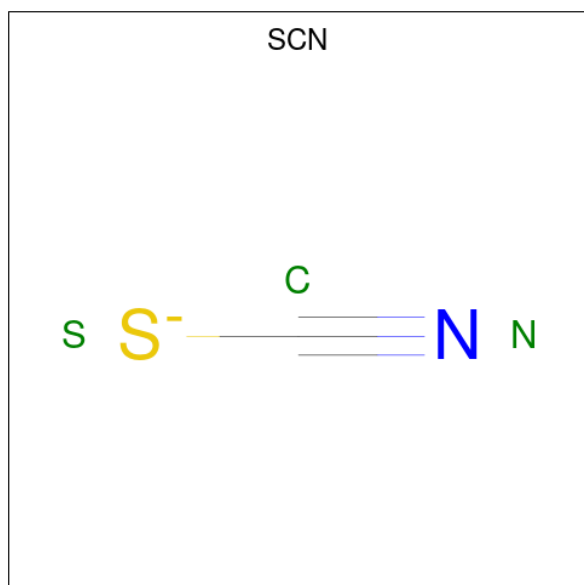
- Molecule 1 is a protein called Prolyl endopeptidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	C	707	Total	C	H	N	O	S	177	8	0
			11290	3670	5576	944	1072	28			
1	A	707	Total	C	H	N	O	S	178	7	0
			11280	3667	5569	943	1073	28			
1	B	707	Total	C	H	N	O	S	177	2	0
			11206	3645	5524	941	1068	28			

There are 3 discrepancies between the modelled and reference sequences:

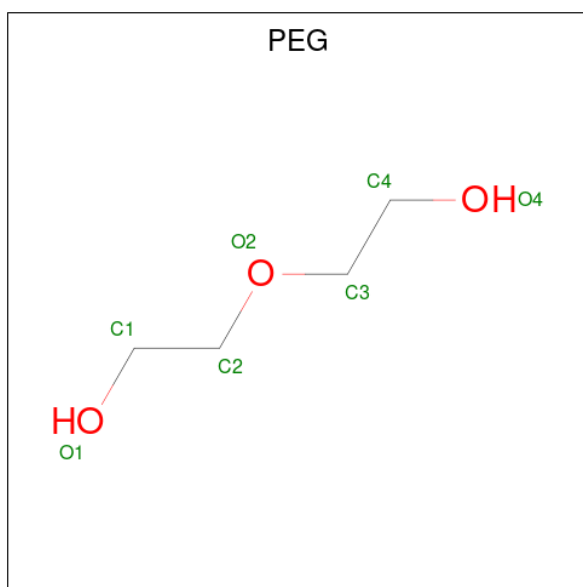
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	GLY	-	expression tag	UNP P48147
A	0	GLY	-	expression tag	UNP P48147
B	0	GLY	-	expression tag	UNP P48147

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



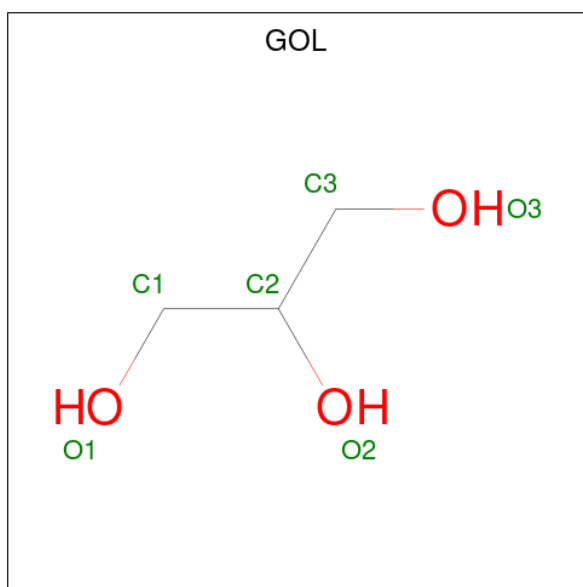
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C N S 3 1 1 1	0	0
2	C	1	Total C N S 3 1 1 1	0	0
2	C	1	Total C N S 3 1 1 1	0	0
2	C	1	Total C N S 3 1 1 1	0	0
2	C	1	Total C N S 3 1 1 1	0	0
2	C	1	Total C N S 3 1 1 1	0	0
2	C	1	Total C N S 3 1 1 1	0	0
2	C	1	Total C N S 3 1 1 1	0	0
2	C	1	Total C N S 3 1 1 1	0	0
2	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	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
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	H	O	2	0
			17	4	10	3		
3	C	1	Total	C	H	O	2	0
			17	4	10	3		
3	C	1	Total	C	H	O	2	0
			17	4	10	3		
3	C	1	Total	C	H	O	2	0
			17	4	10	3		
3	C	1	Total	C	H	O	2	0
			17	4	10	3		
3	A	1	Total	C	H	O	2	0
			17	4	10	3		
3	A	1	Total	C	H	O	4	1
			34	8	20	6		
3	B	1	Total	C	H	O	2	0
			17	4	10	3		

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



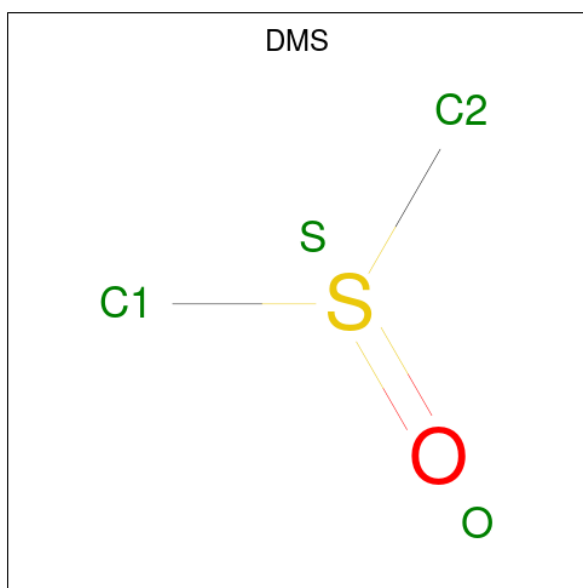
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	H	O	3	0
			14	3	8	3		
4	C	1	Total	C	H	O	3	0
			14	3	8	3		
4	C	1	Total	C	H	O	3	0
			14	3	8	3		
4	C	1	Total	C	H	O	3	0
			14	3	8	3		
4	C	1	Total	C	H	O	3	0
			14	3	8	3		
4	C	1	Total	C	H	O	3	0
			14	3	8	3		
4	C	1	Total	C	H	O	3	0
			14	3	8	3		
4	C	1	Total	C	H	O	3	0
			14	3	8	3		
4	C	1	Total	C	H	O	3	0
			14	3	8	3		
4	C	1	Total	C	H	O	3	0
			14	3	8	3		
4	C	1	Total	C	H	O	6	1
			28	6	16	6		
4	A	1	Total	C	H	O	3	0
			14	3	8	3		
4	A	1	Total	C	H	O	3	0
			14	3	8	3		

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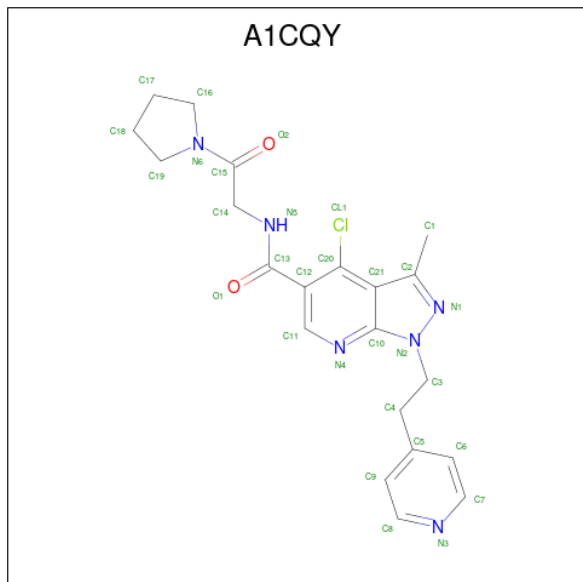
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	3	0
			14	3	8	3		
4	A	1	Total	C	H	O	3	0
			14	3	8	3		
4	A	1	Total	C	H	O	3	0
			14	3	8	3		
4	A	1	Total	C	H	O	3	0
			14	3	8	3		
4	A	1	Total	C	H	O	3	0
			14	3	8	3		
4	A	1	Total	C	H	O	3	0
			14	3	8	3		
4	B	1	Total	C	H	O	3	0
			14	3	8	3		
4	B	1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

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



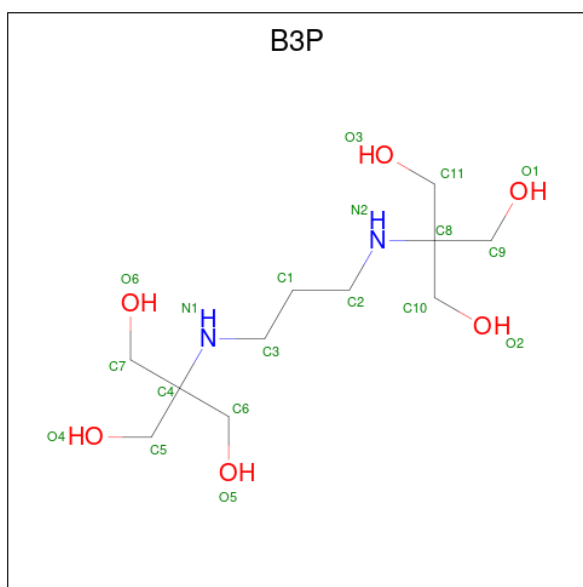
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
5	C	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
5	C	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
5	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
5	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

- Molecule 6 is 3-methyl-N-[2-oxo-2-(pyrrolidin-1-yl)ethyl]-1-[2-(pyridin-4-yl)ethyl]-1H-pyrazolo[3,4-b]pyridine-5-carboxamide (CCD ID: A1CQY) (formula: C₂₁H₂₃ClN₆O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	H	N	O	3	0
			52	21	23	6	2		
6	A	1	Total	C	H	N	O	3	0
			53	21	24	6	2		
6	B	1	Total	C	H	N	O	3	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: C₁₁H₂₆N₂O₆).



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

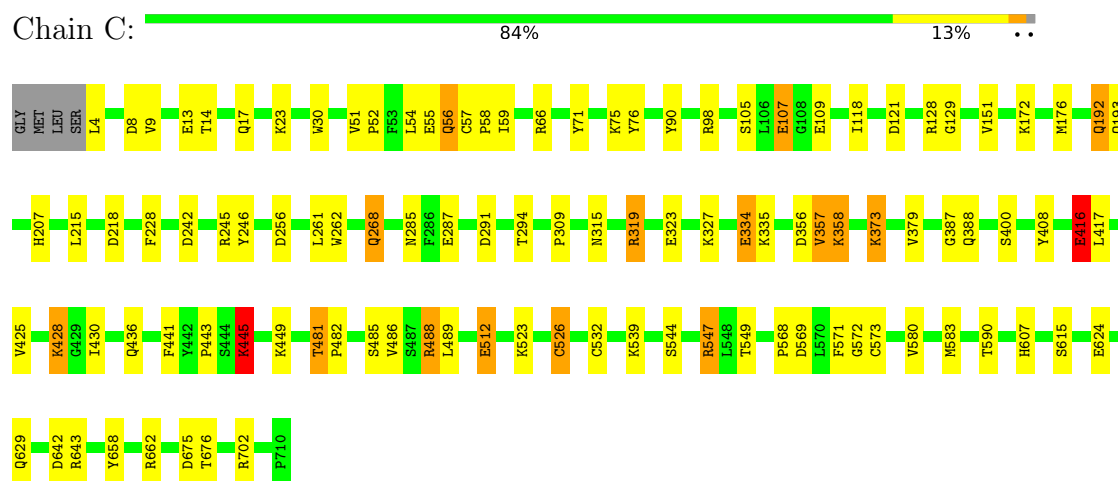
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	596	Total	O	0	0
			596	596		
9	A	582	Total	O	0	0
			582	582		
9	B	483	Total	O	0	1
			484	484		

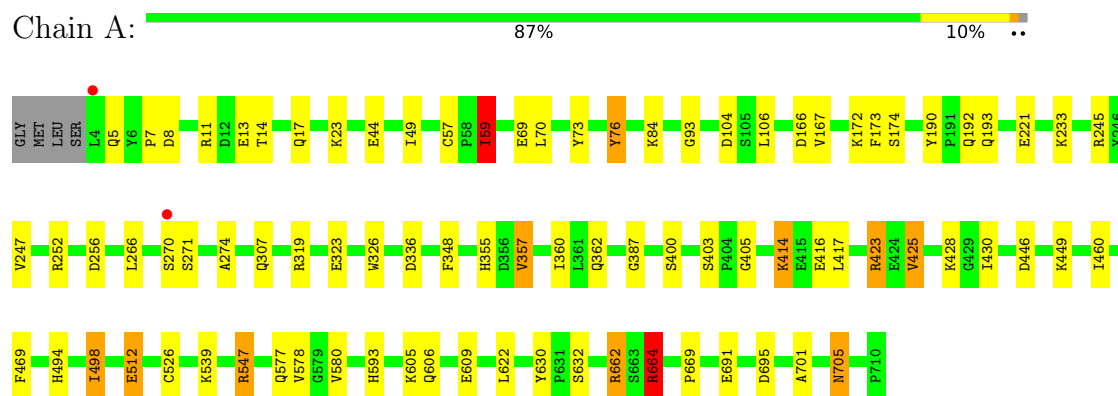
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

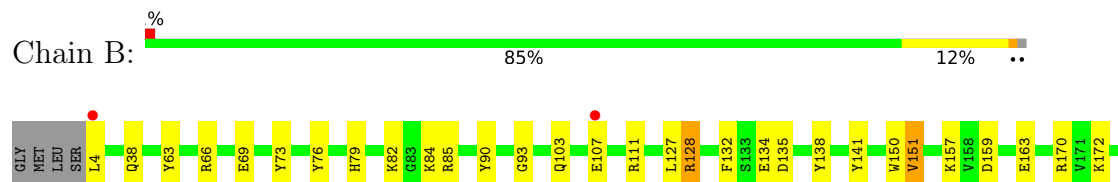
• Molecule 1: Prolyl endopeptidase

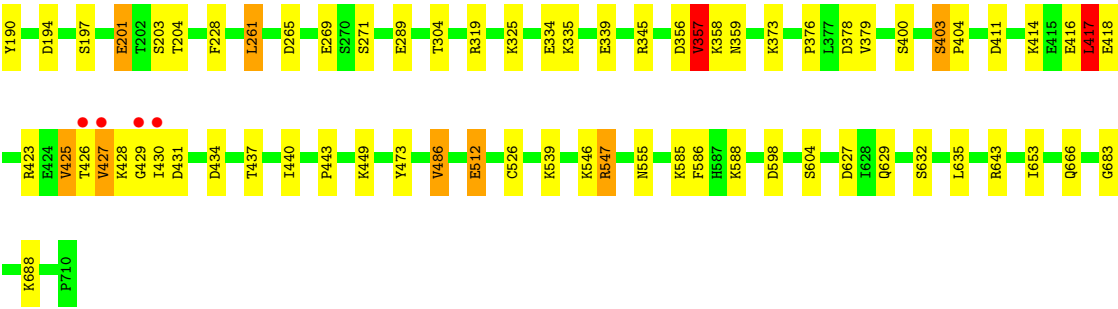


• Molecule 1: Prolyl endopeptidase



• Molecule 1: Prolyl endopeptidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.44Å 66.25Å 156.20Å 90.00° 102.00° 90.00°	Depositor
Resolution (Å)	34.50 – 1.66 34.50 – 1.66	Depositor EDS
% Data completeness (in resolution range)	75.4 (34.50-1.66) 75.6 (34.50-1.66)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 1.66Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.105)	Depositor
R, R_{free}	0.162 , 0.216 0.162 , 0.216	Depositor DCC
R_{free} test set	12151 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	14.6	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	36338	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.36% 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: GOL, PEG, DMS, SCN, A1CQY, NA, 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	0.99	3/5884 (0.1%)	1.37	30/7975 (0.4%)
1	B	0.94	2/5840 (0.0%)	1.39	33/7917 (0.4%)
1	C	0.97	2/5890 (0.0%)	1.37	27/7985 (0.3%)
All	All	0.97	7/17614 (0.0%)	1.38	90/23877 (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	1
1	B	0	4
1	C	0	4
All	All	0	9

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	512	GLU	CD-OE1	7.04	1.38	1.25
1	A	59	ILE	CB-CG1	-6.98	1.39	1.53
1	A	494	HIS	CE1-NE2	-6.56	1.25	1.32
1	A	400	SER	CA-CB	-5.99	1.45	1.53
1	C	544	SER	CA-CB	-5.42	1.47	1.53
1	C	607	HIS	CD2-NE2	-5.13	1.32	1.37
1	B	632	SER	CA-CB	-5.11	1.45	1.53

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	512	GLU	CB-CG-CD	10.24	130.00	112.60
1	B	66	ARG	CG-CD-NE	-8.70	92.86	112.00
1	C	121	ASP	CB-CA-C	-8.11	95.10	110.67
1	B	418	GLU	CB-CA-C	8.10	123.41	111.02
1	B	418	GLU	N-CA-CB	-7.65	101.38	111.40
1	B	437	THR	CA-CB-OG1	-7.39	98.51	109.60
1	C	90	TYR	N-CA-CB	-7.24	98.64	110.81
1	A	416	GLU	CB-CA-C	-7.22	96.81	110.67
1	C	334	GLU	N-CA-CB	7.03	120.45	110.12
1	B	204	THR	OG1-CB-CG2	-7.00	95.29	109.30
1	B	547	ARG	CB-CA-C	-6.78	98.97	110.64
1	B	159	ASP	CA-CB-CG	6.77	119.37	112.60
1	A	348	PHE	CA-CB-CG	6.73	120.53	113.80
1	A	539	LYS	CB-CA-C	6.62	121.78	110.79
1	B	373	LYS	CB-CA-C	-6.55	98.18	110.16
1	C	172	LYS	N-CA-CB	-6.52	99.39	111.52
1	A	705	ASN	CA-CB-CG	-6.52	106.08	112.60
1	B	134	GLU	CB-CA-C	6.44	121.49	110.79
1	A	416	GLU	N-CA-CB	6.43	120.25	110.28
1	A	336	ASP	CA-CB-CG	6.40	119.00	112.60
1	B	269	GLU	N-CA-CB	6.37	119.85	110.49
1	C	107	GLU	CB-CG-CD	6.36	123.41	112.60
1	C	676	THR	OG1-CB-CG2	-6.33	96.65	109.30
1	B	688	LYS	N-CA-CB	6.29	119.58	110.20
1	A	630	TYR	N-CA-CB	6.20	119.16	110.11
1	C	580	VAL	N-CA-CB	6.18	118.70	111.66
1	B	63	TYR	N-CA-C	-6.16	104.49	111.14
1	C	547	ARG	CG-CD-NE	-6.09	98.60	112.00
1	B	423	ARG	CB-CA-C	-6.08	96.98	109.94
1	A	526[A]	CYS	CB-CA-C	-6.08	101.33	110.88
1	A	526[B]	CYS	CB-CA-C	-6.08	101.33	110.88
1	B	269	GLU	CB-CA-C	-6.05	102.85	112.05
1	B	588	LYS	N-CA-CB	6.05	119.87	110.44
1	C	13	GLU	CB-CG-CD	6.01	122.81	112.60
1	A	512	GLU	N-CA-CB	5.95	119.51	110.28
1	B	627	ASP	CA-CB-CG	5.95	118.55	112.60
1	C	642	ASP	CA-CB-CG	5.85	118.45	112.60
1	B	128	ARG	NE-CZ-NH1	-5.78	115.72	121.50
1	C	416	GLU	N-CA-CB	5.76	119.81	110.42
1	C	373	LYS	CD-CE-NZ	-5.75	93.48	111.90
1	B	69	GLU	CB-CG-CD	5.67	122.24	112.60
1	B	66	ARG	N-CA-CB	-5.67	101.77	110.16
1	B	269	GLU	CB-CG-CD	5.63	122.17	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	228	PHE	CB-CA-C	5.61	118.56	111.21
1	A	423	ARG	CD-NE-CZ	-5.61	116.55	124.40
1	B	526[A]	CYS	CB-CA-C	-5.61	102.08	110.88
1	B	526[B]	CYS	CB-CA-C	-5.61	102.08	110.88
1	B	201	GLU	CB-CG-CD	5.59	122.11	112.60
1	C	228	PHE	CA-CB-CG	-5.57	108.23	113.80
1	A	414	LYS	CG-CD-CE	-5.56	98.51	111.30
1	C	245	ARG	CG-CD-NE	-5.56	99.77	112.00
1	A	13	GLU	CB-CG-CD	5.55	122.03	112.60
1	A	691	GLU	N-CA-CB	5.55	118.05	110.01
1	C	512	GLU	CB-CA-C	-5.53	101.61	110.79
1	C	441	PHE	CA-CB-CG	-5.51	108.29	113.80
1	C	481	THR	OG1-CB-CG2	-5.50	98.29	109.30
1	A	695	ASP	CA-CB-CG	5.50	118.10	112.60
1	A	252	ARG	CD-NE-CZ	5.49	132.08	124.40
1	C	66	ARG	CG-CD-NE	-5.47	99.97	112.00
1	C	109	GLU	N-CA-CB	-5.43	101.76	109.85
1	C	14	THR	CA-CB-OG1	-5.42	101.47	109.60
1	A	580	VAL	N-CA-CB	5.42	117.83	111.66
1	A	664	ARG	CA-CB-CG	5.42	124.93	114.10
1	B	376	PRO	CB-CA-C	5.40	118.00	111.46
1	C	624	GLU	N-CA-CB	5.37	118.11	110.16
1	C	526[A]	CYS	CB-CA-C	5.37	119.31	110.88
1	C	526[B]	CYS	CB-CA-C	5.37	119.31	110.88
1	A	11	ARG	N-CA-CB	5.36	118.96	110.55
1	A	44	GLU	CB-CA-C	5.34	119.35	110.81
1	A	8	ASP	CA-CB-CG	5.33	117.93	112.60
1	B	265	ASP	CA-CB-CG	5.33	117.93	112.60
1	C	98	ARG	CG-CD-NE	-5.32	100.29	112.00
1	B	135	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	104	ASP	CB-CA-C	5.31	118.90	109.65
1	A	446	ASP	CA-CB-CG	5.29	117.89	112.60
1	B	151	VAL	O-C-N	-5.29	117.47	123.03
1	C	445	LYS	CA-CB-CG	5.24	124.58	114.10
1	B	63	TYR	N-CA-CB	5.24	117.67	110.07
1	C	55	GLU	CB-CA-C	5.21	120.26	110.63
1	B	325	LYS	CA-CB-CG	5.20	124.50	114.10
1	B	345	ARG	NE-CZ-NH1	-5.20	116.30	121.50
1	A	662	ARG	CD-NE-CZ	5.18	131.65	124.40
1	A	245	ARG	NE-CZ-NH1	-5.17	116.33	121.50
1	C	192	GLN	CG-CD-NE2	5.16	124.14	116.40
1	A	11	ARG	CB-CA-C	-5.15	101.75	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	469	PHE	CA-CB-CG	5.14	118.94	113.80
1	A	76	TYR	CB-CA-C	-5.13	99.20	109.35
1	B	190	TYR	CB-CA-C	5.11	115.79	108.68
1	B	486	VAL	CB-CA-C	-5.08	105.29	112.14
1	A	274	ALA	O-C-N	-5.03	117.01	122.19

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	662	ARG	Sidechain
1	B	111	ARG	Sidechain
1	B	170	ARG	Sidechain
1	B	547	ARG	Sidechain
1	B	643	ARG	Sidechain
1	C	488[A]	ARG	Sidechain
1	C	488[B]	ARG	Sidechain
1	C	643	ARG	Sidechain
1	C	702	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	5711	5569	5545	45	0
1	B	5682	5524	5501	41	1
1	C	5714	5576	5553	87	1
2	A	15	0	0	4	0
2	B	12	0	0	1	0
2	C	27	0	0	12	0
3	A	21	30	30	4	0
3	B	7	10	10	0	0
3	C	42	60	60	22	0
4	A	54	72	72	6	0
4	B	30	40	40	3	0
4	C	78	104	104	14	0
5	A	4	6	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	4	6	6	0	0
5	C	12	18	18	8	0
6	A	29	24	0	0	0
6	B	29	23	0	0	0
6	C	29	23	0	0	0
7	A	19	26	26	0	0
7	B	19	26	26	0	0
8	A	1	0	0	0	0
9	A	582	0	0	14	0
9	B	484	0	0	10	1
9	C	596	0	0	17	1
All	All	19201	17137	16997	186	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (186) 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:903:HOH:O	1.90	1.13
2:C:820:SCN:N	9:C:901:HOH:O	1.82	1.10
1:C:291:ASP:OD1	4:C:805:GOL:H2	1.63	0.95
1:A:425:VAL:HG22	9:A:1336:HOH:O	1.71	0.91
1:C:428:LYS:N	1:C:428:LYS:HD2	1.85	0.90
3:C:813:PEG:H12	9:C:1022:HOH:O	1.74	0.88
1:C:425:VAL:HG22	5:C:821:DMS:H13	1.60	0.82
1:A:57:CYS:HB2	9:A:1317:HOH:O	1.79	0.81
1:C:268:GLN:HE21	1:C:268:GLN:HA	1.47	0.80
1:C:428:LYS:HD2	1:C:428:LYS:H	1.46	0.79
1:C:129:GLY:HA2	4:C:809:GOL:H11	1.64	0.78
1:C:629:GLN:O	3:C:802:PEG:H21	1.87	0.74
1:C:218:ASP:OD1	9:C:902:HOH:O	2.06	0.73
1:A:664:ARG:HB3	1:A:664:ARG:NH1	2.03	0.73
1:C:571:PHE:O	3:C:802:PEG:H31	1.89	0.73
1:C:425:VAL:HG13	5:C:821:DMS:H11	1.71	0.72
1:C:291:ASP:OD1	4:C:805:GOL:C2	2.37	0.72
1:A:192:GLN:HE21	1:A:193:GLN:H	1.38	0.71
1:C:319:ARG:HH11	1:C:319:ARG:HB2	1.54	0.71
1:C:192:GLN:HE21	1:C:193:GLN:H	1.39	0.71
1:C:539:LYS:NZ	9:C:905:HOH:O	2.19	0.70
1:C:443:PRO:HD2	2:C:822:SCN:S	2.33	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:GLU:CG	9:A:903:HOH:O	2.34	0.69
1:A:362:GLN:HE22	3:A:805[B]:PEG:H31	1.57	0.69
1:C:30:TRP:CH2	3:C:813:PEG:H31	2.29	0.67
1:C:285:ASN:HD21	4:C:810:GOL:H32	1.59	0.67
2:C:826:SCN:N	9:C:906:HOH:O	2.28	0.67
1:C:675:ASP:OD2	9:C:903:HOH:O	2.14	0.65
1:A:247:VAL:HG23	1:A:266:LEU:HG	1.77	0.65
4:A:812:GOL:H11	9:A:1145:HOH:O	1.96	0.64
1:A:221:GLU:HG3	9:A:903:HOH:O	1.97	0.64
1:C:30:TRP:CZ2	3:C:813:PEG:H31	2.34	0.63
1:C:207:HIS:CD2	4:C:816:GOL:H2	2.34	0.63
1:A:256:ASP:HB2	9:A:1147:HOH:O	1.99	0.63
1:B:271:SER:HA	9:B:930:HOH:O	1.98	0.63
1:B:339:GLU:OE1	1:B:359:ASN:ND2	2.30	0.61
1:C:430:ILE:HG21	1:C:489:LEU:HD13	1.83	0.60
1:A:512:GLU:OE1	9:A:901:HOH:O	2.17	0.60
1:C:56:GLN:NE2	9:C:914:HOH:O	2.35	0.59
1:C:176:MET:HG3	4:C:809:GOL:H32	1.83	0.59
1:A:59:ILE:HG12	1:A:701:ALA:CB	2.32	0.59
1:B:194:ASP:OD2	9:B:902:HOH:O	2.17	0.58
1:A:174:SER:O	3:A:802:PEG:H21	2.02	0.58
1:B:425:VAL:HB	4:B:806:GOL:H32	1.85	0.58
1:A:190:TYR:HB3	4:A:804:GOL:H12	1.85	0.57
1:C:285:ASN:HD21	4:C:810:GOL:C3	2.17	0.57
4:C:828:GOL:C3	9:C:1086:HOH:O	2.54	0.56
1:A:664:ARG:HB3	1:A:664:ARG:HH11	1.72	0.55
1:C:547:ARG:HG2	3:C:806:PEG:O4	2.07	0.55
1:C:569:ASP:HA	3:C:802:PEG:H22	1.88	0.55
1:B:440:ILE:HD12	1:B:440:ILE:C	2.31	0.55
1:C:443:PRO:O	2:C:822:SCN:S	2.65	0.55
1:B:486:VAL:HG23	9:B:1121:HOH:O	2.07	0.55
1:C:129:GLY:CA	4:C:809:GOL:H11	2.35	0.54
4:A:812:GOL:C1	9:A:1145:HOH:O	2.54	0.54
1:C:425:VAL:HG13	5:C:821:DMS:C1	2.36	0.54
1:C:128:ARG:HD2	1:C:151:VAL:CG2	2.37	0.54
1:C:334:GLU:HG2	9:C:1152:HOH:O	2.08	0.54
1:B:425:VAL:HB	4:B:806:GOL:C3	2.38	0.54
1:C:17:GLN:NE2	2:C:825:SCN:S	2.82	0.53
1:C:268:GLN:HE21	1:C:268:GLN:CA	2.20	0.53
1:A:605:LYS:NZ	1:A:609:GLU:OE2	2.40	0.53
1:C:319:ARG:HH11	1:C:319:ARG:CB	2.19	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:LYS:HD3	3:C:824:PEG:C2	2.39	0.52
1:A:547:ARG:HB3	9:A:988:HOH:O	2.09	0.52
2:C:818:SCN:S	9:C:1123:HOH:O	2.60	0.52
1:C:323:GLU:OE1	4:C:810:GOL:O2	2.28	0.51
1:C:327:LYS:HD3	3:C:824:PEG:O2	2.10	0.51
1:C:268:GLN:HA	1:C:268:GLN:NE2	2.21	0.51
1:C:287[B]:GLU:OE1	9:C:904:HOH:O	2.18	0.51
1:C:549:THR:HA	1:C:573:CYS:O	2.11	0.51
1:C:485:SER:OG	1:C:488[B]:ARG:HD3	2.11	0.50
1:C:572:GLY:HA2	3:C:802:PEG:H42	1.94	0.50
1:B:79:HIS:NE2	1:B:103:GLN:NE2	2.59	0.50
1:C:51:VAL:HB	1:C:52:PRO:HD3	1.93	0.49
1:A:387:GLY:H	2:A:816:SCN:C	2.25	0.49
1:C:400:SER:HB2	2:C:820:SCN:N	2.27	0.49
1:B:404:PRO:HD3	1:B:427:VAL:HG22	1.94	0.49
1:C:327:LYS:HD3	3:C:824:PEG:C3	2.43	0.48
1:C:335:LYS:NZ	1:C:356:ASP:OD1	2.40	0.48
1:B:128:ARG:HD2	1:B:151:VAL:CG2	2.43	0.48
1:C:71:TYR:CZ	1:C:75:LYS:HE2	2.49	0.48
1:C:523:LYS:O	1:C:526[B]:CYS:HB3	2.12	0.48
1:A:664:ARG:HB3	1:A:664:ARG:CZ	2.42	0.48
1:B:197:SER:N	9:B:901:HOH:O	2.10	0.48
1:A:166:ASP:HA	2:A:815:SCN:N	2.27	0.48
1:B:127:LEU:HD11	1:B:141:TYR:HB2	1.96	0.48
1:B:201:GLU:HG3	9:B:901:HOH:O	2.14	0.48
1:C:379:VAL:HG12	2:C:820:SCN:S	2.54	0.47
1:C:416:GLU:HB3	9:C:1435:HOH:O	2.13	0.47
1:A:69:GLU:CD	4:A:813:GOL:H11	2.39	0.47
1:C:547:ARG:NE	3:C:806:PEG:O4	2.45	0.47
1:A:17:GLN:NE2	2:A:818:SCN:N	2.49	0.47
1:C:373:LYS:HE3	1:C:417:LEU:O	2.15	0.47
5:C:821:DMS:H22	9:C:1100:HOH:O	2.15	0.47
1:C:256:ASP:HB2	9:C:967:HOH:O	2.14	0.47
1:C:327:LYS:HD3	3:C:824:PEG:H31	1.97	0.46
1:A:70:LEU:HD13	1:A:430:ILE:HD11	1.96	0.46
1:A:606[A]:GLN:H	1:A:606[A]:GLN:CD	2.23	0.46
1:B:400:SER:OG	1:B:403:SER:OG	2.29	0.46
1:B:138:TYR:OH	1:B:157:LYS:HE2	2.16	0.46
1:B:411:ASP:OD2	1:B:414:LYS:HE2	2.16	0.46
3:C:802:PEG:H12	3:C:802:PEG:H32	1.55	0.46
1:C:568:PRO:O	3:C:802:PEG:H22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:SER:OG	1:A:669:PRO:HD2	2.15	0.45
1:C:9:VAL:HA	3:C:813:PEG:H22	1.97	0.45
1:A:319:ARG:HD3	1:B:334:GLU:HB2	1.97	0.45
1:B:356:ASP:C	1:B:357:VAL:HG23	2.41	0.45
1:A:7:PRO:HD3	1:A:49:ILE:CD1	2.47	0.45
1:A:355:HIS:HB2	1:A:360:ILE:HD12	1.98	0.45
1:C:416:GLU:H	1:C:416:GLU:CD	2.24	0.45
1:C:436:GLN:NE2	3:C:808:PEG:O4	2.50	0.45
1:C:207:HIS:CG	4:C:816:GOL:H2	2.52	0.45
1:B:417:LEU:HD23	1:B:417:LEU:N	2.32	0.45
1:C:327:LYS:CD	3:C:824:PEG:C2	2.94	0.45
1:B:82:LYS:HG3	1:B:132:PHE:CD1	2.52	0.45
3:A:805[A]:PEG:H32	3:A:805[A]:PEG:H11	1.39	0.45
1:B:416:GLU:O	1:B:417:LEU:HB2	2.17	0.45
1:A:69:GLU:OE2	4:A:813:GOL:H11	2.16	0.45
1:C:315:ASN:HD22	3:C:824:PEG:H32	1.81	0.44
1:A:221:GLU:OE1	9:A:903:HOH:O	2.18	0.44
1:B:428:LYS:O	1:B:430:ILE:N	2.49	0.44
1:C:246:TYR:OH	2:C:801:SCN:S	2.65	0.44
1:C:262:TRP:CZ3	4:C:831[B]:GOL:H12	2.53	0.44
1:B:163:GLU:HG2	9:B:1023:HOH:O	2.16	0.44
1:C:4:LEU:N	4:C:828:GOL:HO3	2.16	0.44
2:B:812:SCN:S	9:B:1039:HOH:O	2.61	0.44
1:B:443:PRO:HB3	1:B:449:LYS:HE3	1.98	0.44
1:A:233:LYS:HE2	1:A:593:HIS:HB2	1.99	0.44
1:B:73:TYR:O	1:B:93:GLY:HA2	2.18	0.44
1:B:425:VAL:HG21	4:B:806:GOL:H31	1.99	0.44
1:C:309:PRO:HB3	1:C:512:GLU:HB3	2.00	0.43
1:C:658:TYR:HA	1:C:662:ARG:HD3	1.99	0.43
1:C:242:ASP:OD2	1:C:294:THR:OG1	2.31	0.43
1:B:473:TYR:CZ	1:B:555:ASN:HB3	2.53	0.43
1:B:635:LEU:HD12	1:B:653:ILE:HB	2.00	0.43
1:C:387:GLY:H	2:C:817:SCN:C	2.32	0.43
1:B:261:LEU:C	1:B:261:LEU:HD13	2.44	0.43
1:C:327:LYS:CE	3:C:824:PEG:H31	2.49	0.43
1:C:532:CYS:O	2:C:822:SCN:N	2.52	0.43
1:C:76:TYR:HB2	5:C:821:DMS:H21	2.00	0.43
1:A:405:GLY:O	1:A:425:VAL:HG23	2.19	0.42
1:A:449:LYS:HE3	9:A:987:HOH:O	2.18	0.42
1:B:289:GLU:O	1:B:304:THR:HA	2.18	0.42
1:C:17:GLN:HB3	2:C:826:SCN:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:LYS:HE2	3:C:824:PEG:H22	2.01	0.42
1:C:425:VAL:H	5:C:821:DMS:C1	2.32	0.42
1:C:583:MET:HB2	1:C:615:SER:HB2	2.01	0.42
1:B:150:TRP:CE2	1:B:172:LYS:HE3	2.55	0.42
1:B:585:LYS:O	1:B:586:PHE:C	2.62	0.42
1:C:54:LEU:O	1:C:57:CYS:HB2	2.20	0.42
1:C:425:VAL:H	5:C:821:DMS:H12	1.85	0.42
1:C:481:THR:HB	1:C:482:PRO:HD2	2.02	0.42
1:A:271:SER:N	9:A:940:HOH:O	2.52	0.42
1:C:449:LYS:HE3	9:C:937:HOH:O	2.20	0.41
1:B:683:GLY:HA2	9:B:941:HOH:O	2.20	0.41
1:C:118:ILE:HD13	1:C:118:ILE:HG21	1.88	0.41
1:A:76:TYR:CD1	1:A:423:ARG:HD2	2.55	0.41
1:B:629:GLN:HB2	1:B:666:GLN:OE1	2.21	0.41
1:C:58:PRO:HD2	9:C:1319:HOH:O	2.21	0.41
1:A:460:ILE:CD1	1:A:498:ILE:HD11	2.50	0.41
1:B:378:ASP:HB3	9:B:1247:HOH:O	2.21	0.41
1:B:431:ASP:HB3	1:B:434:ASP:OD2	2.21	0.41
1:C:358:LYS:HE2	1:C:358:LYS:HB2	1.78	0.41
1:B:76:TYR:CE1	1:B:90:TYR:CD1	3.09	0.41
1:A:174:SER:O	3:A:802:PEG:C2	2.69	0.41
4:C:805:GOL:H11	9:C:945:HOH:O	2.20	0.41
1:A:192:GLN:NE2	1:A:192:GLN:HA	2.36	0.41
4:A:813:GOL:C3	9:A:1255:HOH:O	2.68	0.41
1:A:73:TYR:O	1:A:93:GLY:HA2	2.21	0.41
1:B:38:GLN:H	1:B:38:GLN:CD	2.28	0.41
1:A:323:GLU:HA	1:A:326:TRP:CE2	2.56	0.41
1:C:105:SER:O	1:C:107:GLU:O	2.40	0.40
1:A:167:VAL:O	2:A:815:SCN:S	2.79	0.40
1:C:268:GLN:CA	1:C:268:GLN:NE2	2.80	0.40
1:C:425:VAL:N	5:C:821:DMS:C1	2.84	0.40
3:C:813:PEG:H12	3:C:813:PEG:H32	1.94	0.40
1:A:423:ARG:HH21	1:A:423:ARG:HD3	1.59	0.40
1:B:85:ARG:HD2	9:B:1030:HOH:O	2.20	0.40
1:B:358:LYS:HD2	1:B:379:VAL:HG13	2.03	0.40
1:C:445:LYS:HB2	1:C:445:LYS:HE2	1.22	0.40
1:C:215:LEU:HA	1:C:215:LEU:HD12	1.93	0.40
1:A:172:LYS:HD3	1:A:173:PHE:CE2	2.57	0.40
1:A:577:GLN:O	1:A:578:VAL:C	2.65	0.40
1:B:335:LYS:NZ	1:B:356:ASP:OD1	2.54	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:408:TYR:HH	1:B:84:LYS:HE3[1_545]	1.29	0.31
9:C:1226:HOH:O	9:B:1339:HOH:O[2_645]	2.12	0.08

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	712/711 (100%)	687 (96%)	24 (3%)	1 (0%)	48	30
1	B	707/711 (99%)	681 (96%)	23 (3%)	3 (0%)	30	15
1	C	713/711 (100%)	696 (98%)	15 (2%)	2 (0%)	36	21
All	All	2132/2133 (100%)	2064 (97%)	62 (3%)	6 (0%)	36	21

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	429	GLY
1	C	357	VAL
1	C	590	THR
1	B	417	LEU
1	A	357	VAL
1	B	357	VAL

5.3.2 Protein sidechains [i](#)

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	621/617 (101%)	602 (97%)	19 (3%)	35	12
1	B	616/617 (100%)	600 (97%)	16 (3%)	40	17
1	C	622/617 (101%)	608 (98%)	14 (2%)	44	21
All	All	1859/1851 (100%)	1810 (97%)	49 (3%)	39	17

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	8	ASP
1	C	23	LYS
1	C	56	GLN
1	C	59	ILE
1	C	261	LEU
1	C	268	GLN
1	C	319	ARG
1	C	357	VAL
1	C	358	LYS
1	C	388	GLN
1	C	416	GLU
1	C	428	LYS
1	C	445	LYS
1	C	486	VAL
1	A	5	GLN
1	A	14	THR
1	A	23	LYS
1	A	59	ILE
1	A	84	LYS
1	A	106	LEU
1	A	270	SER
1	A	307	GLN
1	A	357	VAL
1	A	403	SER
1	A	414	LYS
1	A	417	LEU
1	A	425	VAL
1	A	428	LYS
1	A	498	ILE
1	A	547	ARG
1	A	622	LEU
1	A	664	ARG
1	A	705	ASN
1	B	4	LEU

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Mol	Chain	Res	Type
1	B	107	GLU
1	B	203	SER
1	B	261	LEU
1	B	319	ARG
1	B	357	VAL
1	B	403	SER
1	B	417	LEU
1	B	425	VAL
1	B	426	THR
1	B	427	VAL
1	B	512	GLU
1	B	539	LYS
1	B	546	LYS
1	B	598	ASP
1	B	604	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) 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	503	ASN
1	C	524	GLN
1	C	531	GLN
1	C	566	GLN
1	C	577	GLN
1	A	5	GLN
1	A	192	GLN
1	A	205	ASN
1	A	267	GLN
1	A	362	GLN
1	A	388	GLN
1	A	483	ASN
1	A	503	ASN
1	A	524	GLN
1	A	531	GLN
1	A	566	GLN
1	A	705	ASN

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Mol	Chain	Res	Type
1	B	103	GLN
1	B	267	GLN
1	B	362	GLN
1	B	436	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	$\# Z > 2$
3	PEG	C	813	-	6,6,6	1.30	1 (16%)	5,5,5	0.98	0
2	SCN	A	818	-	1,2,2	0.49	0	0,1,1	-	-
2	SCN	C	811	-	1,2,2	0.69	0	0,1,1	-	-
5	DMS	C	823	-	3,3,3	0.50	0	3,3,3	0.41	0
2	SCN	C	822	-	1,2,2	0.97	0	0,1,1	-	-
3	PEG	C	806	-	6,6,6	0.66	0	5,5,5	0.53	0
3	PEG	A	802	-	6,6,6	0.52	0	5,5,5	0.76	0
2	SCN	B	810	-	1,2,2	1.29	0	0,1,1	-	-
4	GOL	A	803	-	5,5,5	0.19	0	5,5,5	0.45	0
4	GOL	B	805	-	5,5,5	0.31	0	5,5,5	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SCN	B	812	-	1,2,2	0.41	0	0,1,1	-	-
2	SCN	B	809	-	1,2,2	0.85	0	0,1,1	-	-
3	PEG	C	808	-	6,6,6	0.20	0	5,5,5	0.21	0
4	GOL	C	805	-	5,5,5	0.49	0	5,5,5	1.14	0
6	A1CQY	B	811	1	32,32,33	0.83	1 (3%)	44,44,46	1.64	9 (20%)
2	SCN	C	825	-	1,2,2	0.96	0	0,1,1	-	-
4	GOL	C	812	-	5,5,5	0.37	0	5,5,5	0.81	0
4	GOL	A	813	-	5,5,5	0.11	0	5,5,5	0.32	0
4	GOL	A	809	-	5,5,5	0.15	0	5,5,5	0.67	0
4	GOL	C	807	-	5,5,5	0.29	0	5,5,5	0.85	0
4	GOL	C	809	-	5,5,5	0.59	0	5,5,5	1.83	2 (40%)
3	PEG	C	802	-	6,6,6	0.72	0	5,5,5	0.77	0
4	GOL	C	831[A]	-	5,5,5	0.19	0	5,5,5	0.36	0
5	DMS	C	821	-	3,3,3	0.76	0	3,3,3	0.26	0
2	SCN	A	808	-	1,2,2	0.90	0	0,1,1	-	-
4	GOL	B	802	-	5,5,5	0.32	0	5,5,5	0.18	0
2	SCN	C	818	-	1,2,2	0.86	0	0,1,1	-	-
2	SCN	C	817	-	1,2,2	0.10	0	0,1,1	-	-
4	GOL	A	810	-	5,5,5	0.58	0	5,5,5	1.77	2 (40%)
3	PEG	C	824	-	6,6,6	1.42	1 (16%)	5,5,5	0.86	0
7	B3P	A	801	-	18,18,18	0.60	0	23,23,23	1.33	1 (4%)
2	SCN	A	816	-	1,2,2	0.65	0	0,1,1	-	-
2	SCN	A	815	-	1,2,2	1.03	0	0,1,1	-	-
2	SCN	C	801	-	1,2,2	0.20	0	0,1,1	-	-
4	GOL	A	819	-	5,5,5	0.23	0	5,5,5	0.86	0
5	DMS	A	814	-	3,3,3	0.60	0	3,3,3	0.62	0
4	GOL	C	830	-	5,5,5	0.19	0	5,5,5	0.57	0
2	SCN	B	804	-	1,2,2	2.15	1 (100%)	0,1,1	-	-
3	PEG	A	805[A]	-	6,6,6	0.87	0	5,5,5	0.52	0
4	GOL	A	807	-	5,5,5	0.17	0	5,5,5	0.47	0
4	GOL	C	829	-	5,5,5	0.27	0	5,5,5	0.30	0
5	DMS	C	819	-	3,3,3	0.57	0	3,3,3	0.44	0
4	GOL	C	831[B]	-	5,5,5	0.24	0	5,5,5	0.40	0
4	GOL	B	806	-	5,5,5	0.32	0	5,5,5	0.63	0
4	GOL	C	804	-	5,5,5	0.39	0	5,5,5	0.74	0
4	GOL	B	813	-	5,5,5	0.19	0	5,5,5	0.41	0
4	GOL	A	806	-	5,5,5	0.21	0	5,5,5	0.30	0
5	DMS	B	808	-	3,3,3	0.59	0	3,3,3	0.30	0
6	A1CQY	A	817	1	32,32,33	1.09	2 (6%)	44,44,46	1.78	7 (15%)
7	B3P	B	801	-	18,18,18	0.75	1 (5%)	23,23,23	1.05	1 (4%)
4	GOL	C	810	-	5,5,5	0.11	0	5,5,5	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	812	-	5,5,5	0.53	0	5,5,5	1.18	0
2	SCN	C	826	-	1,2,2	1.35	0	0,1,1	-	-
4	GOL	C	816	-	5,5,5	0.62	0	5,5,5	1.01	0
2	SCN	C	820	-	1,2,2	1.03	0	0,1,1	-	-
4	GOL	C	803	-	5,5,5	0.20	0	5,5,5	0.29	0
2	SCN	C	814	-	1,2,2	2.06	1 (100%)	0,1,1	-	-
4	GOL	B	803	-	5,5,5	0.17	0	5,5,5	0.65	0
2	SCN	A	811	-	1,2,2	2.06	1 (100%)	0,1,1	-	-
6	A1CQY	C	827	1	32,32,33	1.33	3 (9%)	44,44,46	1.73	9 (20%)
3	PEG	B	807	-	6,6,6	0.46	0	5,5,5	0.44	0
3	PEG	C	815	-	6,6,6	0.47	0	5,5,5	0.28	0
4	GOL	C	828	-	5,5,5	0.21	0	5,5,5	0.19	0
3	PEG	A	805[B]	-	6,6,6	1.15	1 (16%)	5,5,5	0.75	0
4	GOL	A	804	-	5,5,5	0.35	0	5,5,5	1.18	1 (20%)

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	PEG	C	813	-	-	3/4/4/4	-
3	PEG	C	806	-	-	4/4/4/4	-
3	PEG	A	802	-	-	3/4/4/4	-
4	GOL	A	803	-	-	0/4/4/4	-
4	GOL	B	805	-	-	2/4/4/4	-
3	PEG	C	808	-	-	2/4/4/4	-
4	GOL	C	805	-	-	2/4/4/4	-
6	A1CQY	B	811	1	-	4/18/25/25	0/4/4/4
4	GOL	C	812	-	-	2/4/4/4	-
4	GOL	A	813	-	-	2/4/4/4	-
4	GOL	A	809	-	-	4/4/4/4	-
4	GOL	C	807	-	-	2/4/4/4	-
4	GOL	C	809	-	-	4/4/4/4	-
3	PEG	C	802	-	-	3/4/4/4	-
4	GOL	C	831[A]	-	-	2/4/4/4	-
4	GOL	B	802	-	-	1/4/4/4	-
4	GOL	A	810	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	B3P	A	801	-	-	0/28/28/28	-
3	PEG	C	824	-	-	3/4/4/4	-
4	GOL	A	819	-	-	2/4/4/4	-
4	GOL	C	830	-	-	0/4/4/4	-
3	PEG	A	805[A]	-	-	2/4/4/4	-
4	GOL	A	807	-	-	3/4/4/4	-
4	GOL	C	829	-	-	2/4/4/4	-
4	GOL	C	831[B]	-	-	0/4/4/4	-
4	GOL	B	806	-	-	2/4/4/4	-
4	GOL	C	804	-	-	2/4/4/4	-
4	GOL	B	813	-	-	0/4/4/4	-
4	GOL	A	806	-	-	4/4/4/4	-
7	B3P	B	801	-	-	0/28/28/28	-
6	A1CQY	A	817	1	-	4/18/25/25	0/4/4/4
4	GOL	C	810	-	-	2/4/4/4	-
4	GOL	A	812	-	-	2/4/4/4	-
4	GOL	C	816	-	-	2/4/4/4	-
4	GOL	C	803	-	-	4/4/4/4	-
4	GOL	B	803	-	-	0/4/4/4	-
6	A1CQY	C	827	1	-	5/18/25/25	0/4/4/4
3	PEG	B	807	-	-	3/4/4/4	-
3	PEG	C	815	-	-	2/4/4/4	-
4	GOL	C	828	-	-	1/4/4/4	-
3	PEG	A	805[B]	-	-	2/4/4/4	-
4	GOL	A	804	-	-	2/4/4/4	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	827	A1CQY	C2-N1	4.95	1.37	1.32
6	A	817	A1CQY	C21-C10	-4.03	1.35	1.41
6	C	827	A1CQY	C3-C4	2.87	1.60	1.52
6	C	827	A1CQY	C11-C12	2.43	1.43	1.39
6	B	811	A1CQY	C21-C10	2.38	1.44	1.41
3	C	824	PEG	O1-C1	2.38	1.54	1.42
2	B	804	SCN	C-N	-2.15	1.07	1.15
3	A	805[B]	PEG	O1-C1	2.11	1.52	1.42
3	C	813	PEG	O4-C4	2.09	1.52	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	801	B3P	C6-C4	2.08	1.55	1.53
2	A	811	SCN	C-N	-2.06	1.08	1.15
2	C	814	SCN	C-N	-2.06	1.08	1.15
6	A	817	A1CQY	C3-C4	2.02	1.57	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	817	A1CQY	C21-C2-N1	-6.54	108.20	110.76
6	B	811	A1CQY	C21-C2-N1	-5.39	108.65	110.76
6	C	827	A1CQY	C10-C21-C2	-5.19	103.48	105.15
6	A	817	A1CQY	C10-C21-C2	4.85	106.71	105.15
6	B	811	A1CQY	C20-C12-C11	4.45	122.50	117.92
6	C	827	A1CQY	C20-C21-C2	4.22	141.16	136.72
6	C	827	A1CQY	C21-C2-N1	-3.56	109.36	110.76
6	C	827	A1CQY	C3-N2-N1	3.49	122.75	119.75
7	A	801	B3P	C7-C4-N1	-3.23	99.37	109.02
6	C	827	A1CQY	C1-C2-C21	3.16	133.03	127.56
6	B	811	A1CQY	C20-C21-C2	3.13	140.01	136.72
6	A	817	A1CQY	C12-C13-N5	-2.99	110.91	117.12
7	B	801	B3P	O3-C11-C8	-2.87	105.84	111.68
6	B	811	A1CQY	C2-N1-N2	2.87	108.21	104.97
6	B	811	A1CQY	C20-C21-C10	-2.84	114.81	117.67
6	C	827	A1CQY	O1-C13-C12	2.83	126.50	120.90
6	C	827	A1CQY	C12-C13-N5	-2.82	111.26	117.12
6	A	817	A1CQY	C18-C17-C16	-2.82	97.30	105.10
4	C	809	GOL	C3-C2-C1	2.77	121.94	111.80
6	A	817	A1CQY	O1-C13-C12	2.68	126.20	120.90
4	C	809	GOL	O3-C3-C2	2.64	122.25	110.38
6	B	811	A1CQY	C4-C3-N2	-2.57	109.22	111.93
4	A	810	GOL	O3-C3-C2	2.47	121.51	110.38
6	A	817	A1CQY	C20-C21-C10	-2.47	115.18	117.67
6	B	811	A1CQY	C1-C2-C21	2.43	131.76	127.56
4	A	810	GOL	O2-C2-C3	2.40	119.11	109.18
6	C	827	A1CQY	C20-C21-C10	-2.32	115.33	117.67
6	B	811	A1CQY	C21-C20-C12	-2.21	117.05	120.70
6	C	827	A1CQY	C21-C10-N2	2.10	108.48	107.18
6	A	817	A1CQY	O2-C15-N6	-2.07	118.43	122.12
4	A	804	GOL	O1-C1-C2	2.03	119.51	110.38
6	B	811	A1CQY	C21-C10-N2	-2.02	105.93	107.18

There are no chirality outliers.

All (93) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	803	GOL	C1-C2-C3-O3
4	C	804	GOL	O1-C1-C2-C3
4	C	805	GOL	O1-C1-C2-C3
4	C	807	GOL	C1-C2-C3-O3
4	C	809	GOL	O1-C1-C2-C3
4	C	809	GOL	C1-C2-C3-O3
4	C	812	GOL	C1-C2-C3-O3
4	C	812	GOL	O2-C2-C3-O3
4	C	816	GOL	C1-C2-C3-O3
4	C	831[A]	GOL	C1-C2-C3-O3
4	A	806	GOL	O1-C1-C2-C3
4	A	807	GOL	C1-C2-C3-O3
4	A	809	GOL	C1-C2-C3-O3
4	A	810	GOL	C1-C2-C3-O3
4	A	812	GOL	O1-C1-C2-C3
4	A	813	GOL	O1-C1-C2-C3
4	A	819	GOL	O1-C1-C2-C3
4	B	805	GOL	C1-C2-C3-O3
3	A	805[A]	PEG	C1-C2-O2-C3
6	A	817	A1CQY	C20-C12-C13-N5
6	A	817	A1CQY	C11-C12-C13-N5
3	C	813	PEG	C1-C2-O2-C3
3	C	802	PEG	C1-C2-O2-C3
3	A	802	PEG	O2-C3-C4-O4
6	B	811	A1CQY	C20-C12-C13-N5
6	C	827	A1CQY	C20-C12-C13-N5
6	C	827	A1CQY	C11-C12-C13-N5
6	B	811	A1CQY	C11-C12-C13-N5
4	C	805	GOL	O1-C1-C2-O2
4	C	809	GOL	O2-C2-C3-O3
4	C	831[A]	GOL	O2-C2-C3-O3
4	A	809	GOL	O2-C2-C3-O3
4	A	812	GOL	O1-C1-C2-O2
3	C	808	PEG	O1-C1-C2-O2
3	A	805[A]	PEG	O1-C1-C2-O2
3	C	802	PEG	O2-C3-C4-O4
3	C	806	PEG	C1-C2-O2-C3
4	C	803	GOL	O1-C1-C2-C3
4	C	810	GOL	O1-C1-C2-C3
4	C	828	GOL	C1-C2-C3-O3
4	A	804	GOL	O1-C1-C2-C3
4	A	809	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	A	810	GOL	O1-C1-C2-C3
4	B	806	GOL	O1-C1-C2-C3
3	C	806	PEG	O2-C3-C4-O4
3	C	813	PEG	O2-C3-C4-O4
4	C	803	GOL	O2-C2-C3-O3
4	C	804	GOL	O1-C1-C2-O2
4	C	807	GOL	O2-C2-C3-O3
4	C	809	GOL	O1-C1-C2-O2
4	C	816	GOL	O2-C2-C3-O3
4	A	806	GOL	O1-C1-C2-O2
4	A	807	GOL	O2-C2-C3-O3
4	A	809	GOL	O1-C1-C2-O2
4	A	810	GOL	O1-C1-C2-O2
4	A	813	GOL	O1-C1-C2-O2
4	B	805	GOL	O2-C2-C3-O3
4	B	806	GOL	O1-C1-C2-O2
3	B	807	PEG	O2-C3-C4-O4
6	A	817	A1CQY	C20-C12-C13-O1
3	C	808	PEG	O2-C3-C4-O4
3	C	806	PEG	O1-C1-C2-O2
3	C	815	PEG	O1-C1-C2-O2
3	C	815	PEG	O2-C3-C4-O4
3	C	824	PEG	O2-C3-C4-O4
4	A	819	GOL	O1-C1-C2-O2
6	A	817	A1CQY	C11-C12-C13-O1
6	C	827	A1CQY	C11-C12-C13-O1
4	C	803	GOL	O1-C1-C2-O2
4	C	829	GOL	O1-C1-C2-O2
3	C	824	PEG	C4-C3-O2-C2
4	A	804	GOL	O1-C1-C2-O2
4	A	806	GOL	O2-C2-C3-O3
4	A	810	GOL	O2-C2-C3-O3
4	B	802	GOL	O2-C2-C3-O3
3	C	813	PEG	C4-C3-O2-C2
3	B	807	PEG	O1-C1-C2-O2
6	C	827	A1CQY	C20-C12-C13-O1
3	C	824	PEG	O1-C1-C2-O2
3	A	805[B]	PEG	O2-C3-C4-O4
6	B	811	A1CQY	C11-C12-C13-O1
3	C	802	PEG	C4-C3-O2-C2
3	A	805[B]	PEG	C1-C2-O2-C3
3	B	807	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
6	B	811	A1CQY	C20-C12-C13-O1
3	A	802	PEG	C4-C3-O2-C2
4	C	829	GOL	O1-C1-C2-C3
4	A	806	GOL	C1-C2-C3-O3
4	C	810	GOL	O1-C1-C2-O2
4	A	807	GOL	O1-C1-C2-O2
3	A	802	PEG	C1-C2-O2-C3
3	C	806	PEG	C4-C3-O2-C2
6	C	827	A1CQY	C15-C14-N5-C13

There are no ring outliers.

30 monomers are involved in 74 short contacts:

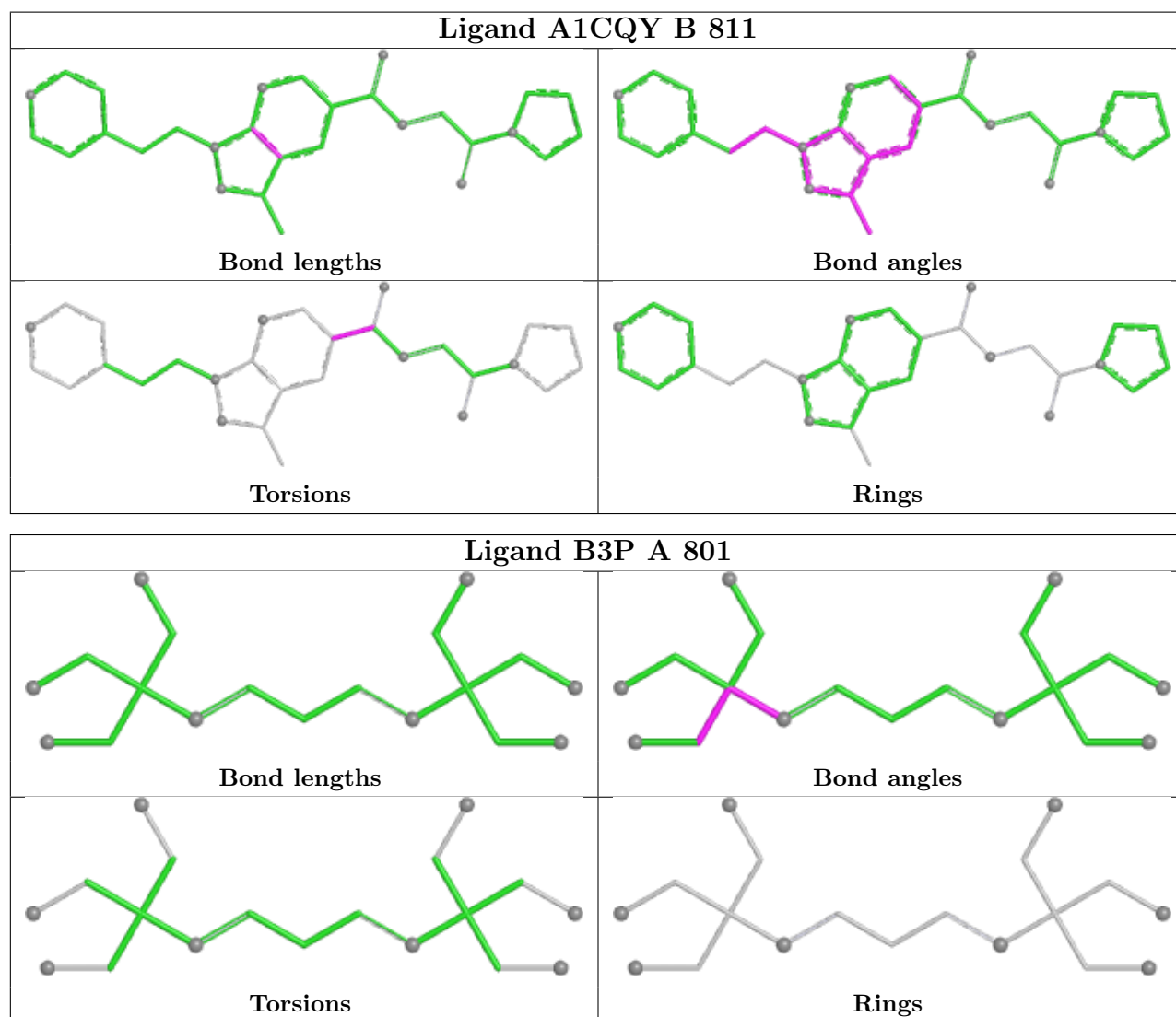
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	813	PEG	5	0
2	A	818	SCN	1	0
2	C	822	SCN	3	0
3	C	806	PEG	2	0
3	A	802	PEG	2	0
2	B	812	SCN	1	0
3	C	808	PEG	1	0
4	C	805	GOL	3	0
2	C	825	SCN	1	0
4	A	813	GOL	3	0
4	C	809	GOL	3	0
3	C	802	PEG	6	0
5	C	821	DMS	8	0
2	C	818	SCN	1	0
2	C	817	SCN	1	0
3	C	824	PEG	8	0
2	A	816	SCN	1	0
2	A	815	SCN	2	0
2	C	801	SCN	1	0
3	A	805[A]	PEG	1	0
4	C	831[B]	GOL	1	0
4	B	806	GOL	3	0
4	C	810	GOL	3	0
4	A	812	GOL	2	0
2	C	826	SCN	2	0
4	C	816	GOL	2	0
2	C	820	SCN	3	0
4	C	828	GOL	2	0

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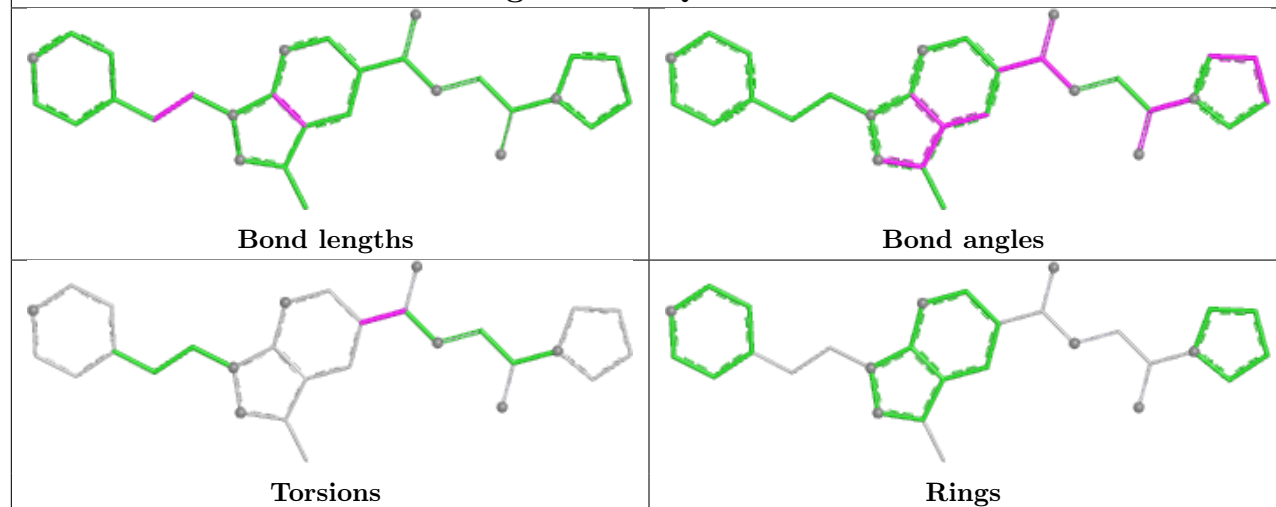
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	805[B]	PEG	1	0
4	A	804	GOL	1	0

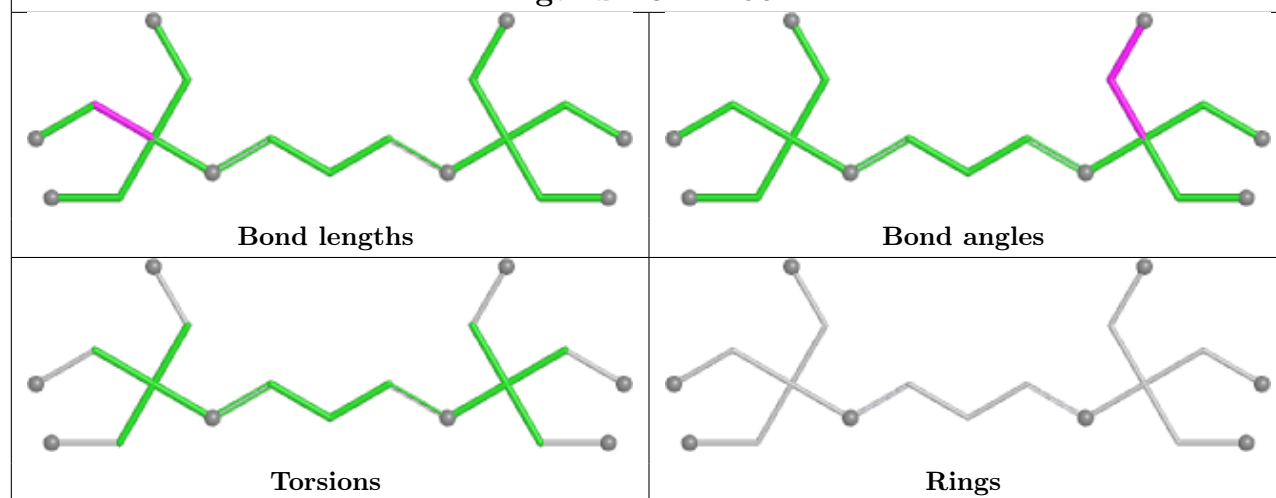
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



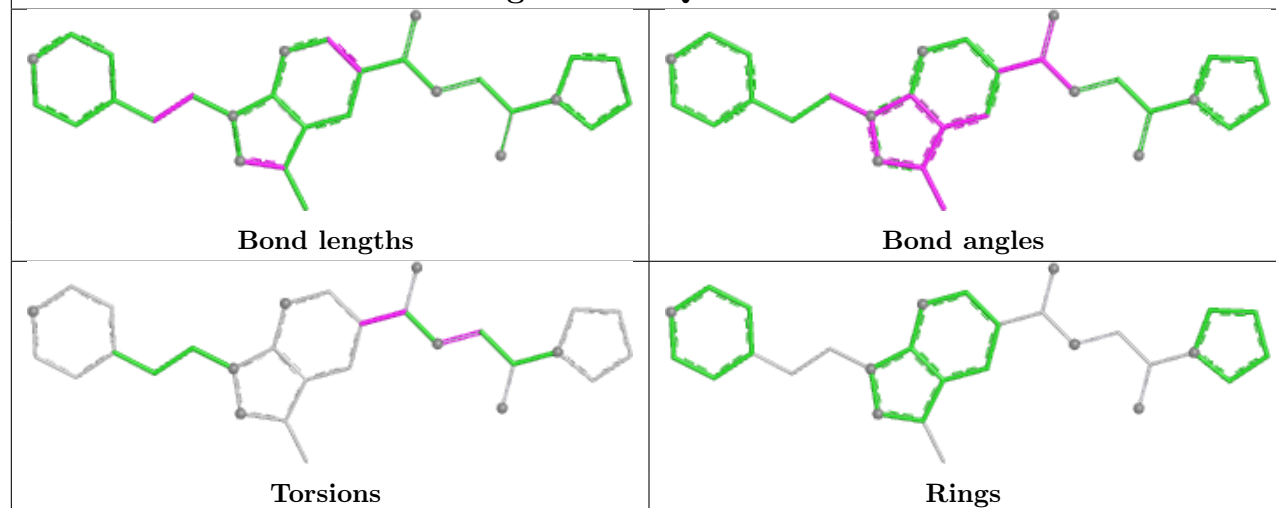
Ligand A1CQY A 817



Ligand B3P B 801



Ligand A1CQY C 827



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%)	-0.82	2 (0%)	90	93	6, 15, 31, 54	7 (0%)
1	B	707/711 (99%)	-0.60	6 (0%)	82	87	6, 19, 37, 61	2 (0%)
1	C	707/711 (99%)	-0.86	0	100	100	5, 14, 30, 52	8 (1%)
All	All	2121/2133 (99%)	-0.76	8 (0%)	88	92	5, 16, 34, 61	17 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	426	THR	3.2
1	A	4	LEU	2.9
1	B	430	ILE	2.7
1	B	4	LEU	2.6
1	B	427	VAL	2.5
1	B	429	GLY	2.4
1	A	270	SER	2.3
1	B	107	GLU	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 [i](#)

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PEG	A	805[A]	7/7	0.70	0.22	24,30,36,37	17
3	PEG	A	805[B]	7/7	0.70	0.22	16,17,30,30	17
4	GOL	C	805	6/6	0.75	0.17	30,39,47,50	3
3	PEG	C	808	7/7	0.78	0.15	30,53,63,65	2
4	GOL	C	812	6/6	0.80	0.15	30,50,54,55	3
4	GOL	C	828	6/6	0.80	0.12	36,41,46,48	3
3	PEG	C	813	7/7	0.81	0.14	28,30,41,42	2
2	SCN	B	810	3/3	0.81	0.19	54,54,54,72	0
4	GOL	C	803	6/6	0.83	0.14	30,39,49,50	3
3	PEG	B	807	7/7	0.83	0.14	30,53,57,57	2
4	GOL	C	816	6/6	0.85	0.13	22,30,35,38	3
4	GOL	C	829	6/6	0.85	0.12	33,39,46,52	3
4	GOL	A	819	6/6	0.85	0.13	36,46,49,53	3
3	PEG	C	815	7/7	0.86	0.11	30,36,44,46	2
3	PEG	C	824	7/7	0.86	0.13	27,37,44,50	2
2	SCN	C	825	3/3	0.86	0.14	47,47,52,60	0
3	PEG	C	806	7/7	0.86	0.12	30,40,42,46	2
2	SCN	C	826	3/3	0.86	0.22	29,29,29,37	3
4	GOL	A	806	6/6	0.86	0.12	30,36,40,50	3
4	GOL	A	807	6/6	0.86	0.13	30,40,48,50	3
4	GOL	A	813	6/6	0.86	0.11	30,41,42,42	3
2	SCN	B	804	3/3	0.86	0.11	25,25,29,54	0
4	GOL	B	803	6/6	0.86	0.12	30,42,46,46	3
4	GOL	B	806	6/6	0.86	0.11	30,38,43,45	3
3	PEG	A	802	7/7	0.87	0.14	22,30,44,44	2
2	SCN	A	816	3/3	0.87	0.16	37,37,41,47	0
4	GOL	A	810	6/6	0.87	0.12	23,30,32,37	3
4	GOL	A	812	6/6	0.87	0.15	21,33,35,35	3
4	GOL	C	831[A]	6/6	0.88	0.12	22,29,36,36	14
4	GOL	C	831[B]	6/6	0.88	0.12	15,16,36,36	14
2	SCN	B	809	3/3	0.88	0.13	34,34,43,64	0
4	GOL	C	809	6/6	0.88	0.10	24,30,34,38	3
2	SCN	C	811	3/3	0.88	0.13	50,50,51,62	0
3	PEG	C	802	7/7	0.89	0.10	24,30,36,37	2
2	SCN	C	814	3/3	0.89	0.12	22,22,24,44	0
2	SCN	C	818	3/3	0.89	0.12	35,35,45,54	0
5	DMS	C	821	4/4	0.89	0.12	30,35,44,56	0
4	GOL	B	805	6/6	0.90	0.12	27,37,46,52	3
4	GOL	C	807	6/6	0.91	0.11	20,35,38,42	3
2	SCN	A	818	3/3	0.91	0.09	37,37,45,57	0
2	SCN	A	811	3/3	0.91	0.13	28,28,31,60	0

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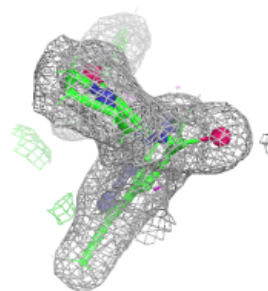
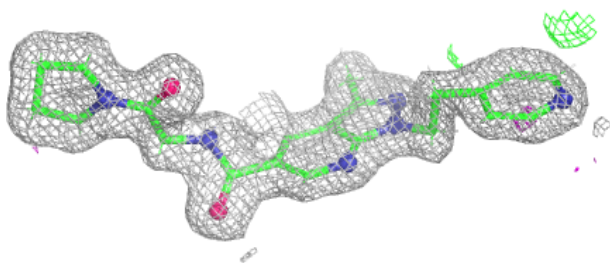
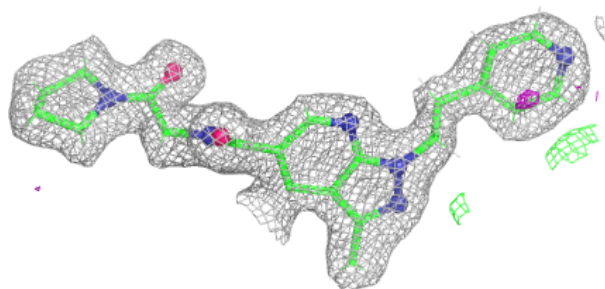
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	C	830	6/6	0.92	0.08	31,34,36,39	3
4	GOL	B	813	6/6	0.92	0.08	28,34,37,55	3
4	GOL	B	802	6/6	0.92	0.10	30,36,43,50	3
4	GOL	C	810	6/6	0.93	0.09	26,39,48,49	3
2	SCN	A	808	3/3	0.93	0.09	20,20,35,54	0
2	SCN	C	822	3/3	0.93	0.16	24,24,34,49	0
4	GOL	C	804	6/6	0.93	0.08	18,25,30,31	3
4	GOL	A	804	6/6	0.94	0.07	15,25,30,36	3
4	GOL	A	809	6/6	0.94	0.06	25,27,30,30	3
2	SCN	B	812	3/3	0.94	0.07	35,35,35,50	0
2	SCN	C	817	3/3	0.95	0.12	32,32,34,52	0
5	DMS	C	823	4/4	0.95	0.09	31,44,47,48	0
4	GOL	A	803	6/6	0.96	0.06	16,20,30,30	3
2	SCN	A	815	3/3	0.96	0.11	22,22,23,23	3
2	SCN	C	820	3/3	0.96	0.16	37,37,37,43	0
2	SCN	C	801	3/3	0.96	0.11	21,21,29,29	0
6	A1CQY	C	827	29/30	0.97	0.05	10,14,27,30	3
6	A1CQY	A	817	29/30	0.97	0.05	10,14,30,32	3
6	A1CQY	B	811	29/30	0.97	0.05	14,16,36,40	3
7	B3P	A	801	19/19	0.97	0.05	12,18,30,30	8
7	B3P	B	801	19/19	0.97	0.04	13,16,30,30	8
5	DMS	C	819	4/4	0.98	0.05	14,15,17,18	0
5	DMS	B	808	4/4	0.99	0.06	16,17,19,19	0
5	DMS	A	814	4/4	0.99	0.03	13,17,18,18	0
8	NA	A	820	1/1	0.99	0.07	13,13,13,13	0

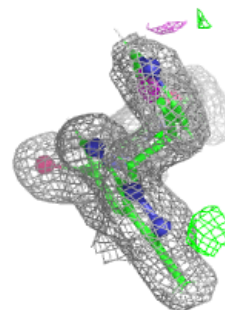
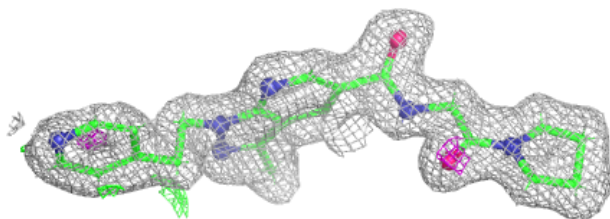
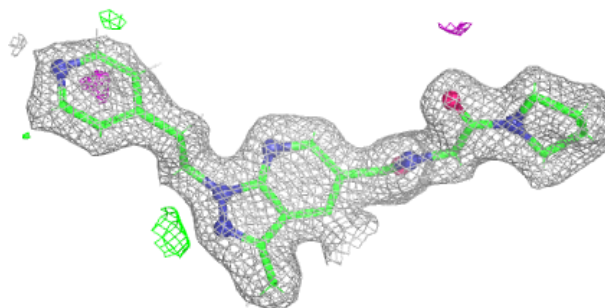
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1CQY C 827:

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

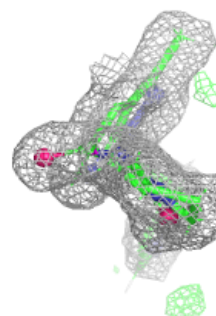
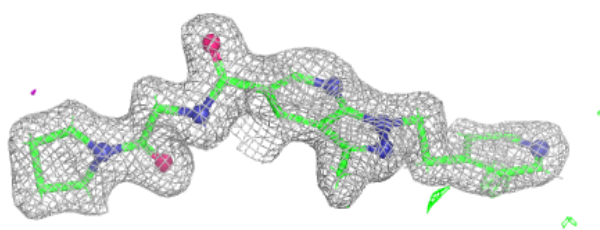
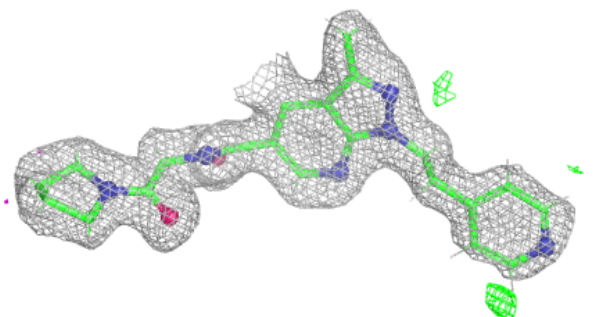
**Electron density around A1CQY A 817:**

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

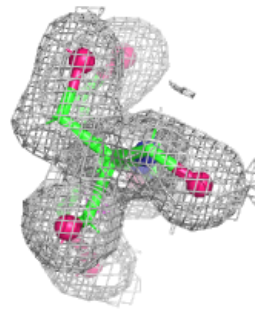
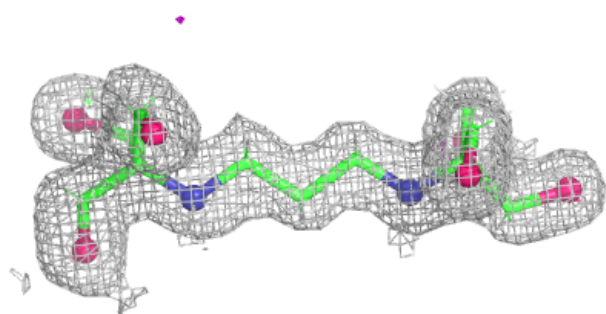
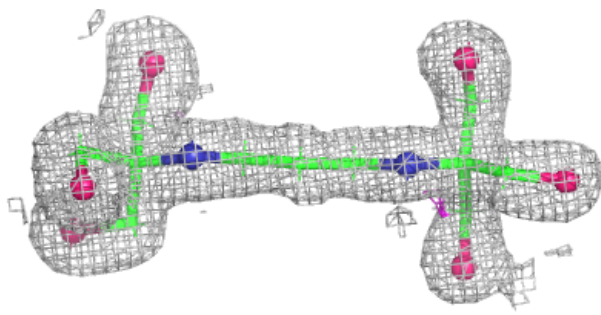


Electron density around A1CQY B 811:

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

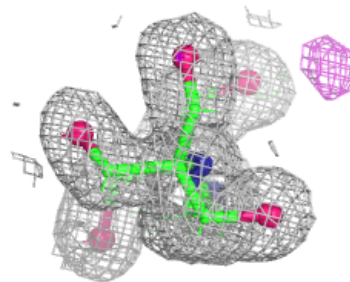
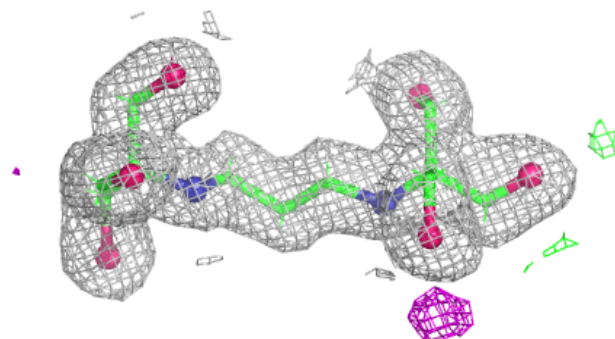
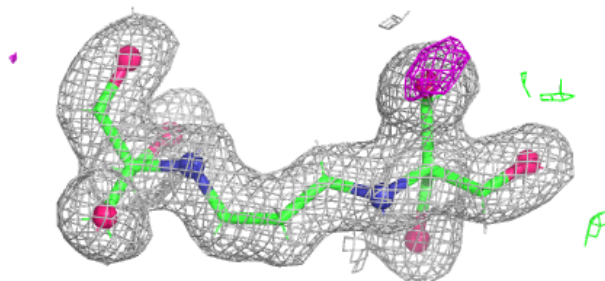
**Electron density around B3P A 801:**

$2mF_o-DF_c$ (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.