



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:42 AM UTC

PDB ID : 9XYK / pdb_00009xyk
Title : Human prolyl endopeptidase (PREP) - complex with JP-7-1-7
Authors : Fucci, I.J.; Thakur, K.; Pandian, J.; Yoo, E.; Monteiro, D.C.F.
Deposited on : 2025-08-26
Resolution : 1.73 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

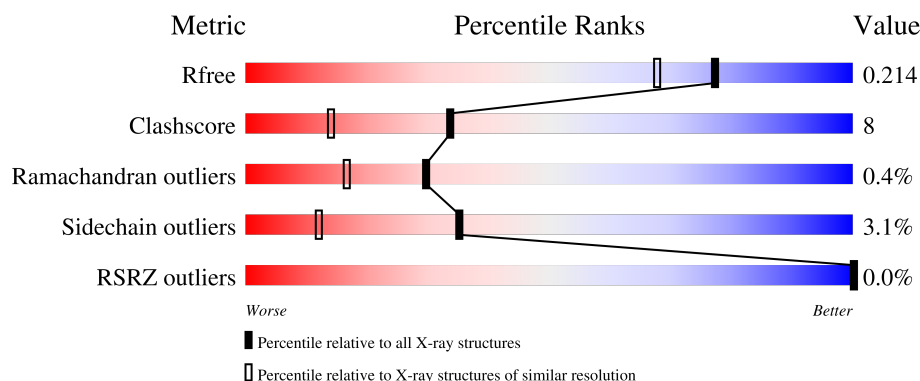
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.73 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	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	
1	B	711	
1	C	711	

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	820	-	-	X	-
2	SCN	C	822	-	-	X	-
3	PEG	A	802	-	-	X	-
3	PEG	C	802	-	-	X	-
3	PEG	C	824	-	-	X	-
4	GOL	C	805	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 36320 atoms, of which 17148 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.

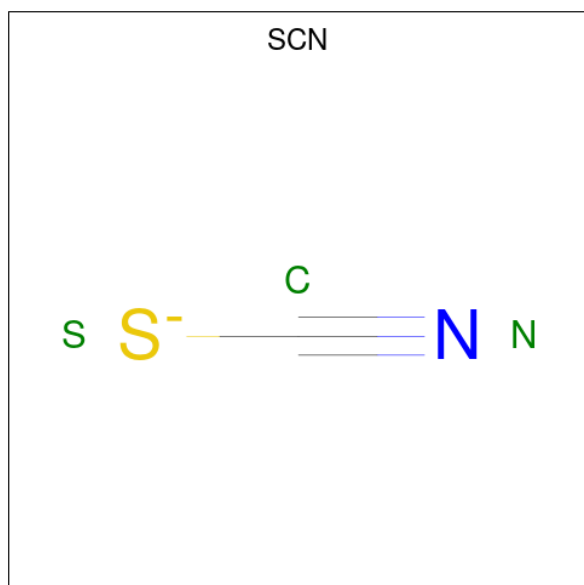
- Molecule 1 is a protein called Prolyl endopeptidase.

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	177	7	0
			11279	3667	5568	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: $C_3H_8O_3$).



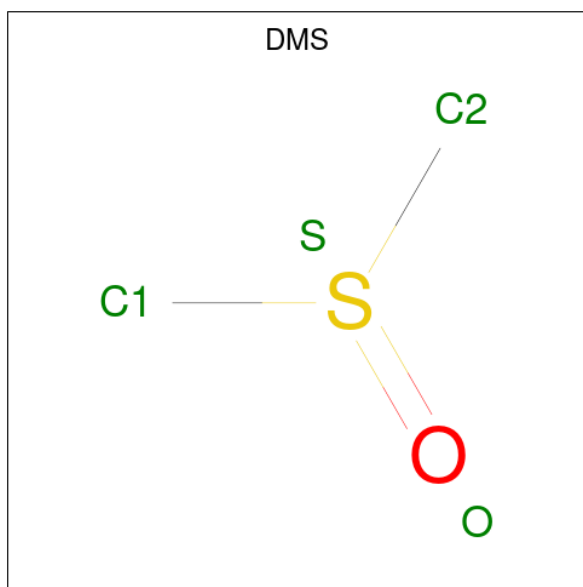
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	H	O	3	0
			14	3	8	3		
4	C	1	Total	C	H	O	3	0
			14	3	8	3		
4	C	1	Total	C	H	O	3	0
			14	3	8	3		
4	C	1	Total	C	H	O	3	0
			14	3	8	3		
4	C	1	Total	C	H	O	3	0
			14	3	8	3		
4	C	1	Total	C	H	O	3	0
			14	3	8	3		
4	C	1	Total	C	H	O	3	0
			14	3	8	3		
4	C	1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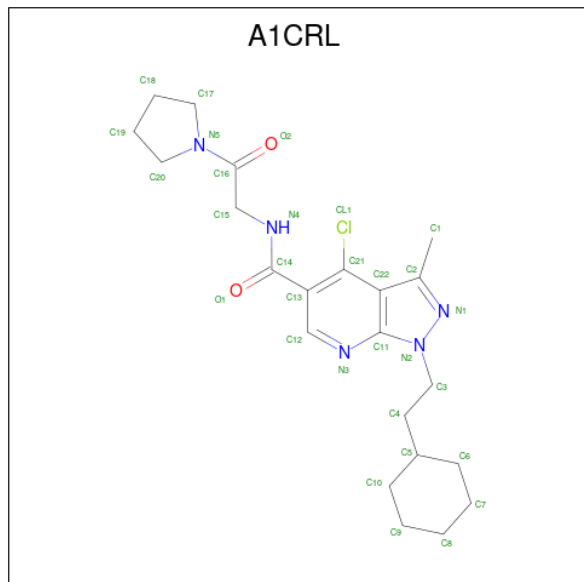
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	3	0
			14	3	8	3		
4	A	1	Total	C	H	O	3	0
			14	3	8	3		
4	A	1	Total	C	H	O	3	0
			14	3	8	3		
4	A	1	Total	C	H	O	3	0
			14	3	8	3		
4	A	1	Total	C	H	O	3	0
			14	3	8	3		
4	B	1	Total	C	H	O	3	0
			14	3	8	3		
4	B	1	Total	C	H	O	3	0
			14	3	8	3		
4	B	1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



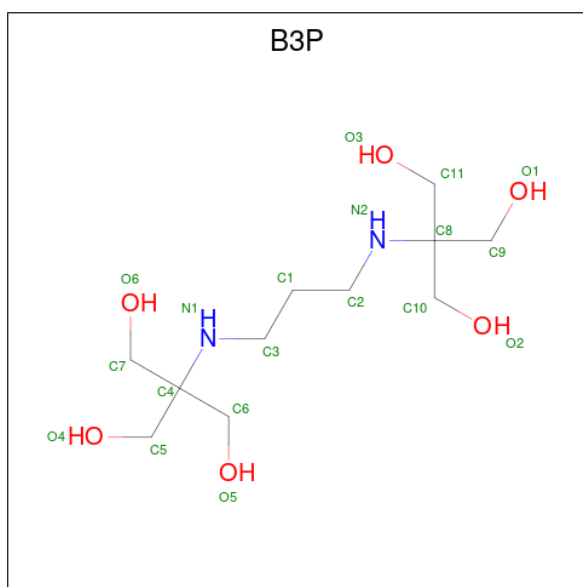
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
5	C	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
5	C	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
5	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
5	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

- Molecule 6 is 4-chloro-1-(2-cyclohexylethyl)-3-methyl-N-[2-oxo-2-(pyrrolidin-1-yl)ethyl]-1H-pyrazolo[3,4-b]pyridine-5-carboxamide (CCD ID: A1CRL) (formula: $C_{22}H_{30}ClN_5O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	H	N	O	3	0
			59	22	30	5	2		
6	A	1	Total	C	H	N	O	3	0
			59	22	30	5	2		
6	B	1	Total	C	H	N	O	3	0
			59	22	30	5	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	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	B	1	Total	Na	0	0
			1	1		

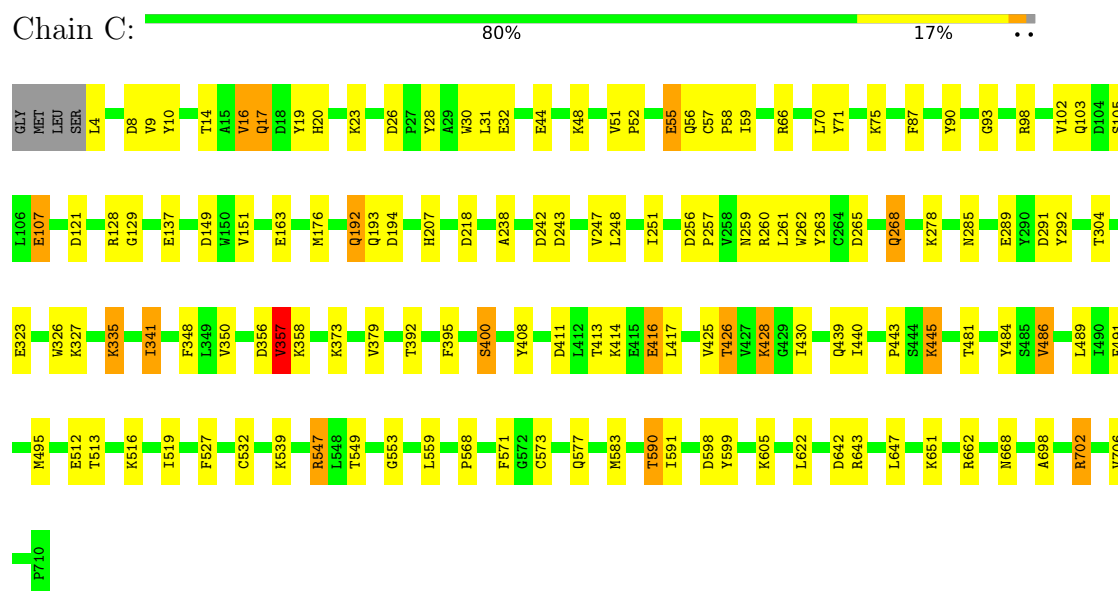
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	591	Total	O	0	0
			591	591		
9	A	577	Total	O	0	0
			577	577		
9	B	470	Total	O	0	1
			471	471		

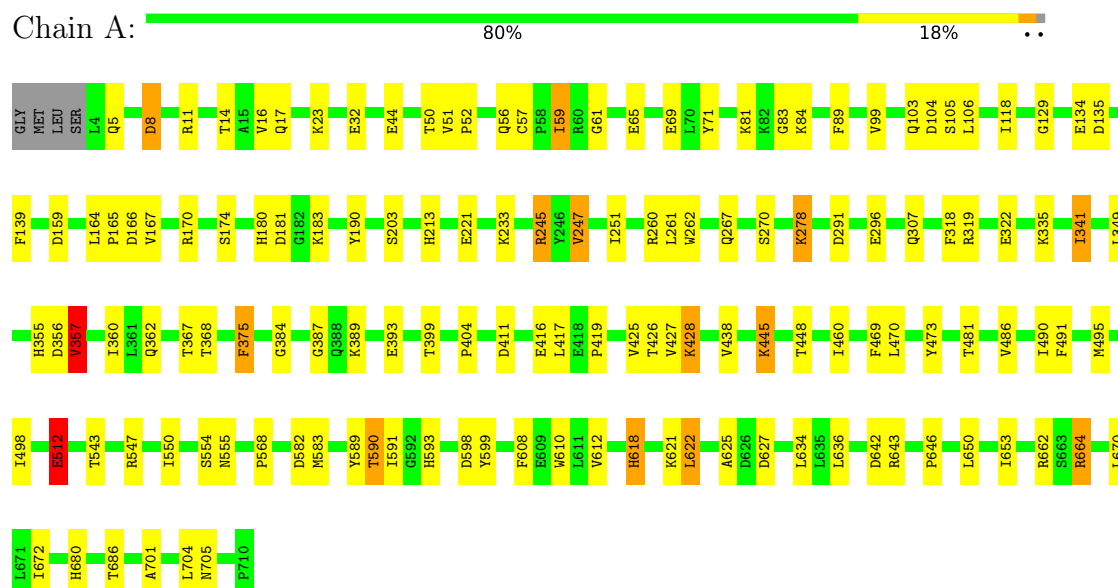
3 Residue-property plots

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

• Molecule 1: Prolyl endopeptidase

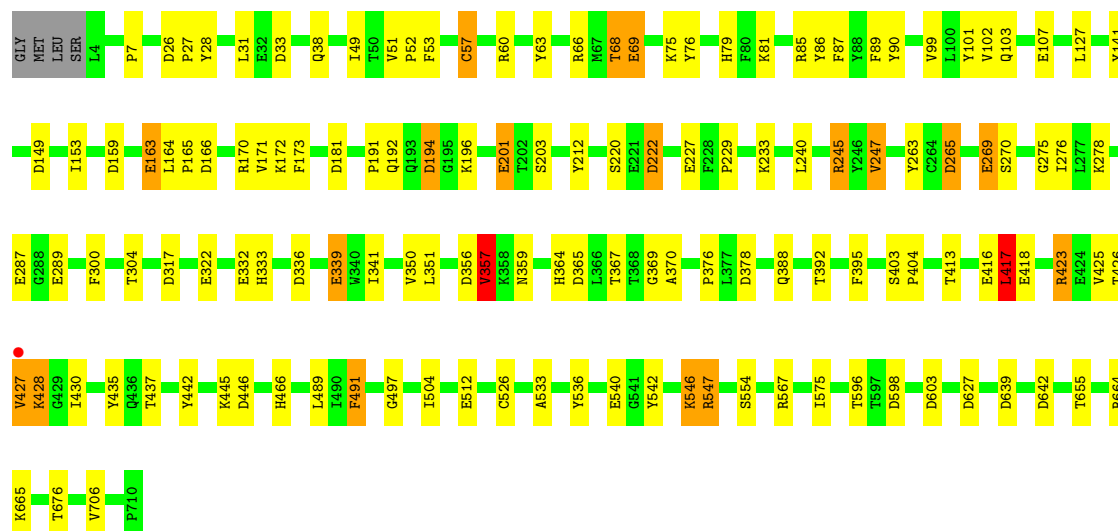


• Molecule 1: Prolyl endopeptidase



● Molecule 1: Prolyl endopeptidase

Chain B:  80% 16% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.54Å 66.30Å 156.24Å 90.00° 102.10° 90.00°	Depositor
Resolution (Å)	34.50 – 1.73 34.50 – 1.73	Depositor EDS
% Data completeness (in resolution range)	64.3 (34.50-1.73) 64.4 (34.50-1.73)	Depositor EDS
R_{merge}	0.36	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 1.73Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.105)	Depositor
R, R_{free}	0.189 , 0.255 0.157 , 0.214	Depositor DCC
R_{free} test set	84478 reflections (38.95%)	wwPDB-VP
Wilson B-factor (Å ²)	17.8	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	36320	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.04% 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: B3P, SCN, PEG, NA, A1CRL, DMS, GOL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.76	1/5884 (0.0%)	1.29	30/7975 (0.4%)
1	B	0.70	0/5840	1.34	41/7917 (0.5%)
1	C	0.74	1/5890 (0.0%)	1.30	23/7985 (0.3%)
All	All	0.73	2/17614 (0.0%)	1.31	94/23877 (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	4
1	B	0	3
1	C	0	3
All	All	0	10

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	213	HIS	CG-CD2	-5.72	1.29	1.35
1	C	400	SER	CA-CB	-5.19	1.47	1.53

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	512	GLU	CB-CG-CD	8.38	126.85	112.60
1	B	428	LYS	CB-CA-C	-8.12	96.89	109.89
1	B	437	THR	CA-CB-OG1	-7.87	97.79	109.60
1	C	445	LYS	N-CA-CB	-7.69	97.99	110.14
1	B	163	GLU	CB-CA-C	-7.64	97.97	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	322	GLU	N-CA-CB	7.51	121.70	110.29
1	A	411	ASP	CA-CB-CG	7.36	119.96	112.60
1	A	416	GLU	CB-CA-C	-7.31	96.64	110.67
1	A	448	THR	CA-CB-OG1	-7.19	98.82	109.60
1	B	159	ASP	CA-CB-CG	7.07	119.67	112.60
1	C	194	ASP	CA-CB-CG	7.04	119.64	112.60
1	C	149	ASP	CA-CB-CG	7.00	119.60	112.60
1	C	103	GLN	CB-CA-C	-6.97	95.46	110.45
1	C	107	GLU	CB-CA-C	6.96	122.07	109.62
1	B	222	ASP	CA-CB-CG	6.87	119.47	112.60
1	B	596	THR	CA-CB-OG1	-6.84	99.34	109.60
1	B	27	PRO	CB-CA-C	-6.83	102.16	111.85
1	B	395	PHE	CA-CB-CG	6.71	120.51	113.80
1	B	163	GLU	N-CA-CB	6.69	119.92	109.69
1	B	446	ASP	CA-CB-CG	6.68	119.28	112.60
1	A	291	ASP	CA-CB-CG	6.61	119.20	112.60
1	C	426	THR	CA-CB-OG1	-6.60	99.70	109.60
1	C	268	GLN	N-CA-CB	6.58	120.17	110.56
1	C	107	GLU	CB-CG-CD	6.57	123.76	112.60
1	B	339	GLU	CB-CA-C	-6.54	100.57	110.90
1	C	121	ASP	CA-CB-CG	6.52	119.12	112.60
1	C	55	GLU	CB-CG-CD	6.49	123.64	112.60
1	B	66	ARG	N-CA-CB	-6.44	100.61	110.20
1	C	192	GLN	CB-CA-C	6.43	120.39	109.72
1	B	423	ARG	CB-CA-C	-6.39	99.43	109.72
1	B	445	LYS	N-CA-CB	-6.31	100.59	110.06
1	A	469	PHE	CA-CB-CG	6.25	120.05	113.80
1	B	166	ASP	CB-CA-C	6.21	119.82	109.89
1	C	622	LEU	O-C-N	-6.17	116.66	121.47
1	A	247	VAL	N-CA-CB	6.14	118.00	111.00
1	A	686	THR	CA-CB-OG1	-6.11	100.44	109.60
1	A	416	GLU	N-CA-CB	6.10	119.73	110.28
1	A	318	PHE	CA-CB-CG	5.98	119.78	113.80
1	A	428	LYS	CB-CA-C	5.96	120.51	109.54
1	B	317	ASP	CA-CB-CG	5.96	118.56	112.60
1	A	44	GLU	CB-CA-C	5.95	120.32	110.81
1	B	68	THR	CA-CB-OG1	-5.94	100.69	109.60
1	C	348	PHE	CA-CB-CG	5.92	119.72	113.80
1	B	194	ASP	CA-CB-CG	5.90	118.50	112.60
1	B	547	ARG	CB-CA-C	-5.88	100.52	110.64
1	C	547	ARG	CG-CD-NE	-5.88	99.07	112.00
1	A	166	ASP	CA-CB-CG	5.88	118.48	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	322	GLU	CB-CG-CD	5.83	122.50	112.60
1	A	278	LYS	N-CA-CB	5.82	118.68	110.24
1	C	121	ASP	CB-CA-C	-5.79	99.56	110.67
1	A	135	ASP	CA-CB-CG	5.79	118.39	112.60
1	A	642	ASP	CA-CB-CG	5.78	118.38	112.60
1	A	705	ASN	CB-CA-C	-5.76	104.44	111.82
1	B	676	THR	CA-CB-OG1	-5.74	100.99	109.60
1	C	414	LYS	CB-CA-C	-5.72	99.01	109.54
1	C	242	ASP	CA-CB-CG	5.71	118.31	112.60
1	B	181	ASP	CA-CB-CG	5.58	118.18	112.60
1	A	610	TRP	CB-CA-C	-5.56	102.15	110.88
1	A	393	GLU	CB-CG-CD	5.55	122.03	112.60
1	C	411	ASP	CA-CB-CG	5.51	118.11	112.60
1	B	149	ASP	CA-CB-CG	5.51	118.11	112.60
1	C	481	THR	OG1-CB-CG2	-5.44	98.41	109.30
1	A	291	ASP	CB-CA-C	5.44	119.11	110.19
1	B	192	GLN	N-CA-CB	5.44	118.04	109.83
1	A	159	ASP	CA-CB-CG	5.43	118.03	112.60
1	A	50	THR	CA-CB-OG1	-5.37	101.54	109.60
1	B	69	GLU	CB-CG-CD	5.36	121.70	112.60
1	B	26	ASP	CB-CA-C	5.34	119.12	111.27
1	B	201	GLU	CB-CG-CD	5.30	121.61	112.60
1	B	526[A]	CYS	CB-CA-C	-5.27	101.89	110.85
1	B	526[B]	CYS	CB-CA-C	-5.27	101.89	110.85
1	A	375	PHE	CB-CA-C	5.26	117.93	109.41
1	C	590	THR	CA-CB-OG1	5.22	117.44	109.60
1	C	256	ASP	CA-CB-CG	5.22	117.82	112.60
1	B	265	ASP	CA-CB-CG	5.21	117.81	112.60
1	B	491	PHE	N-CA-C	-5.20	105.62	111.28
1	B	247	VAL	N-CA-CB	5.17	117.26	111.21
1	B	655	THR	OG1-CB-CG2	-5.17	98.97	109.30
1	A	8	ASP	CA-CB-CG	5.16	117.76	112.60
1	B	367	THR	CA-CB-OG1	-5.15	101.87	109.60
1	B	53	PHE	CA-CB-CG	-5.14	108.66	113.80
1	B	269	GLU	N-CA-CB	5.12	118.07	110.49
1	A	368	THR	CA-CB-OG1	-5.12	101.93	109.60
1	B	63	TYR	N-CA-CB	5.10	117.41	110.01
1	A	618	HIS	CB-CA-C	5.10	118.78	110.17
1	B	322	GLU	CB-CA-C	-5.10	100.08	109.46
1	A	139	PHE	CA-CB-CG	5.09	118.89	113.80
1	B	627	ASP	CA-CB-CG	5.08	117.68	112.60
1	C	445	LYS	CB-CA-C	5.05	120.26	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	ASP	CB-CA-C	5.03	118.44	109.29
1	B	57	CYS	CB-CA-C	5.03	118.12	109.82
1	B	300	PHE	CA-CB-CG	-5.03	108.77	113.80
1	A	481	THR	CA-CB-OG1	-5.01	102.09	109.60
1	C	137	GLU	N-CA-C	-5.00	107.73	113.88

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	ARG	Sidechain
1	A	245	ARG	Sidechain
1	A	319	ARG	Sidechain
1	A	662	ARG	Sidechain
1	B	245	ARG	Sidechain
1	B	567	ARG	Sidechain
1	B	60	ARG	Sidechain
1	C	259	ASN	Peptide
1	C	643	ARG	Sidechain
1	C	702	ARG	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5711	5568	5545	76	0
1	B	5682	5524	5501	75	0
1	C	5714	5576	5553	102	0
2	A	15	0	0	3	0
2	B	12	0	0	3	0
2	C	27	0	0	10	0
3	A	21	30	30	6	0
3	B	7	10	10	0	0
3	C	42	60	60	14	0
4	A	48	64	64	8	0
4	B	30	40	40	3	0
4	C	78	104	104	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	4	6	6	0	0
5	B	4	6	6	0	0
5	C	12	18	18	3	0
6	A	29	30	0	1	0
6	B	29	30	0	0	0
6	C	29	30	0	0	0
7	A	19	26	26	1	0
7	B	19	26	26	0	0
8	B	1	0	0	0	0
9	A	577	0	0	16	0
9	B	471	0	0	21	0
9	C	591	0	0	23	1
All	All	19172	17148	16989	265	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (265) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:425:VAL:HG22	5:C:821:DMS:H13	1.38	1.03
1:C:285:ASN:HD21	4:C:810:GOL:H32	1.30	0.95
1:C:571:PHE:O	3:C:802:PEG:H31	1.73	0.88
1:C:285:ASN:HD21	4:C:810:GOL:C3	1.88	0.86
1:B:425:VAL:HB	4:B:806:GOL:H31	1.59	0.84
2:C:820:SCN:N	9:C:903:HOH:O	2.12	0.82
1:C:218:ASP:OD1	9:C:901:HOH:O	1.98	0.81
1:A:17:GLN:NE2	2:A:816:SCN:N	2.29	0.79
2:B:811:SCN:S	9:B:1036:HOH:O	2.39	0.79
1:C:425:VAL:HG22	5:C:821:DMS:C1	2.13	0.79
2:C:817:SCN:N	9:C:905:HOH:O	2.16	0.79
1:C:358:LYS:HG2	1:C:379:VAL:HG13	1.64	0.78
1:C:163:GLU:HB3	9:C:1330:HOH:O	1.84	0.77
1:C:291:ASP:OD1	4:C:805:GOL:H2	1.83	0.77
1:C:335:LYS:NZ	1:C:356:ASP:OD1	2.20	0.74
7:A:801:B3P:H61	6:A:817:A1CRL:C6	2.17	0.73
1:C:539:LYS:NZ	9:C:907:HOH:O	2.16	0.72
3:C:813:PEG:H12	9:C:910:HOH:O	1.92	0.70
1:C:285:ASN:ND2	4:C:810:GOL:H32	2.04	0.70
1:B:388:GLN:OE1	9:B:901:HOH:O	2.10	0.70
1:C:428:LYS:HD2	1:C:428:LYS:N	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:706:VAL:O	9:C:902:HOH:O	2.11	0.69
1:B:665:LYS:O	9:B:903:HOH:O	2.12	0.68
1:B:38:GLN:O	9:B:904:HOH:O	2.12	0.68
1:C:547:ARG:NE	3:C:806:PEG:O4	2.27	0.67
1:B:33:ASP:OD2	9:B:902:HOH:O	2.11	0.67
4:C:804:GOL:H31	9:C:1172:HOH:O	1.95	0.66
1:B:127:LEU:CD1	1:B:141:TYR:HB2	2.24	0.66
1:A:445:LYS:NZ	9:A:909:HOH:O	2.28	0.65
1:C:51:VAL:O	1:C:55:GLU:HG3	1.97	0.65
1:B:269:GLU:OE2	9:B:905:HOH:O	2.13	0.65
1:B:270:SER:O	9:B:906:HOH:O	2.14	0.65
1:B:127:LEU:HD11	1:B:141:TYR:HB2	1.79	0.65
1:C:17:GLN:HG2	1:C:19:TYR:CE1	2.31	0.65
1:A:57:CYS:HB2	9:A:1311:HOH:O	1.95	0.65
1:A:460:ILE:HD13	1:A:498:ILE:HD11	1.80	0.64
1:C:327:LYS:HD3	3:C:824:PEG:C2	2.28	0.63
2:C:826:SCN:N	9:C:913:HOH:O	2.30	0.63
1:C:105:SER:C	1:C:107:GLU:O	2.41	0.63
1:B:227:GLU:HG3	1:B:229:PRO:HD3	1.80	0.62
1:C:105:SER:O	1:C:107:GLU:O	2.17	0.62
1:C:291:ASP:OD1	4:C:805:GOL:C2	2.46	0.62
1:C:192:GLN:HE21	1:C:193:GLN:H	1.48	0.61
1:C:58:PRO:HD2	9:C:1212:HOH:O	2.01	0.61
1:C:265:ASP:OD2	9:C:906:HOH:O	2.16	0.61
1:A:129:GLY:HA3	3:A:802:PEG:H12	1.82	0.61
1:C:129:GLY:HA2	4:C:809:GOL:H11	1.83	0.61
1:B:706:VAL:O	9:B:907:HOH:O	2.16	0.61
1:C:668:ASN:HD21	3:C:802:PEG:H41	1.67	0.60
1:A:278:LYS:HE3	9:A:1010:HOH:O	2.00	0.60
1:C:207:HIS:CD2	4:C:816:GOL:H2	2.37	0.59
1:C:327:LYS:HD3	3:C:824:PEG:C1	2.33	0.59
1:B:194:ASP:OD2	9:B:908:HOH:O	2.16	0.58
1:C:71:TYR:CZ	1:C:75:LYS:HE2	2.39	0.57
1:C:87:PHE:CE2	1:C:102:VAL:HG23	2.39	0.57
1:A:512:GLU:OE1	9:A:901:HOH:O	2.17	0.57
1:A:118:ILE:HD11	9:A:1220:HOH:O	2.04	0.57
1:B:170:ARG:N	2:B:810:SCN:S	2.68	0.57
1:C:662:ARG:NH2	9:C:917:HOH:O	2.31	0.57
1:A:399:THR:HG21	9:A:1283:HOH:O	2.04	0.56
1:A:221:GLU:CD	9:A:1145:HOH:O	2.48	0.56
1:C:549:THR:HA	1:C:573:CYS:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:668:ASN:ND2	3:C:802:PEG:H41	2.21	0.56
1:A:568:PRO:O	4:A:808:GOL:H2	2.06	0.56
1:B:201:GLU:HG3	9:B:939:HOH:O	2.03	0.56
1:B:87:PHE:CE2	1:B:102:VAL:HG23	2.40	0.56
1:A:164:LEU:HB3	1:A:165:PRO:HD2	1.88	0.56
1:A:251:ILE:HB	1:A:260:ARG:HB2	1.88	0.56
1:A:664:ARG:HB3	1:A:664:ARG:NH1	2.21	0.55
1:A:367:THR:O	9:A:902:HOH:O	2.18	0.55
1:A:71:TYR:CE1	4:A:809:GOL:H31	2.41	0.55
1:C:262:TRP:CZ3	4:C:831[B]:GOL:H12	2.41	0.55
1:C:98:ARG:NH2	2:C:814:SCN:S	2.77	0.54
1:C:428:LYS:HD2	1:C:428:LYS:H	1.72	0.54
1:A:59:ILE:HG12	1:A:701:ALA:CB	2.38	0.54
1:B:417:LEU:N	1:B:417:LEU:HD23	2.22	0.54
1:C:57:CYS:HA	1:C:702:ARG:HD2	1.89	0.53
1:B:639:ASP:OD2	9:B:910:HOH:O	2.19	0.53
1:B:339:GLU:OE1	1:B:359:ASN:ND2	2.42	0.53
1:B:442:TYR:CZ	1:B:533:ALA:HB2	2.44	0.53
1:C:9:VAL:HA	3:C:813:PEG:H22	1.91	0.53
1:C:26:ASP:HB2	9:C:913:HOH:O	2.08	0.53
1:B:430:ILE:HD13	1:B:489:LEU:HB3	1.91	0.53
1:A:384:GLY:HA2	4:A:818:GOL:H2	1.91	0.52
1:B:356:ASP:C	1:B:357:VAL:HG23	2.33	0.52
1:B:430:ILE:HG23	1:B:435:TYR:HE2	1.73	0.52
1:C:547:ARG:CD	3:C:806:PEG:O4	2.57	0.52
1:A:404:PRO:CG	1:A:427:VAL:HG23	2.40	0.52
1:C:327:LYS:HD3	3:C:824:PEG:H11	1.92	0.52
1:C:400:SER:HB2	2:C:820:SCN:N	2.25	0.52
1:C:66:ARG:HG3	1:C:70:LEU:HD12	1.93	0.51
1:A:134[B]:GLU:HG3	1:A:180:HIS:CE1	2.45	0.51
1:A:61:GLY:O	1:A:65[B]:GLU:HG3	2.10	0.51
1:A:591:ILE:O	1:A:591:ILE:HG13	2.09	0.51
1:B:287:GLU:OE1	9:B:911:HOH:O	2.19	0.51
1:A:387:GLY:H	2:A:815:SCN:C	2.24	0.51
1:C:90:TYR:OH	9:C:908:HOH:O	2.19	0.51
1:C:17:GLN:NE2	2:C:825:SCN:S	2.84	0.51
1:A:653:ILE:HG21	1:A:672:ILE:HG21	1.92	0.51
1:C:379:VAL:HG12	2:C:820:SCN:S	2.51	0.50
1:B:546:LYS:HG2	9:B:1210:HOH:O	2.10	0.50
1:C:443:PRO:HD2	2:C:822:SCN:S	2.52	0.50
1:A:134[B]:GLU:HG3	1:A:180:HIS:ND1	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:SER:O	3:A:802:PEG:H21	2.12	0.50
1:A:245:ARG:HG3	1:A:267:GLN:HG3	1.93	0.50
1:C:583:MET:HE1	1:C:599:TYR:CD2	2.47	0.49
1:C:289:GLU:O	1:C:304:THR:HA	2.12	0.49
1:A:634:LEU:HD21	1:A:636:LEU:HD21	1.93	0.49
1:B:57:CYS:HB3	9:B:1024:HOH:O	2.11	0.49
1:A:486:VAL:O	1:A:490:ILE:HG13	2.12	0.49
1:B:642:ASP:HB2	9:B:926:HOH:O	2.11	0.49
1:A:103:GLN:NE2	1:A:105:SER:O	2.35	0.49
1:B:81:LYS:HE3	1:B:86:TYR:CZ	2.48	0.49
1:B:430:ILE:HG23	1:B:435:TYR:CE2	2.47	0.49
1:A:362:GLN:HE22	3:A:804[B]:PEG:H31	1.78	0.49
1:A:547:ARG:HA	1:A:704:LEU:HD13	1.95	0.49
1:B:425:VAL:CB	4:B:806:GOL:H31	2.36	0.48
1:C:416:GLU:CD	1:C:416:GLU:H	2.21	0.48
1:B:227:GLU:HG3	1:B:229:PRO:CD	2.43	0.48
1:C:358:LYS:HG2	1:C:379:VAL:CG1	2.39	0.48
1:A:174:SER:O	3:A:802:PEG:C2	2.61	0.48
1:A:81:LYS:HE2	1:A:83:GLY:O	2.14	0.48
1:A:355:HIS:CB	1:A:360:ILE:HD12	2.43	0.48
1:A:32:GLU:OE1	9:A:903:HOH:O	2.20	0.48
1:A:356:ASP:C	1:A:357:VAL:HG23	2.38	0.48
1:B:536:TYR:CZ	1:B:540:GLU:HG3	2.49	0.48
1:A:170:ARG:NH1	9:A:923:HOH:O	2.37	0.48
1:C:358:LYS:NZ	1:C:439:GLN:OE1	2.47	0.48
1:B:376:PRO:HD2	9:B:1114:HOH:O	2.13	0.48
1:A:375:PHE:CD1	1:A:419:PRO:HG3	2.49	0.47
1:C:57:CYS:HB3	9:C:1212:HOH:O	2.13	0.47
1:A:51:VAL:HB	1:A:52:PRO:HD3	1.95	0.47
1:B:378:ASP:HB3	9:B:1247:HOH:O	2.13	0.47
1:A:621:LYS:HE2	1:A:622:LEU:O	2.15	0.47
1:C:591:ILE:O	1:C:591:ILE:HG13	2.14	0.47
1:A:69:GLU:OE2	4:A:812:GOL:H11	2.15	0.47
1:A:643:ARG:HG2	1:A:680:HIS:CD2	2.50	0.47
1:A:355:HIS:HB3	1:A:360:ILE:HD12	1.97	0.47
1:B:76:TYR:CZ	1:B:90:TYR:CE1	3.03	0.47
1:B:7:PRO:HD3	1:B:49:ILE:CD1	2.45	0.47
1:C:392:THR:HB	1:C:413:THR:CG2	2.45	0.46
1:A:233:LYS:HE2	1:A:593:HIS:HB2	1.97	0.46
1:A:262:TRP:CZ3	4:A:811:GOL:H11	2.50	0.46
1:B:75:LYS:HA	4:B:806:GOL:O2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:ARG:HD2	1:C:151:VAL:CG2	2.45	0.46
1:B:90:TYR:HB3	1:B:101:TYR:CE1	2.51	0.46
1:C:341:ILE:HA	1:C:350:VAL:O	2.15	0.46
1:B:163:GLU:HG2	9:B:1170:HOH:O	2.16	0.46
5:C:821:DMS:H22	9:C:1258:HOH:O	2.15	0.46
1:B:79:HIS:HE1	1:B:423:ARG:HH11	1.64	0.46
1:A:89:PHE:HA	1:A:99:VAL:O	2.16	0.46
1:C:243:ASP:OD2	2:C:801:SCN:N	2.49	0.45
1:C:395:PHE:HA	1:C:408:TYR:O	2.16	0.45
1:B:51:VAL:HB	1:B:52:PRO:HD3	1.98	0.45
1:B:85:ARG:HD2	9:B:985:HOH:O	2.16	0.45
1:C:4:LEU:N	4:C:829:GOL:HO3	2.13	0.45
1:A:664:ARG:HB3	1:A:664:ARG:CZ	2.47	0.45
1:C:30:TRP:CH2	3:C:813:PEG:H31	2.51	0.45
1:C:32:GLU:HG2	1:C:647:LEU:HD22	1.99	0.45
1:A:167:VAL:O	2:A:814:SCN:S	2.75	0.45
1:A:170:ARG:HD3	9:A:1035:HOH:O	2.15	0.45
1:A:262:TRP:HZ3	4:A:811:GOL:H11	1.81	0.45
1:B:87:PHE:CE2	1:B:102:VAL:CG2	3.00	0.45
1:A:622:LEU:HD23	1:A:622:LEU:HA	1.91	0.45
1:B:341:ILE:HA	1:B:350:VAL:O	2.16	0.45
1:B:392:THR:HB	1:B:413:THR:CG2	2.47	0.45
1:B:416:GLU:HB3	1:B:418:GLU:HB2	1.98	0.45
1:A:646:PRO:O	1:A:650:LEU:HG	2.17	0.45
1:A:296:GLU:OE2	1:A:389:LYS:NZ	2.44	0.45
1:C:10:TYR:HA	4:C:812:GOL:H12	1.98	0.45
3:A:804[A]:PEG:H32	3:A:804[A]:PEG:H11	1.44	0.45
1:C:532:CYS:O	2:C:822:SCN:N	2.49	0.44
1:C:553:GLY:HA2	1:C:577:GLN:O	2.17	0.44
1:A:181:ASP:CG	1:A:183:LYS:HG3	2.43	0.44
1:C:75:LYS:NZ	1:C:93:GLY:O	2.51	0.44
1:C:484:TYR:CE2	1:C:486:VAL:HG23	2.52	0.44
1:C:513:THR:O	4:C:807:GOL:O2	2.36	0.44
1:C:14:THR:O	1:C:16[A]:VAL:HG22	2.18	0.44
4:C:805:GOL:H11	9:C:959:HOH:O	2.17	0.44
1:B:89:PHE:HA	1:B:99:VAL:O	2.18	0.44
1:C:706:VAL:HG13	3:C:806:PEG:H22	2.00	0.44
1:B:233:LYS:NZ	9:B:966:HOH:O	2.50	0.44
1:C:416:GLU:HB3	9:C:1446:HOH:O	2.18	0.44
1:A:491:PHE:O	1:A:495:MET:HB2	2.18	0.44
1:B:69:GLU:OE2	1:B:428:LYS:CE	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:HIS:HB3	1:B:336:ASP:O	2.17	0.44
1:A:625:ALA:HB1	1:A:627:ASP:OD1	2.18	0.44
1:C:44:GLU:O	1:C:48:LYS:HG3	2.18	0.43
1:C:662:ARG:NE	9:C:917:HOH:O	2.42	0.43
1:A:426:THR:HA	9:A:926:HOH:O	2.17	0.43
1:B:69:GLU:OE2	1:B:428:LYS:NZ	2.50	0.43
1:B:603:ASP:HB2	2:B:809:SCN:N	2.33	0.43
1:A:335:LYS:NZ	1:A:356:ASP:OD1	2.51	0.43
1:A:404:PRO:HG2	1:A:427:VAL:HG23	2.00	0.43
1:A:425:VAL:HG13	9:A:1269:HOH:O	2.18	0.43
1:B:69:GLU:OE2	1:B:428:LYS:HE2	2.18	0.43
1:B:332:GLU:HG2	1:B:333:HIS:O	2.19	0.43
1:B:351:LEU:N	1:B:351:LEU:HD12	2.33	0.43
1:C:251:ILE:HB	1:C:260:ARG:HB2	2.01	0.43
4:C:829:GOL:C3	9:C:1062:HOH:O	2.66	0.43
1:C:323:GLU:HG3	1:C:326:TRP:CE3	2.53	0.43
1:B:212:TYR:O	1:B:222:ASP:HB3	2.18	0.43
1:C:356:ASP:C	1:C:357:VAL:HG23	2.44	0.43
1:C:87:PHE:CE2	1:C:102:VAL:CG2	3.02	0.43
1:B:79:HIS:HE1	1:B:423:ARG:NH1	2.16	0.43
1:C:440:ILE:C	1:C:440:ILE:HD12	2.44	0.43
1:B:364:HIS:HA	1:B:370:ALA:O	2.18	0.43
1:A:174:SER:O	3:A:802:PEG:O2	2.37	0.43
1:C:176:MET:HG3	4:C:809:GOL:H31	2.01	0.42
1:B:269:GLU:OE2	1:B:278:LYS:HE3	2.19	0.42
1:A:389:LYS:N	9:A:956:HOH:O	2.49	0.42
1:B:491:PHE:CE2	1:B:497:GLY:HA3	2.54	0.42
4:A:812:GOL:C3	9:A:971:HOH:O	2.67	0.42
1:B:404:PRO:HD3	1:B:427:VAL:HG22	2.01	0.42
1:A:460:ILE:CD1	1:A:498:ILE:HD11	2.48	0.42
1:A:473:TYR:CE1	1:A:555:ASN:HB3	2.54	0.42
1:A:583:MET:HE1	1:A:599:TYR:CD2	2.55	0.42
1:C:32:GLU:OE2	1:C:651:LYS:NZ	2.48	0.42
1:A:106:LEU:HA	1:A:106:LEU:HD23	1.82	0.42
1:B:153:ILE:HD11	1:B:171:VAL:HG11	2.02	0.42
1:C:662:ARG:CZ	9:C:917:HOH:O	2.68	0.42
1:C:268:GLN:HE21	1:C:268:GLN:HA	1.84	0.42
1:C:445:LYS:HE2	1:C:445:LYS:HB2	1.90	0.42
1:A:341:ILE:HD11	1:A:349:LEU:HD22	2.02	0.42
1:B:164:LEU:HB3	1:B:165:PRO:CD	2.50	0.42
1:B:245:ARG:HH21	1:B:265:ASP:CG	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:TYR:HB3	1:C:31:LEU:HD12	2.01	0.41
1:C:292:TYR:O	4:C:805:GOL:H2	2.20	0.41
1:C:549:THR:OG1	1:C:573:CYS:HB3	2.20	0.41
1:C:642:ASP:HB2	9:C:935:HOH:O	2.20	0.41
1:A:608:PHE:O	1:A:612:VAL:HG12	2.19	0.41
1:B:466:HIS:HB2	1:B:542:TYR:O	2.20	0.41
1:C:257:PRO:HB3	4:C:804:GOL:H12	2.02	0.41
1:A:582:ASP:OD1	1:A:618:HIS:HE1	2.02	0.41
1:C:20:HIS:HB3	1:C:605:LYS:HG3	2.02	0.41
1:B:247:VAL:O	1:B:263:TYR:HA	2.20	0.41
1:C:491:PHE:O	1:C:495:MET:HB2	2.20	0.41
1:B:365:ASP:O	1:B:369:GLY:N	2.52	0.41
1:C:238:ALA:HA	1:C:248:LEU:O	2.21	0.41
1:C:516:LYS:HA	1:C:519:ILE:HG12	2.02	0.41
1:C:568:PRO:O	3:C:802:PEG:C2	2.69	0.41
1:C:57:CYS:HB2	1:C:698:ALA:HB1	2.03	0.41
1:C:247:VAL:O	1:C:263:TYR:HA	2.21	0.41
1:A:52:PRO:O	1:A:56:GLN:HG3	2.21	0.41
1:B:289:GLU:O	1:B:304:THR:HA	2.20	0.41
1:B:172:LYS:HG2	1:B:173:PHE:CD2	2.55	0.41
1:C:129:GLY:CA	4:C:809:GOL:H11	2.49	0.41
1:C:430:ILE:HG21	1:C:489:LEU:HD13	2.03	0.41
1:A:203:SER:HA	9:A:1183:HOH:O	2.20	0.41
1:A:589:TYR:O	1:A:590:THR:C	2.64	0.41
1:B:38:GLN:N	1:B:38:GLN:CD	2.79	0.41
1:C:373:LYS:HE3	1:C:417:LEU:O	2.21	0.41
1:A:653:ILE:HD11	1:A:670:LEU:C	2.46	0.41
1:B:28:TYR:HB3	1:B:31:LEU:HD12	2.03	0.40
1:B:240:LEU:HD13	1:B:240:LEU:HA	1.94	0.40
1:B:275:GLY:O	1:B:276:ILE:C	2.63	0.40
1:C:51:VAL:HB	1:C:52:PRO:HD3	2.03	0.40
1:B:87:PHE:CZ	1:B:102:VAL:HG23	2.56	0.40
1:C:207:HIS:HB2	9:C:1131:HOH:O	2.20	0.40
1:A:190:TYR:HB3	4:A:803:GOL:H12	2.02	0.40
1:B:270:SER:C	9:B:906:HOH:O	2.64	0.40
1:C:327:LYS:CD	3:C:824:PEG:C1	2.99	0.40
1:C:527:PHE:HD1	1:C:559:LEU:HD12	1.85	0.40
1:B:245:ARG:NH2	1:B:265:ASP:OD2	2.48	0.40
1:A:470:LEU:HB3	1:A:550:ILE:HG22	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:1371:HOH:O	9:C:1424:HOH:O[2_645]	1.98	0.22

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%)	22 (3%)	3 (0%)	30	16
1	B	707/711 (99%)	678 (96%)	26 (4%)	3 (0%)	30	16
1	C	713/711 (100%)	690 (97%)	21 (3%)	2 (0%)	36	23
All	All	2132/2133 (100%)	2055 (96%)	69 (3%)	8 (0%)	30	16

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	357	VAL
1	C	590	THR
1	A	590	THR
1	B	417	LEU
1	B	554	SER
1	A	357	VAL
1	A	554	SER
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%)	599 (96%)	22 (4%)	32	9
1	B	616/617 (100%)	597 (97%)	19 (3%)	35	12
1	C	622/617 (101%)	604 (97%)	18 (3%)	37	14
All	All	1859/1851 (100%)	1800 (97%)	59 (3%)	35	11

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	8	ASP
1	C	16[A]	VAL
1	C	16[B]	VAL
1	C	17	GLN
1	C	23	LYS
1	C	56	GLN
1	C	59	ILE
1	C	261	LEU
1	C	278	LYS
1	C	335	LYS
1	C	341	ILE
1	C	357	VAL
1	C	416	GLU
1	C	426	THR
1	C	428	LYS
1	C	486	VAL
1	C	512	GLU
1	C	598	ASP
1	A	5	GLN
1	A	8	ASP
1	A	14	THR
1	A	16	VAL
1	A	23	LYS
1	A	59	ILE
1	A	84	LYS
1	A	247	VAL
1	A	261	LEU
1	A	270	SER
1	A	307	GLN
1	A	341	ILE
1	A	357	VAL
1	A	417	LEU
1	A	428	LYS
1	A	438	VAL

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Mol	Chain	Res	Type
1	A	445	LYS
1	A	512	GLU
1	A	543	THR
1	A	598	ASP
1	A	622	LEU
1	A	664	ARG
1	B	68	THR
1	B	103	GLN
1	B	107	GLU
1	B	191	PRO
1	B	196	LYS
1	B	203	SER
1	B	220	SER
1	B	357	VAL
1	B	403	SER
1	B	417	LEU
1	B	426	THR
1	B	427	VAL
1	B	504	ILE
1	B	512	GLU
1	B	546	LYS
1	B	547	ARG
1	B	575	ILE
1	B	598	ASP
1	B	664	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	56	GLN
1	C	103	GLN
1	C	192	GLN
1	C	205	ASN
1	C	268	GLN
1	C	285	ASN
1	C	436	GLN
1	C	483	ASN
1	C	524	GLN
1	C	531	GLN
1	C	551	ASN
1	C	566	GLN
1	C	577	GLN

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Mol	Chain	Res	Type
1	A	205	ASN
1	A	362	GLN
1	A	483	ASN
1	A	551	ASN
1	A	577	GLN
1	B	103	GLN
1	B	267	GLN
1	B	388	GLN
1	B	436	GLN
1	B	477	ASN
1	B	555	ASN
1	B	577	GLN
1	B	640	HIS

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 65 ligands modelled in this entry, 1 is monoatomic - leaving 64 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	815	-	6,6,6	0.59	0	5,5,5	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SCN	C	814	-	1,2,2	0.09	0	0,1,1	-	-
2	SCN	A	810	-	1,2,2	0.27	0	0,1,1	-	-
2	SCN	C	826	-	1,2,2	0.38	0	0,1,1	-	-
4	GOL	C	804	-	5,5,5	0.28	0	5,5,5	0.42	0
4	GOL	C	829	-	5,5,5	0.18	0	5,5,5	0.38	0
4	GOL	A	806	-	5,5,5	0.22	0	5,5,5	0.38	0
3	PEG	C	824	-	6,6,6	1.02	0	5,5,5	0.57	0
4	GOL	C	807	-	5,5,5	0.22	0	5,5,5	0.44	0
2	SCN	B	810	-	1,2,2	0.12	0	0,1,1	-	-
4	GOL	A	805	-	5,5,5	0.27	0	5,5,5	0.50	0
4	GOL	C	809	-	5,5,5	0.27	0	5,5,5	0.76	0
4	GOL	C	812	-	5,5,5	0.35	0	5,5,5	0.83	0
4	GOL	A	812	-	5,5,5	0.24	0	5,5,5	0.62	0
2	SCN	C	817	-	1,2,2	0.03	0	0,1,1	-	-
4	GOL	B	805	-	5,5,5	0.22	0	5,5,5	0.19	0
3	PEG	A	802	-	6,6,6	0.47	0	5,5,5	0.33	0
3	PEG	A	804[A]	-	6,6,6	0.31	0	5,5,5	0.21	0
3	PEG	C	808	-	6,6,6	0.22	0	5,5,5	0.07	0
2	SCN	B	811	-	1,2,2	0.69	0	0,1,1	-	-
3	PEG	B	807	-	6,6,6	0.34	0	5,5,5	0.28	0
4	GOL	B	802	-	5,5,5	0.17	0	5,5,5	0.42	0
4	GOL	B	803	-	5,5,5	0.13	0	5,5,5	0.37	0
4	GOL	C	816	-	5,5,5	0.37	0	5,5,5	0.69	0
5	DMS	C	819	-	3,3,3	0.14	0	3,3,3	0.30	0
2	SCN	B	809	-	1,2,2	0.19	0	0,1,1	-	-
4	GOL	A	818	-	5,5,5	0.21	0	5,5,5	0.58	0
4	GOL	C	828	-	5,5,5	0.22	0	5,5,5	0.53	0
4	GOL	C	805	-	5,5,5	0.28	0	5,5,5	0.73	0
4	GOL	A	811	-	5,5,5	0.34	0	5,5,5	0.83	0
2	SCN	A	807	-	1,2,2	0.53	0	0,1,1	-	-
6	A1CRL	C	827	1	32,32,33	1.07	2 (6%)	44,44,46	1.60	10 (22%)
3	PEG	C	802	-	6,6,6	0.62	0	5,5,5	0.60	0
2	SCN	C	818	-	1,2,2	0.11	0	0,1,1	-	-
4	GOL	C	831[B]	-	5,5,5	0.17	0	5,5,5	0.41	0
4	GOL	A	809	-	5,5,5	0.38	0	5,5,5	0.94	0
6	A1CRL	B	812	1	32,32,33	0.76	0	44,44,46	1.45	9 (20%)
5	DMS	A	813	-	3,3,3	0.39	0	3,3,3	0.40	0
2	SCN	C	820	-	1,2,2	0.06	0	0,1,1	-	-
2	SCN	C	825	-	1,2,2	0.13	0	0,1,1	-	-
2	SCN	C	801	-	1,2,2	0.73	0	0,1,1	-	-
2	SCN	A	816	-	1,2,2	0.44	0	0,1,1	-	-
2	SCN	B	804	-	1,2,2	0.84	0	0,1,1	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	B	813	-	5,5,5	0.06	0	5,5,5	0.34	0
5	DMS	C	823	-	3,3,3	0.42	0	3,3,3	0.28	0
2	SCN	C	822	-	1,2,2	1.07	0	0,1,1	-	-
4	GOL	B	806	-	5,5,5	0.19	0	5,5,5	0.66	0
7	B3P	A	801	-	18,18,18	0.47	0	23,23,23	1.03	1 (4%)
2	SCN	A	815	-	1,2,2	0.48	0	0,1,1	-	-
4	GOL	A	808	-	5,5,5	0.08	0	5,5,5	0.21	0
3	PEG	C	813	-	6,6,6	0.71	0	5,5,5	0.66	0
7	B3P	B	801	-	18,18,18	0.37	0	23,23,23	1.16	3 (13%)
4	GOL	A	803	-	5,5,5	0.28	0	5,5,5	1.14	0
4	GOL	C	803	-	5,5,5	0.22	0	5,5,5	0.52	0
4	GOL	C	830	-	5,5,5	0.24	0	5,5,5	0.50	0
5	DMS	C	821	-	3,3,3	0.39	0	3,3,3	0.24	0
5	DMS	B	808	-	3,3,3	0.37	0	3,3,3	0.33	0
4	GOL	C	831[A]	-	5,5,5	0.23	0	5,5,5	0.43	0
2	SCN	A	814	-	1,2,2	0.51	0	0,1,1	-	-
3	PEG	C	806	-	6,6,6	0.30	0	5,5,5	0.28	0
2	SCN	C	811	-	1,2,2	0.49	0	0,1,1	-	-
3	PEG	A	804[B]	-	6,6,6	0.26	0	5,5,5	0.15	0
6	A1CRL	A	817	1	32,32,33	0.92	2 (6%)	44,44,46	1.24	6 (13%)
4	GOL	C	810	-	5,5,5	0.18	0	5,5,5	0.36	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
3	PEG	C	815	-	-	2/4/4/4	-
4	GOL	C	829	-	-	2/4/4/4	-
4	GOL	A	806	-	-	2/4/4/4	-
3	PEG	C	824	-	-	4/4/4/4	-
4	GOL	C	807	-	-	2/4/4/4	-
4	GOL	A	805	-	-	2/4/4/4	-
4	GOL	C	812	-	-	2/4/4/4	-
4	GOL	C	809	-	-	2/4/4/4	-
4	GOL	A	812	-	-	4/4/4/4	-
4	GOL	B	805	-	-	2/4/4/4	-
3	PEG	A	802	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	A	804[A]	-	-	3/4/4/4	-
3	PEG	C	808	-	-	3/4/4/4	-
3	PEG	B	807	-	-	1/4/4/4	-
4	GOL	B	802	-	-	2/4/4/4	-
4	GOL	B	803	-	-	0/4/4/4	-
4	GOL	C	816	-	-	3/4/4/4	-
4	GOL	A	818	-	-	3/4/4/4	-
4	GOL	C	828	-	-	0/4/4/4	-
4	GOL	C	805	-	-	4/4/4/4	-
4	GOL	A	811	-	-	4/4/4/4	-
6	A1CRL	C	827	1	-	8/18/33/33	0/4/4/4
3	PEG	C	802	-	-	3/4/4/4	-
4	GOL	C	831[B]	-	-	0/4/4/4	-
4	GOL	A	809	-	-	2/4/4/4	-
6	A1CRL	B	812	1	-	4/18/33/33	0/4/4/4
4	GOL	B	813	-	-	4/4/4/4	-
4	GOL	B	806	-	-	1/4/4/4	-
7	B3P	A	801	-	-	3/28/28/28	-
4	GOL	A	808	-	-	4/4/4/4	-
3	PEG	C	813	-	-	2/4/4/4	-
7	B3P	B	801	-	-	3/28/28/28	-
4	GOL	A	803	-	-	2/4/4/4	-
4	GOL	C	803	-	-	2/4/4/4	-
4	GOL	C	830	-	-	0/4/4/4	-
4	GOL	C	831[A]	-	-	2/4/4/4	-
3	PEG	C	806	-	-	3/4/4/4	-
4	GOL	C	804	-	-	3/4/4/4	-
3	PEG	A	804[B]	-	-	1/4/4/4	-
6	A1CRL	A	817	1	-	6/18/33/33	0/4/4/4
4	GOL	C	810	-	-	0/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	827	A1CRL	C2-N1	4.07	1.36	1.32
6	A	817	A1CRL	C2-N1	3.25	1.35	1.32
6	A	817	A1CRL	C12-C13	2.23	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	827	A1CRL	C12-C13	2.00	1.42	1.39

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	817	A1CRL	C22-C2-N1	-4.09	109.16	110.76
6	C	827	A1CRL	C22-C2-N1	-4.05	109.17	110.76
6	B	812	A1CRL	C22-C2-N1	-3.79	109.27	110.76
6	C	827	A1CRL	C11-C22-C2	-3.77	103.94	105.15
6	B	812	A1CRL	C3-C4-C5	3.54	122.70	114.85
6	C	827	A1CRL	C3-C4-C5	3.29	122.14	114.85
6	C	827	A1CRL	C4-C5-C6	3.23	120.16	112.05
6	C	827	A1CRL	C21-C22-C2	3.08	139.96	136.72
6	B	812	A1CRL	C21-C22-C2	2.83	139.70	136.72
6	A	817	A1CRL	C3-C4-C5	2.80	121.04	114.85
6	B	812	A1CRL	C2-N1-N2	2.70	108.01	104.97
6	C	827	A1CRL	C4-C5-C10	-2.69	105.29	112.05
6	C	827	A1CRL	C2-N1-N2	2.53	107.82	104.97
6	A	817	A1CRL	C7-C6-C5	2.42	117.18	112.08
7	A	801	B3P	O6-C7-C4	2.31	116.39	111.68
7	B	801	B3P	O6-C7-C4	2.29	116.34	111.68
7	B	801	B3P	C7-C4-N1	2.28	115.83	109.02
6	A	817	A1CRL	C22-C11-N3	-2.20	124.40	127.01
6	B	812	A1CRL	C3-N2-N1	2.19	121.63	119.75
6	B	812	A1CRL	C9-C8-C7	2.18	117.68	111.19
6	A	817	A1CRL	C13-C14-N4	-2.17	112.62	117.12
6	A	817	A1CRL	C2-N1-N2	2.16	107.40	104.97
6	B	812	A1CRL	C11-C22-C2	-2.14	104.46	105.15
6	B	812	A1CRL	C4-C5-C6	2.14	117.44	112.05
6	C	827	A1CRL	O2-C16-N5	-2.14	118.31	122.12
6	C	827	A1CRL	C22-C11-N2	2.08	108.47	107.18
6	C	827	A1CRL	C3-N2-N1	2.06	121.52	119.75
6	B	812	A1CRL	C21-C13-C12	2.04	120.02	117.92
7	B	801	B3P	C7-C4-C5	-2.01	105.62	110.02

There are no chirality outliers.

All (101) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	804	GOL	O1-C1-C2-C3
4	C	805	GOL	O1-C1-C2-C3
4	C	805	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	C	807	GOL	C1-C2-C3-O3
4	C	809	GOL	O1-C1-C2-C3
4	C	812	GOL	C1-C2-C3-O3
4	C	816	GOL	C1-C2-C3-O3
4	C	831[A]	GOL	C1-C2-C3-O3
4	C	831[A]	GOL	O2-C2-C3-O3
4	A	805	GOL	C1-C2-C3-O3
4	A	806	GOL	C1-C2-C3-O3
4	A	808	GOL	O1-C1-C2-C3
4	A	809	GOL	O1-C1-C2-O2
4	A	809	GOL	O1-C1-C2-C3
4	A	811	GOL	O1-C1-C2-O2
4	A	811	GOL	O1-C1-C2-C3
4	A	812	GOL	O1-C1-C2-C3
4	A	812	GOL	C1-C2-C3-O3
4	A	818	GOL	C1-C2-C3-O3
4	B	802	GOL	C1-C2-C3-O3
4	B	805	GOL	C1-C2-C3-O3
6	C	827	A1CRL	C3-C4-C5-C10
6	B	812	A1CRL	C3-C4-C5-C10
3	A	804[A]	PEG	C1-C2-O2-C3
6	A	817	A1CRL	C21-C13-C14-N4
6	A	817	A1CRL	C12-C13-C14-N4
4	C	804	GOL	O1-C1-C2-O2
4	C	805	GOL	O1-C1-C2-O2
4	A	812	GOL	O2-C2-C3-O3
3	C	806	PEG	O2-C3-C4-O4
3	C	808	PEG	O1-C1-C2-O2
3	C	813	PEG	O2-C3-C4-O4
6	C	827	A1CRL	C21-C13-C14-N4
3	C	808	PEG	O2-C3-C4-O4
3	C	815	PEG	O2-C3-C4-O4
3	A	802	PEG	O2-C3-C4-O4
3	C	824	PEG	C4-C3-O2-C2
4	C	803	GOL	O1-C1-C2-C3
4	C	829	GOL	O1-C1-C2-C3
4	A	803	GOL	O1-C1-C2-C3
4	A	808	GOL	C1-C2-C3-O3
4	B	813	GOL	O1-C1-C2-C3
3	C	806	PEG	O1-C1-C2-O2
3	A	804[A]	PEG	O1-C1-C2-O2
4	C	803	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	C	807	GOL	O2-C2-C3-O3
4	C	812	GOL	O2-C2-C3-O3
4	C	829	GOL	O1-C1-C2-O2
4	A	805	GOL	O2-C2-C3-O3
4	A	806	GOL	O2-C2-C3-O3
4	A	808	GOL	O1-C1-C2-O2
4	A	808	GOL	O2-C2-C3-O3
4	A	812	GOL	O1-C1-C2-O2
4	A	818	GOL	O2-C2-C3-O3
4	B	802	GOL	O2-C2-C3-O3
4	B	805	GOL	O2-C2-C3-O3
4	B	813	GOL	O1-C1-C2-O2
6	A	817	A1CRL	C21-C13-C14-O1
6	C	827	A1CRL	C12-C13-C14-N4
7	A	801	B3P	N1-C4-C7-O6
3	C	824	PEG	O2-C3-C4-O4
3	C	824	PEG	O1-C1-C2-O2
6	A	817	A1CRL	C12-C13-C14-O1
6	B	812	A1CRL	C21-C13-C14-N4
4	C	809	GOL	O1-C1-C2-O2
4	C	816	GOL	O2-C2-C3-O3
7	A	801	B3P	C9-C8-N2-C2
6	B	812	A1CRL	C12-C13-C14-N4
6	A	817	A1CRL	N2-C3-C4-C5
4	C	805	GOL	O2-C2-C3-O3
4	A	803	GOL	O1-C1-C2-O2
4	B	806	GOL	O2-C2-C3-O3
4	A	811	GOL	O2-C2-C3-O3
4	A	818	GOL	O1-C1-C2-O2
3	C	802	PEG	O2-C3-C4-O4
6	C	827	A1CRL	C21-C13-C14-O1
4	A	811	GOL	C1-C2-C3-O3
4	B	813	GOL	C1-C2-C3-O3
3	A	804[B]	PEG	O2-C3-C4-O4
3	C	808	PEG	C4-C3-O2-C2
3	A	804[A]	PEG	C4-C3-O2-C2
7	B	801	B3P	C7-C4-C6-O5
7	B	801	B3P	O2-C10-C8-C11
6	C	827	A1CRL	C12-C13-C14-O1
3	C	813	PEG	C1-C2-O2-C3
3	C	802	PEG	C4-C3-O2-C2
7	A	801	B3P	C5-C4-C7-O6

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Mol	Chain	Res	Type	Atoms
4	C	804	GOL	C1-C2-C3-O3
6	C	827	A1CRL	C3-C4-C5-C6
6	A	817	A1CRL	C3-C4-C5-C6
6	B	812	A1CRL	C3-C4-C5-C6
7	B	801	B3P	O2-C10-C8-N2
3	C	815	PEG	C4-C3-O2-C2
6	C	827	A1CRL	N2-C3-C4-C5
3	C	806	PEG	C1-C2-O2-C3
6	C	827	A1CRL	C16-C15-N4-C14
3	B	807	PEG	O2-C3-C4-O4
3	C	824	PEG	C1-C2-O2-C3
4	C	816	GOL	O1-C1-C2-O2
4	B	813	GOL	O2-C2-C3-O3
3	C	802	PEG	C1-C2-O2-C3

There are no ring outliers.

39 monomers are involved in 69 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	814	SCN	1	0
2	C	826	SCN	1	0
4	C	804	GOL	2	0
4	C	829	GOL	2	0
3	C	824	PEG	4	0
4	C	807	GOL	1	0
2	B	810	SCN	1	0
4	C	809	GOL	3	0
4	C	812	GOL	1	0
4	A	812	GOL	2	0
2	C	817	SCN	1	0
3	A	802	PEG	4	0
3	A	804[A]	PEG	1	0
2	B	811	SCN	1	0
4	C	816	GOL	1	0
2	B	809	SCN	1	0
4	A	818	GOL	1	0
4	C	805	GOL	4	0
4	A	811	GOL	2	0
3	C	802	PEG	4	0
4	C	831[B]	GOL	1	0
4	A	809	GOL	1	0
2	C	820	SCN	3	0

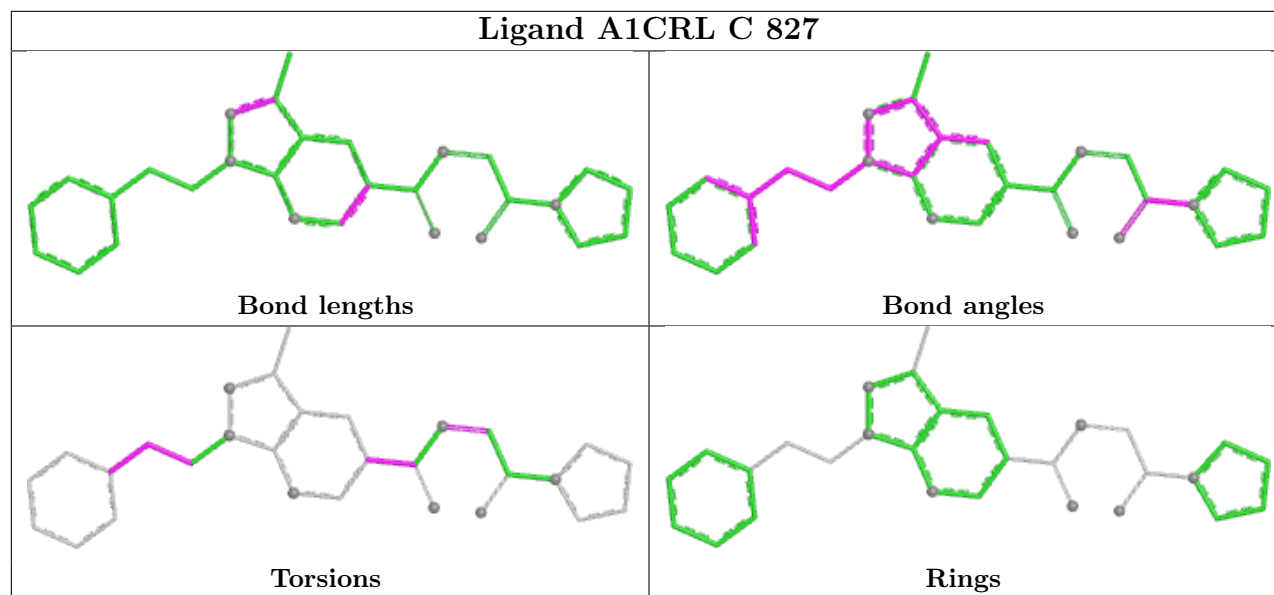
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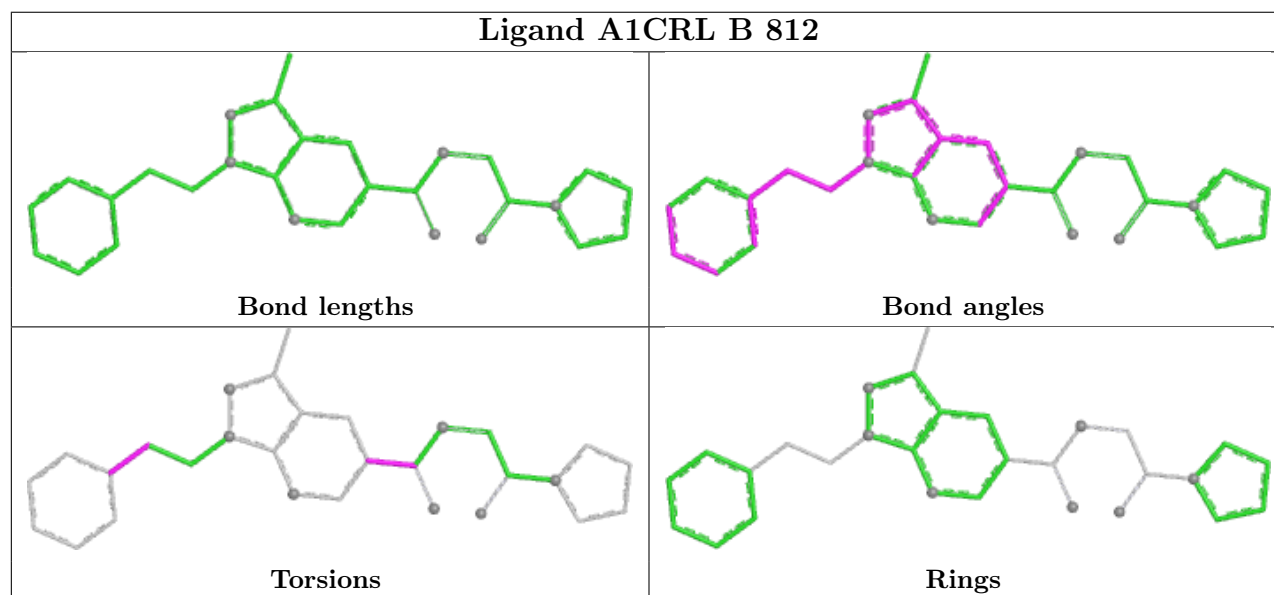
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	825	SCN	1	0
2	C	801	SCN	1	0
2	A	816	SCN	1	0
2	C	822	SCN	2	0
4	B	806	GOL	3	0
7	A	801	B3P	1	0
2	A	815	SCN	1	0
4	A	808	GOL	1	0
3	C	813	PEG	3	0
4	A	803	GOL	1	0
5	C	821	DMS	3	0
2	A	814	SCN	1	0
3	C	806	PEG	3	0
3	A	804[B]	PEG	1	0
6	A	817	A1CRL	1	0
4	C	810	GOL	3	0

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.

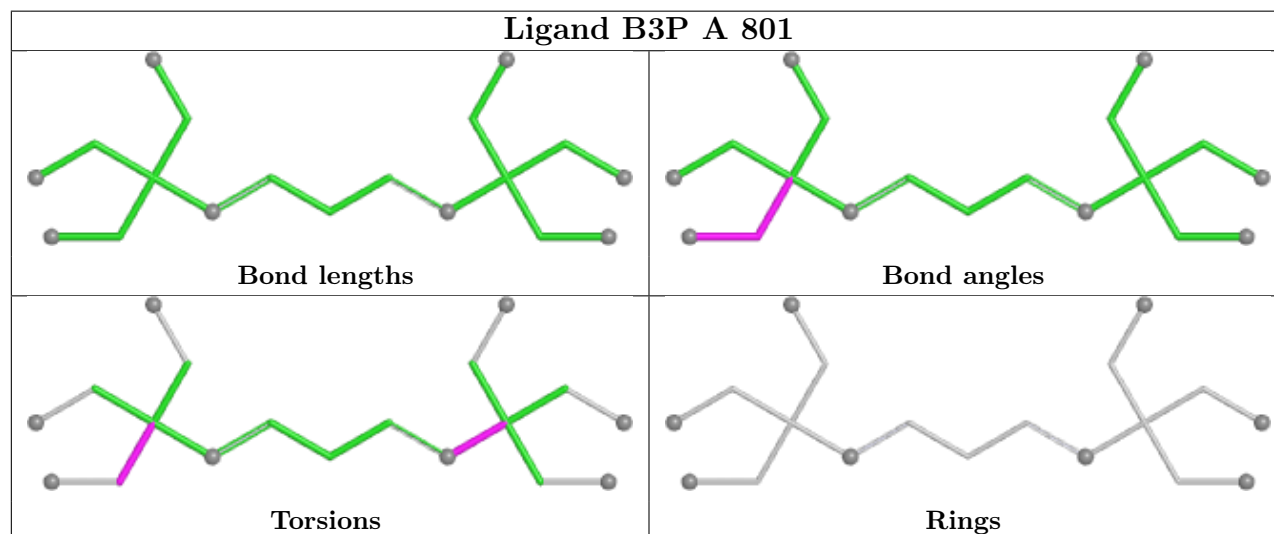
Ligand A1CRL C 827

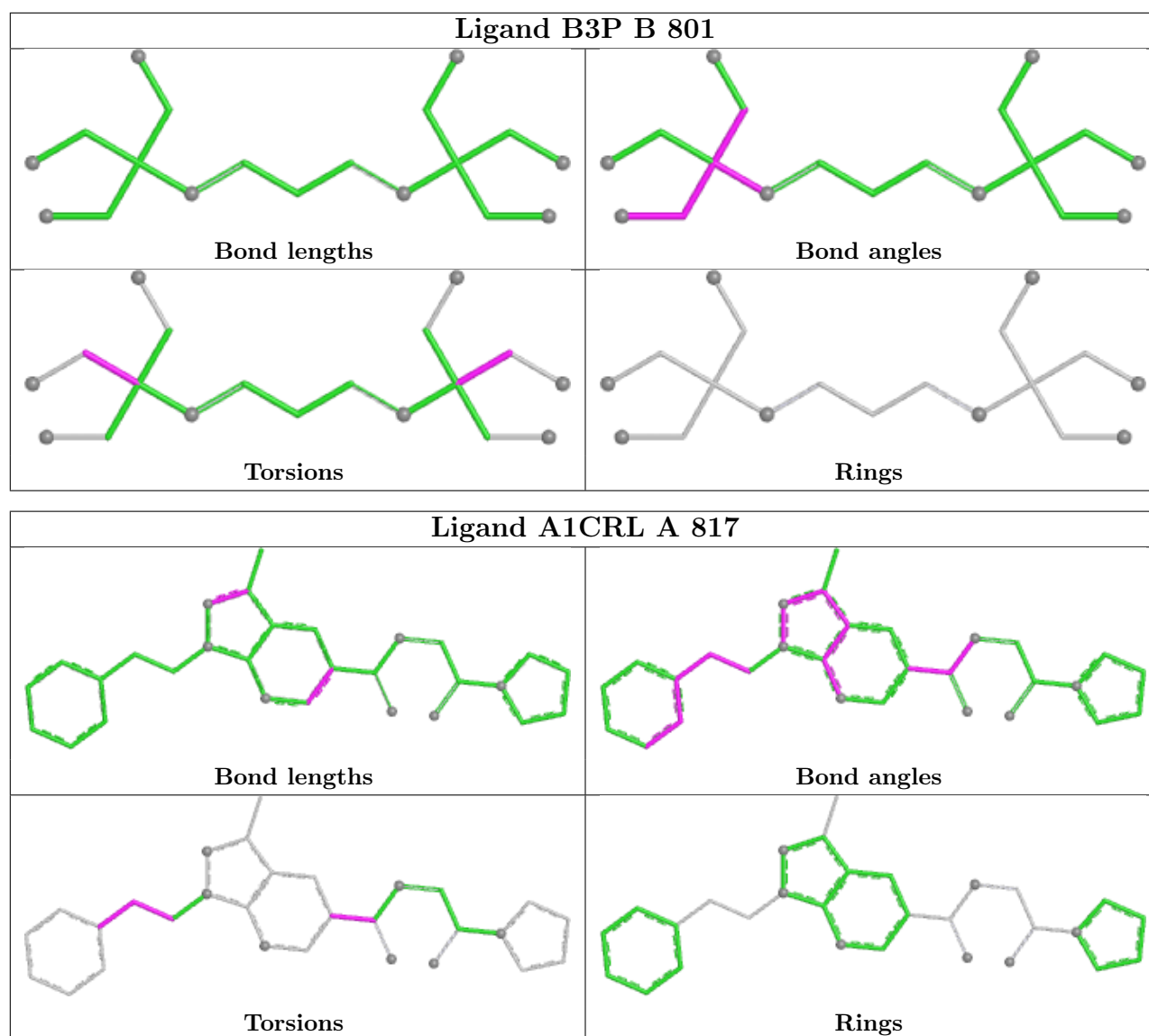


Ligand A1CRL B 812



Ligand B3P A 801





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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%)	-0.62	0 100 100	7, 16, 25, 37	7 (0%)
1	B	707/711 (99%)	-0.40	1 (0%) 92 93	9, 20, 32, 49	2 (0%)
1	C	707/711 (99%)	-0.62	0 100 100	6, 15, 24, 36	8 (1%)
All	All	2121/2133 (99%)	-0.55	1 (0%) 100 100	6, 17, 28, 49	17 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	427	VAL	2.6

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
2	SCN	B	804	3/3	0.82	0.13	25,25,27,34	0
4	GOL	C	829	6/6	0.83	0.09	33,34,37,39	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PEG	A	804[A]	7/7	0.84	0.12	19,21,30,30	17
3	PEG	A	804[B]	7/7	0.84	0.12	16,18,30,30	17
4	GOL	C	816	6/6	0.84	0.16	22,26,30,30	3
3	PEG	C	824	7/7	0.84	0.11	22,27,30,30	2
4	GOL	A	809	6/6	0.84	0.12	18,21,30,30	3
4	GOL	C	831[B]	6/6	0.87	0.09	15,17,33,33	14
4	GOL	C	831[A]	6/6	0.87	0.09	17,20,33,33	14
2	SCN	B	810	3/3	0.88	0.11	32,32,39,43	0
4	GOL	A	811	6/6	0.88	0.12	19,24,30,30	3
4	GOL	A	806	6/6	0.89	0.09	24,27,30,31	3
2	SCN	C	820	3/3	0.89	0.18	26,26,26,30	0
4	GOL	C	809	6/6	0.89	0.15	23,27,30,30	3
4	GOL	B	805	6/6	0.89	0.12	21,25,31,36	3
3	PEG	B	807	7/7	0.90	0.09	30,37,38,38	2
4	GOL	C	803	6/6	0.90	0.10	24,30,32,33	3
4	GOL	C	804	6/6	0.90	0.09	19,25,30,30	3
2	SCN	A	810	3/3	0.90	0.13	27,27,34,42	0
3	PEG	C	813	7/7	0.90	0.12	21,22,30,30	2
3	PEG	C	815	7/7	0.90	0.09	21,23,30,30	2
7	B3P	A	801	19/19	0.90	0.08	18,22,30,30	8
4	GOL	C	812	6/6	0.91	0.10	26,29,30,31	3
3	PEG	C	808	7/7	0.91	0.08	30,36,39,39	2
4	GOL	A	818	6/6	0.91	0.08	23,25,33,33	3
4	GOL	A	805	6/6	0.91	0.07	26,27,30,32	3
4	GOL	B	806	6/6	0.91	0.10	23,26,30,30	3
4	GOL	B	813	6/6	0.91	0.10	26,28,33,35	3
3	PEG	C	802	7/7	0.91	0.10	21,22,30,30	2
4	GOL	A	803	6/6	0.92	0.09	16,20,30,30	3
4	GOL	C	810	6/6	0.92	0.08	27,30,34,35	3
3	PEG	C	806	7/7	0.92	0.07	29,30,31,31	2
4	GOL	B	802	6/6	0.92	0.08	24,28,30,32	3
2	SCN	B	809	3/3	0.93	0.14	38,38,40,43	0
4	GOL	B	803	6/6	0.93	0.07	27,28,30,30	3
3	PEG	A	802	7/7	0.93	0.11	21,24,30,30	2
2	SCN	A	814	3/3	0.94	0.13	17,17,17,18	3
2	SCN	B	811	3/3	0.94	0.11	26,26,33,35	0
4	GOL	A	812	6/6	0.94	0.07	25,28,30,33	3
2	SCN	C	826	3/3	0.94	0.10	24,24,24,28	3
6	A1CRL	B	812	29/30	0.94	0.06	15,17,22,30	3
2	SCN	C	822	3/3	0.94	0.09	18,18,20,29	0
2	SCN	C	818	3/3	0.95	0.12	22,22,26,32	0
4	GOL	C	828	6/6	0.95	0.06	17,19,30,30	3

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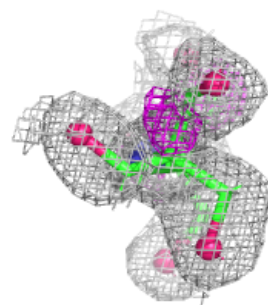
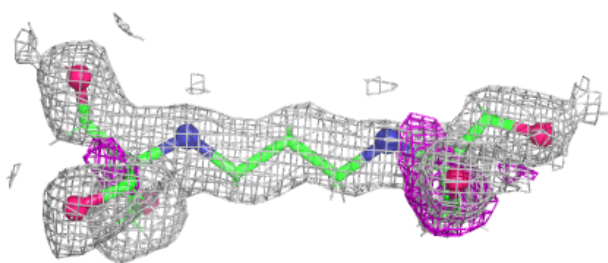
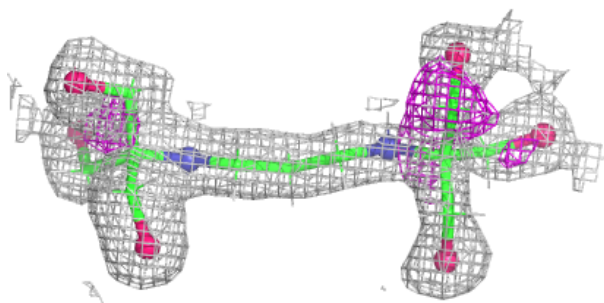
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SCN	A	815	3/3	0.95	0.17	25,25,26,26	0
5	DMS	C	821	4/4	0.95	0.12	26,29,29,31	0
6	A1CRL	A	817	29/30	0.95	0.06	11,15,23,30	3
4	GOL	C	830	6/6	0.95	0.07	21,22,33,33	3
4	GOL	C	805	6/6	0.95	0.07	18,22,30,30	3
4	GOL	C	807	6/6	0.96	0.10	20,22,30,30	3
4	GOL	A	808	6/6	0.96	0.06	20,22,30,30	3
6	A1CRL	C	827	29/30	0.96	0.05	11,13,22,30	3
2	SCN	A	807	3/3	0.96	0.09	20,20,24,30	0
2	SCN	C	811	3/3	0.96	0.06	26,26,28,38	0
2	SCN	C	814	3/3	0.96	0.08	16,16,20,25	0
8	NA	B	814	1/1	0.96	0.06	22,22,22,22	0
2	SCN	C	825	3/3	0.97	0.07	26,26,28,33	0
7	B3P	B	801	19/19	0.97	0.04	13,18,30,30	8
2	SCN	A	816	3/3	0.97	0.07	23,23,26,31	0
2	SCN	C	817	3/3	0.98	0.14	26,26,29,30	0
2	SCN	C	801	3/3	0.98	0.13	22,22,22,23	0
5	DMS	C	823	4/4	0.98	0.10	24,28,31,33	0
5	DMS	C	819	4/4	0.99	0.04	14,15,16,16	0
5	DMS	A	813	4/4	0.99	0.03	13,13,14,14	0
5	DMS	B	808	4/4	0.99	0.04	15,16,17,18	0

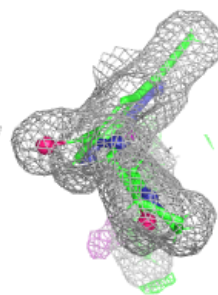
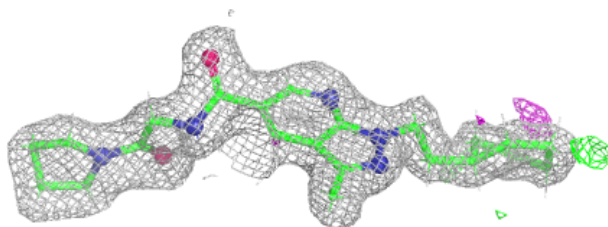
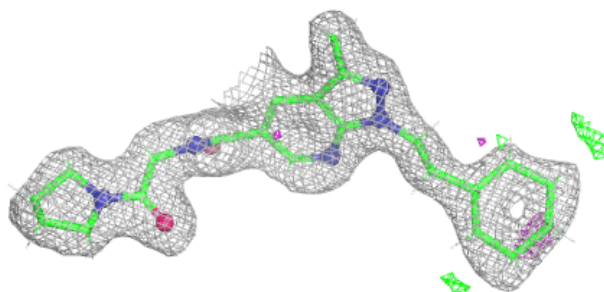
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around B3P A 801:

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

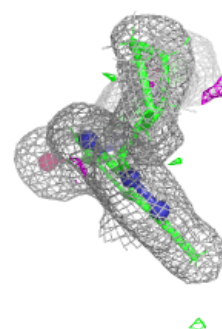
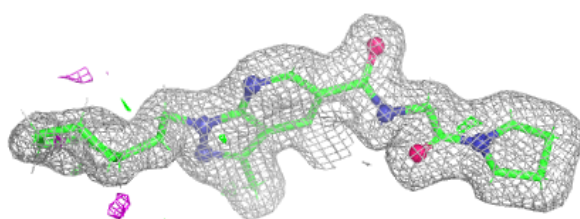
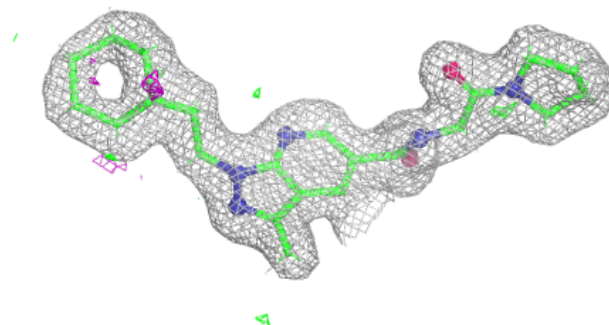
**Electron density around A1CRL B 812:**

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

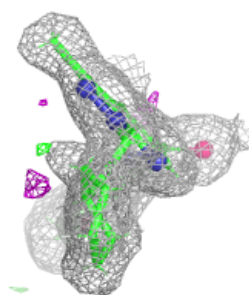
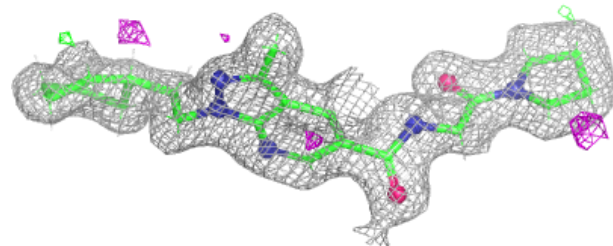
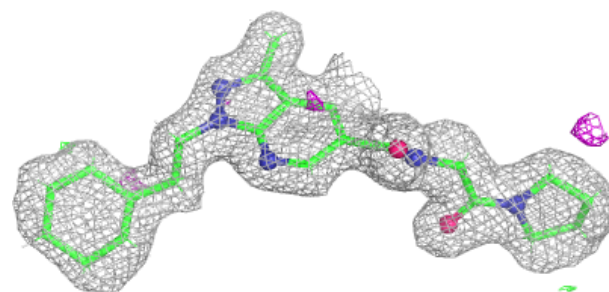


Electron density around A1CRL A 817:

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

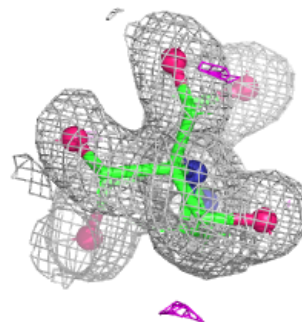
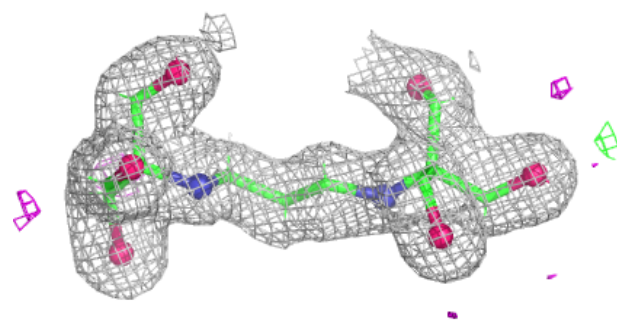
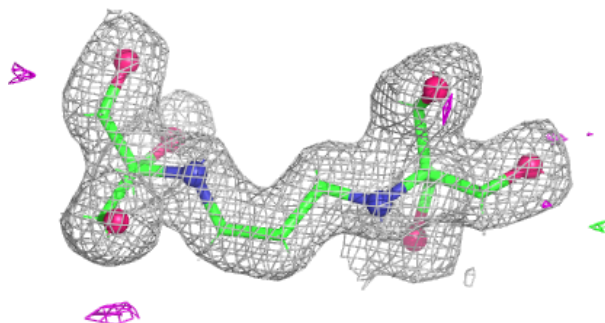
**Electron density around A1CRL C 827:**

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



Electron density around 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.