



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:36 PM UTC

PDB ID : 8DH1 / pdb_00008dh1
Title : T7 RNA polymerase elongation complex with unnatural base dDs-PaTP pair
Authors : Oh, J.; Wang, D.
Deposited on : 2022-06-24
Resolution : 2.65 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

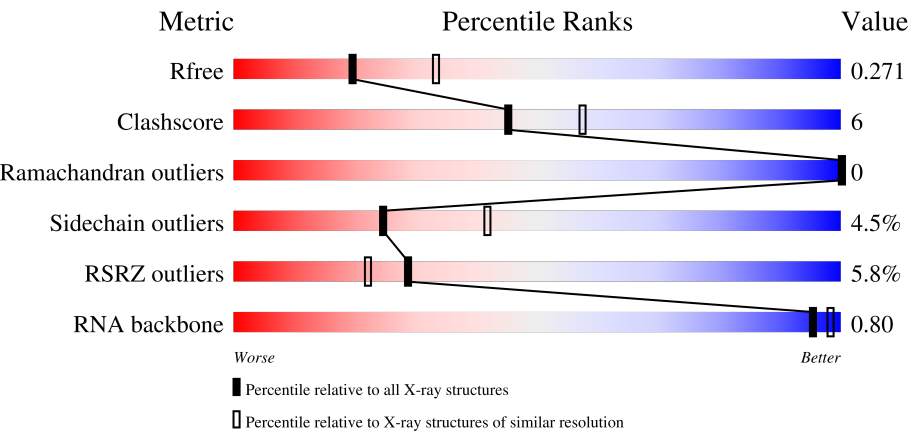
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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.



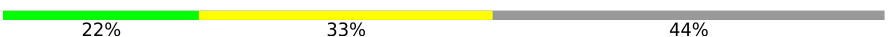
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)
RNA backbone	3983	1090 (2.90-2.42)

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	B	883	4% 83% 14%
1	E	883	5% 73% 15% 11%
1	I	883	7% 73% 19% 7%
1	L	883	5% 67% 12% 20%

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Mol	Chain	Length	Quality of chain
2	A	18	
2	F	18	
2	J	18	
2	M	18	
3	C	12	
3	G	12	
3	K	12	
3	N	12	
4	D	9	
4	H	9	
4	O	9	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 27087 atoms, of which 0 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 T7 RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	855	Total	C	N	O	S	0	0	0
			6719	4280	1169	1235	35			
1	E	785	Total	C	N	O	S	0	0	0
			6125	3908	1060	1125	32			
1	I	825	Total	C	N	O	S	0	0	0
			6478	4133	1118	1192	35			
1	L	702	Total	C	N	O	S	0	0	0
			5358	3402	936	990	30			

- Molecule 2 is a DNA chain called Template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	16	Total	C	N	O	P	S	0	0
			332	160	62	93	16	1		
2	F	17	Total	C	N	O	P	S	0	0
			351	170	67	97	16	1		
2	J	12	Total	C	N	O	P	S	0	0
			248	120	45	70	12	1		
2	M	14	Total	C	N	O	P	S	0	0
			289	140	52	82	14	1		

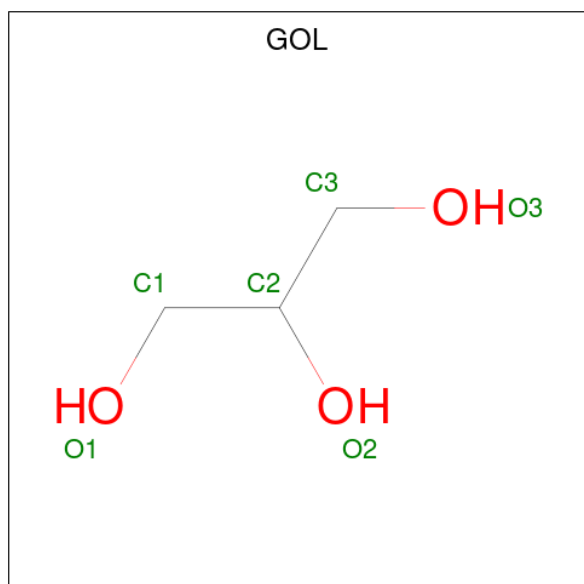
- Molecule 3 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	8	Total	C	N	O	P	0	0
			174	77	33	56	8		
3	G	8	Total	C	N	O	P	0	0
			174	77	33	56	8		
3	K	8	Total	C	N	O	P	0	0
			174	77	33	56	8		
3	N	8	Total	C	N	O	P	0	0
			171	77	33	54	7		

- Molecule 4 is a DNA chain called Non-template strand DNA.

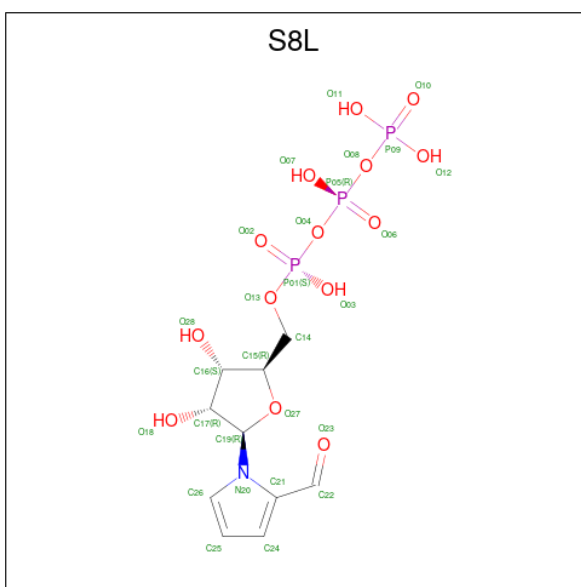
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	6	Total	C	N	O	P	0	0	0
			121	58	20	37	6			
4	H	8	Total	C	N	O	P	0	0	0
			160	77	25	50	8			
4	O	5	Total	C	N	O	P	0	0	0
			102	49	17	31	5			

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	I	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is 1-{5-O-[(S)-hydroxy{[(R)-hydroxy(phosphonooxy)phosphoryl]oxy}phosphoryl]-beta-D-ribofuranosyl}-1H-pyrrole-2-carbaldehyde (CCD ID: S8L) (formula: $C_{10}H_{16}NO_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
6	B	1	Total 28	C 10	N 1	O 14	P 3	0	0

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Mg 1 1	0	0
7	C	1	Total Mg 1 1	0	0

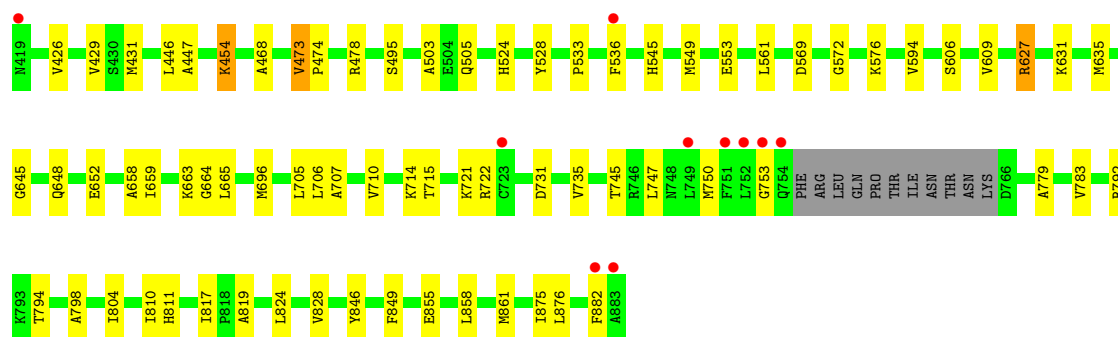
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	38	Total O 38 38	0	0
8	C	3	Total O 3 3	0	0
8	E	14	Total O 14 14	0	0
8	F	1	Total O 1 1	0	0
8	I	4	Total O 4 4	0	0
8	L	2	Total O 2 2	0	0

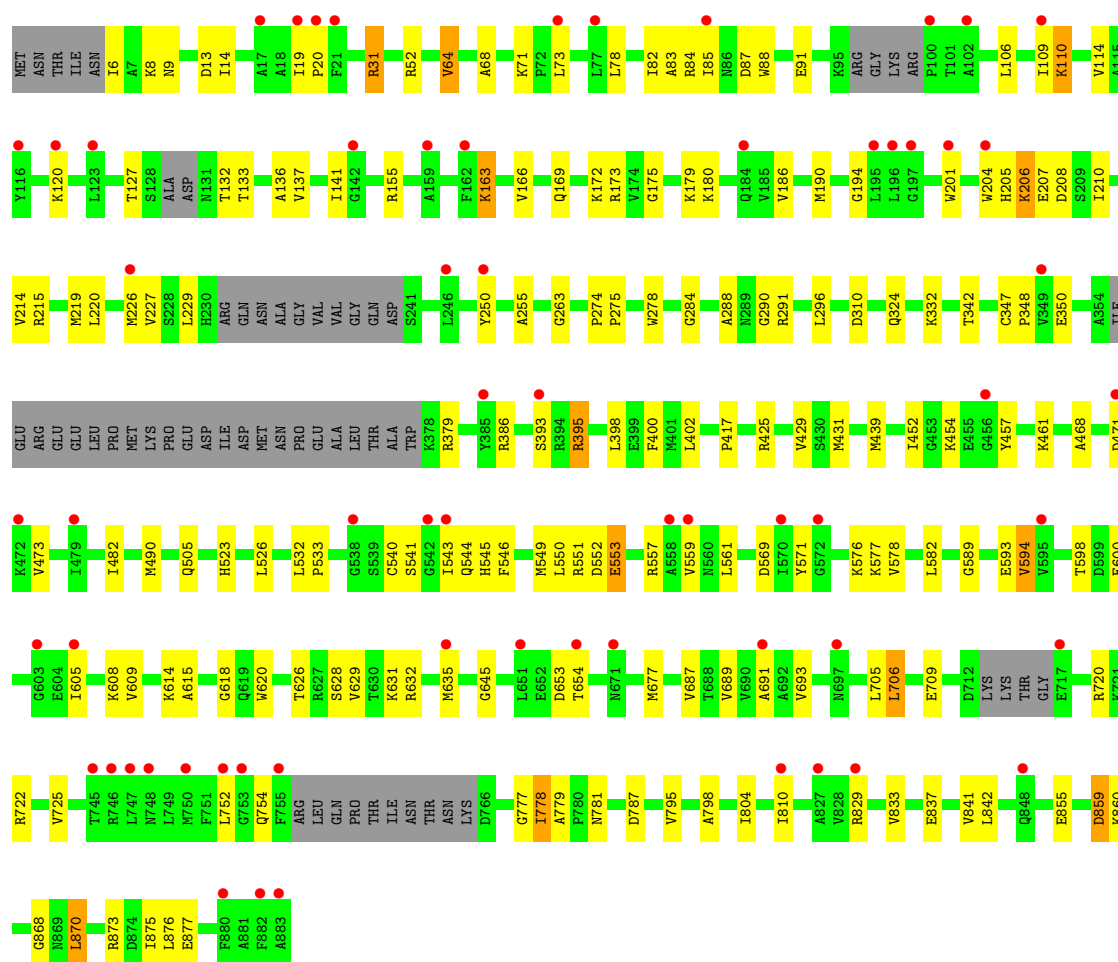
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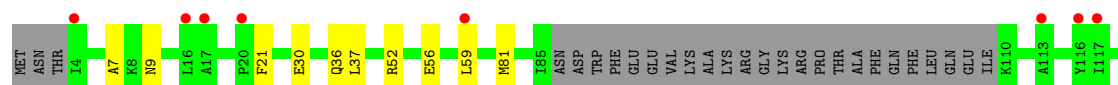
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	O	1	Total	O	0	0
			1	1		

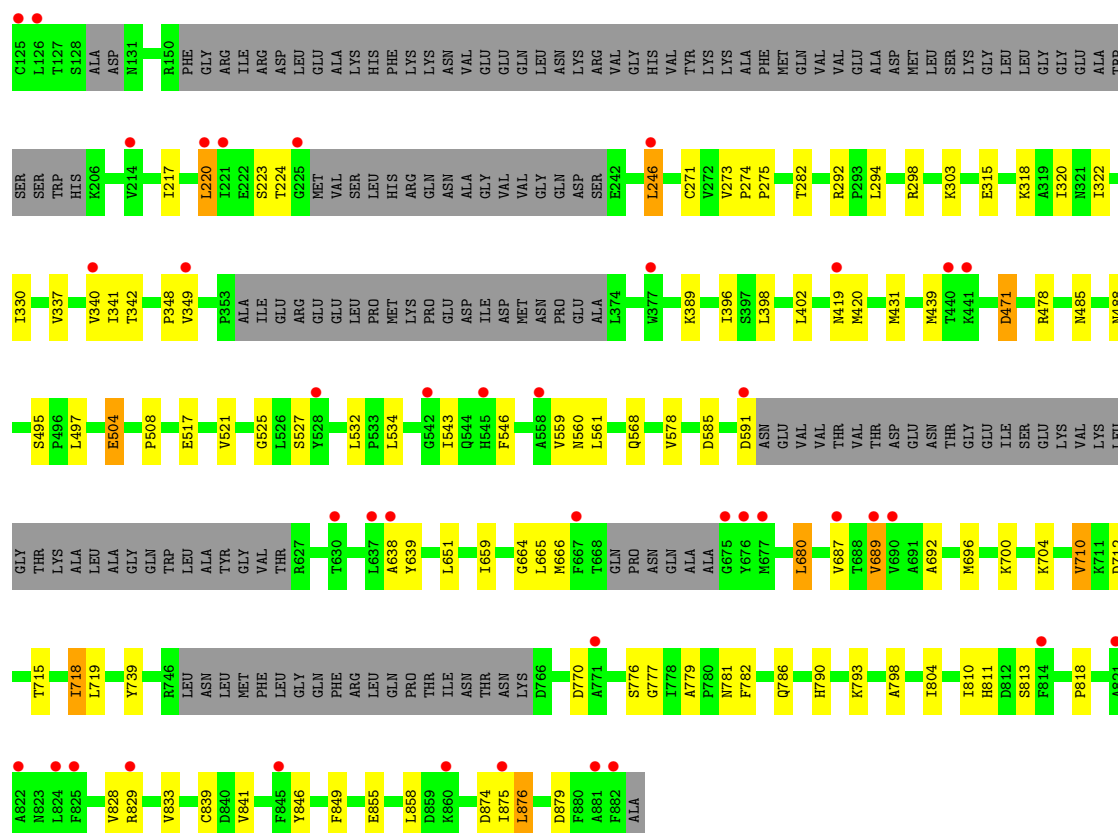


• Molecule 1: T7 RNA polymerase



• Molecule 1: T7 RNA polymerase

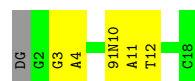




- Molecule 2: Template strand DNA



- Molecule 2: Template strand DNA



- Molecule 2: Template strand DNA



- Molecule 2: Template strand DNA





- Molecule 3: RNA



- Molecule 3: RNA



- Molecule 3: RNA



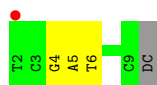
- Molecule 3: RNA



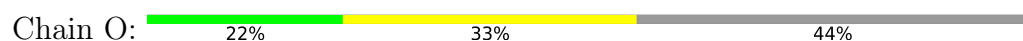
- Molecule 4: Non-template strand DNA



- Molecule 4: Non-template strand DNA



- Molecule 4: Non-template strand DNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	78.87Å 86.16Å 201.68Å 89.85° 85.09° 69.56°	Depositor
Resolution (Å)	39.34 – 2.65 39.34 – 2.65	Depositor EDS
% Data completeness (in resolution range)	89.6 (39.34-2.65) 89.6 (39.34-2.65)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.19	Depositor
R, R_{free}	0.230 , 0.272 0.231 , 0.271	Depositor DCC
R_{free} test set	6388 reflections (4.44%)	wwPDB-VP
Wilson B-factor (Å ²)	65.0	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 69.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	27087	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 91N, MG, S8L, 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	B	0.19	0/6869	0.39	0/9291
1	E	0.18	0/6262	0.37	0/8472
1	I	0.20	0/6623	0.41	0/8957
1	L	0.19	0/5474	0.40	0/7411
2	A	0.23	0/343	0.39	0/524
2	F	0.21	0/365	0.34	0/559
2	J	0.21	0/248	0.37	0/377
2	M	0.20	0/294	0.33	0/448
3	C	0.20	0/194	0.33	0/301
3	G	0.12	0/194	0.21	0/301
3	K	0.12	0/194	0.20	0/301
3	N	0.10	0/191	0.18	0/297
4	D	0.17	0/134	0.35	0/204
4	H	0.18	0/177	0.38	0/270
4	O	0.22	0/113	0.46	0/172
All	All	0.19	0/27675	0.39	0/37885

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	I	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	31	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	B	6719	0	6670	64	0
1	E	6125	0	6043	68	0
1	I	6478	0	6406	106	1
1	L	5358	0	5131	60	0
2	A	332	0	168	4	0
2	F	351	0	180	4	0
2	J	248	0	123	3	0
2	M	289	0	146	2	0
3	C	174	0	88	0	0
3	G	174	0	88	1	0
3	K	174	0	88	1	0
3	N	171	0	89	0	0
4	D	121	0	69	2	0
4	H	160	0	92	2	0
4	O	102	0	58	2	0
5	B	6	0	8	0	0
5	C	6	0	8	0	0
5	I	6	0	8	0	0
6	B	28	0	0	1	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	38	0	0	2	0
8	C	3	0	0	0	0
8	E	14	0	0	0	0
8	F	1	0	0	0	0
8	I	4	0	0	0	0
8	L	2	0	0	0	0
8	O	1	0	0	0	0
All	All	27087	0	25463	309	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 6.

All (309) 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)
6:B:902:S8L:C19	6:B:902:S8L:O27	1.66	1.23
1:I:155:ARG:HA	1:I:163:LYS:HG3	1.63	0.81
1:B:6:ILE:HD12	1:B:291:ARG:HH22	1.50	0.76
1:B:632:ARG:NH1	2:A:10:91N:S8	2.62	0.73
1:I:163:LYS:HA	1:I:166:VAL:HG12	1.70	0.72
1:B:69:ALA:HA	1:B:257:ARG:HG2	1.71	0.72
1:I:19:ILE:HG22	1:I:20:PRO:HD3	1.73	0.71
1:I:169:GLN:HA	1:I:172:LYS:HG3	1.73	0.71
1:L:36:GLN:HE22	1:L:271:CYS:HA	1.56	0.69
1:I:778:ILE:HD12	1:I:779:ALA:H	1.58	0.68
1:I:342:THR:HG22	1:I:348:PRO:HG3	1.76	0.67
1:E:696:MET:HG2	1:E:779:ALA:HB1	1.78	0.66
1:L:798:ALA:HB1	1:L:804:ILE:HD11	1.78	0.66
1:E:159:ALA:HB1	1:E:162:PHE:HB3	1.77	0.65
1:E:707:ALA:O	1:E:722:ARG:NH1	2.29	0.65
1:E:68:ALA:HA	1:E:71:LYS:HG3	1.79	0.64
1:E:798:ALA:HB1	1:E:804:ILE:HD12	1.79	0.64
1:I:166:VAL:HG21	1:I:186:VAL:HG21	1.79	0.64
1:B:154:ILE:HG23	1:B:190:MET:HE1	1.80	0.63
1:B:564:SER:OG	1:B:566:THR:O	2.16	0.63
1:I:68:ALA:HA	1:I:71:LYS:HG3	1.79	0.63
1:L:666:MET:SD	1:L:666:MET:N	2.73	0.62
1:I:594:VAL:HA	1:I:609:VAL:HA	1.81	0.62
1:I:778:ILE:HD12	1:I:779:ALA:N	2.13	0.62
1:L:638:ALA:HA	1:L:696:MET:HE1	1.82	0.60
1:E:51:PHE:HE2	1:E:55:PHE:HD1	1.49	0.60
1:B:159:ALA:O	1:B:163:LYS:N	2.30	0.60
1:E:705:LEU:HD12	1:E:861:MET:HG2	1.84	0.59
1:E:156:ASP:HB3	1:E:157:LEU:HD22	1.84	0.59
1:B:347:CYS:HB3	1:B:350:GLU:HB2	1.85	0.58
1:I:206:LYS:O	1:I:210:ILE:HD12	2.04	0.58
1:L:217:ILE:HA	1:L:220:LEU:HB2	1.85	0.58
1:L:342:THR:HG22	1:L:348:PRO:HG3	1.86	0.58
1:I:829:ARG:HG2	1:I:875:ILE:HG22	1.85	0.58
1:I:14:ILE:HA	1:I:290:GLY:HA2	1.86	0.57
1:I:190:MET:O	1:I:194:GLY:N	2.37	0.57
1:I:754:GLN:N	1:I:754:GLN:OE1	2.37	0.57
1:E:109:ILE:HG13	1:E:153:ARG:HH22	1.70	0.56
1:E:122:THR:O	1:E:126:LEU:HD22	2.06	0.56
1:L:471:ASP:O	1:L:478:ARG:NH2	2.38	0.56
1:B:804:ILE:HG12	1:B:820:ASP:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:6:ILE:HD11	1:I:52:ARG:CZ	2.36	0.56
1:I:398:LEU:HG	1:I:439:MET:HE1	1.88	0.56
1:I:275:PRO:HG2	1:I:324:GLN:HB3	1.88	0.55
1:I:64:VAL:HG21	1:I:127:THR:HG21	1.87	0.55
1:I:543:ILE:HA	1:I:546:PHE:HB2	1.87	0.55
1:B:602:THR:HG23	1:B:604:GLU:H	1.72	0.55
1:I:577:LYS:HE2	1:I:687:VAL:HG21	1.88	0.55
1:E:536:PHE:HB3	1:E:882:PHE:HB3	1.89	0.54
1:E:349:VAL:HG12	1:E:503:ALA:HB1	1.88	0.54
1:L:7:ALA:O	1:L:52:ARG:NH1	2.41	0.54
1:E:248:PRO:HA	1:E:251:ALA:HB3	1.90	0.54
1:L:349:VAL:HG21	1:L:508:PRO:HG3	1.88	0.54
1:E:44:TYR:HA	1:E:266:PRO:HB3	1.90	0.54
1:E:81:MET:HE3	1:E:85:ILE:HD11	1.89	0.54
1:B:215:ARG:HH21	1:B:219:MET:HE1	1.72	0.53
1:E:110:LYS:HD2	1:E:111:PRO:HD2	1.89	0.53
1:I:777:GLY:O	1:I:781:ASN:ND2	2.41	0.53
1:I:347:CYS:HB2	1:I:350:GLU:HB2	1.91	0.53
1:E:648:GLN:NE2	1:E:652:GLU:OE2	2.41	0.53
1:B:599:ASP:HB2	1:B:602:THR:HG22	1.90	0.53
1:B:677:MET:HE2	1:B:681:ILE:HG13	1.90	0.53
1:E:180:LYS:HG3	1:E:750:MET:HE3	1.91	0.53
1:I:417:PRO:HG2	1:I:429:VAL:HB	1.89	0.53
1:E:645:GLY:HA3	2:F:10:91N:OP2	2.08	0.53
1:I:626:THR:HG23	1:I:628:SER:H	1.74	0.53
1:I:169:GLN:NE2	1:I:169:GLN:H	2.06	0.52
1:I:582:LEU:HD21	1:I:620:TRP:HB3	1.91	0.52
1:L:340:VAL:HG11	1:L:497:LEU:HD21	1.91	0.52
1:E:48:GLU:HG2	1:E:262:ALA:HB1	1.92	0.52
1:E:118:THR:O	1:E:122:THR:OG1	2.23	0.52
1:B:50:ARG:HH12	1:B:431:MET:HE1	1.73	0.52
1:E:84:ARG:HD3	1:E:223:SER:HB3	1.91	0.52
1:B:468:ALA:HA	1:B:505:GLN:HB3	1.90	0.52
1:E:117:ILE:O	1:E:121:THR:OG1	2.26	0.52
1:I:798:ALA:HB1	1:I:804:ILE:HD12	1.91	0.52
1:I:837:GLU:OE2	1:I:873:ARG:NH2	2.43	0.52
1:L:485:ASN:HB3	1:L:488:ASN:HB2	1.92	0.52
1:E:706:LEU:HD11	1:E:849:PHE:HB2	1.91	0.52
1:E:30:GLU:OE1	1:E:34:ARG:NH1	2.43	0.51
1:I:629:VAL:HA	1:I:654:THR:HG21	1.93	0.51
1:L:36:GLN:OE1	1:L:273:VAL:HG12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:561:LEU:HB2	1:L:875:ILE:HD12	1.93	0.51
1:L:689:VAL:HG22	1:L:692:ALA:H	1.75	0.51
1:I:645:GLY:HA3	2:J:10:91N:OP2	2.11	0.51
1:L:318:LYS:O	1:L:322:ILE:HG13	2.12	0.50
1:L:81:MET:HE2	1:L:220:LEU:HD22	1.92	0.50
1:B:118:THR:HG22	1:B:141:ILE:HG21	1.92	0.50
1:I:207:GLU:CD	1:I:207:GLU:H	2.20	0.50
1:L:639:TYR:HE2	2:M:11:DA:C4	2.28	0.50
1:E:123:LEU:H	1:E:123:LEU:HD12	1.77	0.50
1:I:220:LEU:HD12	1:I:227:VAL:HG22	1.94	0.50
1:B:332:LYS:NZ	1:B:409:ALA:O	2.45	0.49
1:B:839:CYS:SG	8:B:1037:HOH:O	2.60	0.49
1:I:705:LEU:O	1:I:720:ARG:NH2	2.45	0.49
1:B:76:THR:HG23	1:B:77:LEU:HD12	1.93	0.49
1:B:84:ARG:NH1	1:B:222:GLU:OE1	2.46	0.49
1:B:379:ARG:NH2	1:B:660:ASP:OD1	2.45	0.49
1:B:686:SER:HA	1:B:693:VAL:HG21	1.93	0.49
1:I:615:ALA:O	1:I:618:GLY:N	2.41	0.49
1:L:560:ASN:HD21	1:L:568:GLN:H	1.59	0.49
1:B:118:THR:O	1:B:122:THR:HG22	2.13	0.49
1:B:226:MET:HA	1:B:250:TYR:HD1	1.78	0.49
1:I:550:LEU:HD21	1:I:842:LEU:HD12	1.94	0.49
1:E:347:CYS:HB3	1:E:350:GLU:HB2	1.95	0.48
1:I:632:ARG:NH1	1:I:653:ASP:OD1	2.46	0.48
1:I:551:ARG:HB2	1:I:868:GLY:H	1.78	0.48
1:I:578:VAL:HG11	1:I:677:MET:HE1	1.95	0.48
1:I:571:TYR:OH	1:I:635:MET:HE2	2.12	0.48
1:L:320:ILE:HD11	1:L:420:MET:HE3	1.96	0.48
1:E:173:ARG:O	1:E:179:LYS:NZ	2.47	0.48
1:B:59:LEU:HD12	1:B:64:VAL:HG12	1.96	0.48
1:B:163:LYS:O	1:B:167:GLU:N	2.47	0.48
1:I:8:LYS:HD2	1:I:9:ASN:H	1.79	0.48
1:I:461:LYS:HG2	1:I:482:ILE:HG21	1.95	0.48
1:L:710:VAL:HG22	1:L:719:LEU:HB2	1.95	0.48
1:B:148:GLU:OE2	1:B:746:ARG:NH2	2.47	0.47
1:L:829:ARG:HD3	1:L:875:ILE:HG22	1.96	0.47
1:E:386:ARG:HE	3:G:4:G:H5'	1.79	0.47
1:I:6:ILE:HD11	1:I:52:ARG:NE	2.29	0.47
1:I:87:ASP:OD2	1:I:88:TRP:N	2.47	0.47
1:I:137:VAL:O	1:I:141:ILE:HG13	2.13	0.47
1:L:517:GLU:HG3	1:L:532:LEU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:VAL:HG12	1:B:503:ALA:HB1	1.97	0.47
1:B:709:GLU:HB2	1:B:722:ARG:HH11	1.78	0.47
1:E:524:HIS:HB2	1:E:528:TYR:HB2	1.96	0.47
1:I:210:ILE:O	1:I:214:VAL:HG23	2.14	0.47
1:I:82:ILE:HD12	1:I:83:ALA:N	2.29	0.47
1:L:855:GLU:HA	1:L:858:LEU:HD13	1.96	0.47
1:E:545:HIS:O	1:E:549:MET:HG3	2.15	0.47
1:L:521:VAL:O	1:L:525:GLY:N	2.46	0.47
1:E:446:LEU:HG	1:E:533:PRO:HG3	1.97	0.47
1:B:24:LEU:HD11	1:B:273:VAL:HG21	1.95	0.47
1:I:571:TYR:CE1	1:I:635:MET:HE2	2.49	0.47
1:B:446:LEU:HD13	1:B:806:SER:HB3	1.97	0.47
1:I:6:ILE:HG22	1:I:255:ALA:HA	1.96	0.47
1:I:706:LEU:HD23	1:I:725:VAL:HG22	1.96	0.47
1:I:543:ILE:HD13	1:I:689:VAL:HG11	1.97	0.47
1:L:559:VAL:HG13	1:L:561:LEU:HD23	1.96	0.47
1:E:400:PHE:CZ	1:E:431:MET:HE2	2.50	0.46
1:E:561:LEU:HG	1:E:875:ILE:HD12	1.95	0.46
1:E:747:LEU:HA	1:E:753:GLY:HA3	1.97	0.46
1:I:332:LYS:HB2	1:I:332:LYS:HE2	1.71	0.46
1:I:608:LYS:HA	1:I:608:LYS:HD3	1.79	0.46
1:I:169:GLN:HB2	1:I:173:ARG:HH12	1.81	0.46
1:I:454:LYS:HG2	1:I:526:LEU:HD21	1.97	0.46
1:I:709:GLU:HG3	1:I:722:ARG:HG2	1.97	0.46
1:I:829:ARG:HD3	1:I:875:ILE:O	2.16	0.46
1:B:137:VAL:O	1:B:141:ILE:HG13	2.16	0.46
1:I:84:ARG:HG3	1:I:219:MET:HE2	1.96	0.46
1:I:133:THR:HG23	1:I:136:ALA:H	1.81	0.46
2:J:10:91N:O5'	2:J:10:91N:C2'	2.63	0.46
1:E:794:THR:HG21	1:E:828:VAL:HG22	1.98	0.46
1:I:31:ARG:HA	1:I:31:ARG:HD3	1.58	0.46
1:I:78:LEU:O	1:I:82:ILE:HG13	2.16	0.46
1:I:263:GLY:HA3	1:I:291:ARG:HH21	1.79	0.46
1:I:571:TYR:CD1	1:I:631:LYS:HA	2.50	0.46
1:I:576:LYS:HD3	1:I:576:LYS:HA	1.71	0.46
1:L:659:ILE:HD13	1:L:664:GLY:HA3	1.97	0.46
1:L:777:GLY:O	1:L:781:ASN:ND2	2.47	0.46
1:I:545:HIS:O	1:I:549:MET:HG3	2.15	0.46
1:I:14:ILE:O	1:I:288:ALA:HB1	2.16	0.46
1:I:468:ALA:HA	1:I:505:GLN:HB3	1.97	0.46
1:B:50:ARG:NH1	1:B:431:MET:HE1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:712:ASP:OD1	1:L:715:THR:OG1	2.32	0.46
1:E:478:ARG:HH12	1:E:882:PHE:HZ	1.63	0.46
1:I:226:MET:HA	1:I:250:TYR:HD2	1.81	0.46
1:I:278:TRP:CD2	1:I:284:GLY:HA3	2.51	0.46
1:I:490:MET:HE1	1:I:523:HIS:HE1	1.81	0.46
4:O:3:DC:H2''	4:O:4:DG:C8	2.52	0.46
1:I:274:PRO:HA	1:I:275:PRO:HD3	1.86	0.45
1:B:303:LYS:NZ	1:I:310:ASP:OD1	2.49	0.45
1:B:692:ALA:O	1:B:696:MET:HG3	2.16	0.45
1:L:874:ASP:OD2	1:L:874:ASP:N	2.48	0.45
2:A:5:DA:H61	4:D:6:DT:H3	1.64	0.45
1:B:596:THR:HA	1:B:607:GLU:HG2	1.99	0.45
1:B:829:ARG:NH2	1:B:882:PHE:H	2.14	0.45
1:E:294:LEU:HD21	1:E:429:VAL:HG11	1.99	0.45
1:B:281:ILE:HD11	1:B:308:TYR:HB2	1.99	0.45
1:E:569:ASP:CG	1:E:627:ARG:HH21	2.24	0.45
1:E:855:GLU:HA	1:E:858:LEU:HD23	1.99	0.45
1:I:13:ASP:OD1	1:I:291:ARG:NH1	2.49	0.45
1:I:400:PHE:CE2	1:I:431:MET:HE2	2.52	0.45
1:I:833:VAL:HG21	1:I:876:LEU:HG	1.98	0.45
1:E:24:LEU:HD12	1:E:24:LEU:HA	1.82	0.45
1:E:658:ALA:HB1	1:E:663:LYS:HB3	1.98	0.45
1:B:721:LYS:HD2	1:B:722:ARG:H	1.82	0.45
1:B:857:GLN:HA	1:B:860:LYS:HD3	1.99	0.45
2:F:3:DG:H2''	2:F:4:DA:C8	2.52	0.45
1:E:824:LEU:O	1:E:828:VAL:HG23	2.17	0.45
1:I:82:ILE:O	1:I:85:ILE:N	2.47	0.45
1:L:700:LYS:NZ	1:L:779:ALA:H	2.15	0.45
4:D:4:DG:H2''	4:D:5:DA:H5''	1.99	0.44
1:B:854:HIS:H	1:B:857:GLN:HE21	1.65	0.44
1:I:425:ARG:NH1	1:I:787:ASP:OD2	2.50	0.44
1:E:721:LYS:HD2	1:E:722:ARG:H	1.82	0.44
1:B:59:LEU:HA	1:B:64:VAL:HG12	1.99	0.44
1:L:471:ASP:OD1	1:L:471:ASP:N	2.50	0.44
1:I:206:LYS:H	1:I:206:LYS:HG2	1.51	0.44
1:E:329:LYS:HE2	1:E:447:ALA:HA	1.99	0.44
2:J:14:DG:H2'	2:J:15:DC:C6	2.53	0.44
1:L:292:ARG:HH12	1:L:294:LEU:HD23	1.82	0.44
1:L:389:LYS:HD2	1:L:389:LYS:HA	1.78	0.44
1:L:398:LEU:HG	1:L:439:MET:HE1	2.00	0.44
1:L:790:HIS:NE2	1:L:828:VAL:O	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:LEU:HD13	1:B:287:TRP:CD2	2.52	0.44
1:E:342:THR:HG22	1:E:348:PRO:HG3	1.99	0.44
1:E:731:ASP:OD1	1:E:792:ARG:NE	2.44	0.44
1:E:72:PRO:HG3	1:E:257:ARG:HD2	2.00	0.44
1:I:490:MET:HE1	1:I:523:HIS:CE1	2.53	0.44
1:L:56:GLU:HA	1:L:59:LEU:HD12	1.99	0.43
1:I:226:MET:HA	1:I:250:TYR:CD2	2.53	0.43
1:L:829:ARG:HD2	1:L:876:LEU:HA	1.99	0.43
1:B:269:GLN:O	1:B:286:TYR:OH	2.29	0.43
1:B:551:ARG:NH2	1:B:836:TYR:O	2.51	0.43
1:B:557:ARG:HB2	1:B:562:LEU:HD12	2.00	0.43
1:E:126:LEU:HD11	1:E:244:ILE:HG23	1.99	0.43
1:I:540:CYS:O	1:I:544:GLN:HB2	2.18	0.43
1:I:180:LYS:HB2	1:I:180:LYS:HE2	1.65	0.43
1:I:205:HIS:HB2	1:I:208:ASP:HB2	1.99	0.43
1:I:386:ARG:NH2	3:K:4:G:OP1	2.52	0.43
1:L:739:TYR:O	1:L:770:ASP:N	2.43	0.43
1:B:21:PHE:HE2	1:B:34:ARG:HG3	1.84	0.43
1:B:92:VAL:HA	1:B:95:LYS:HE2	2.00	0.43
1:I:52:ARG:HA	1:I:52:ARG:HD2	1.76	0.43
1:B:831:THR:O	1:B:835:THR:HG23	2.18	0.43
1:L:431:MET:H	1:L:431:MET:HG2	1.59	0.43
1:B:812:ASP:OD1	1:B:812:ASP:N	2.50	0.43
1:E:153:ARG:HA	1:E:153:ARG:HD3	1.69	0.43
1:E:561:LEU:HG	1:E:875:ILE:CD1	2.49	0.43
1:I:395:ARG:HE	1:I:395:ARG:HB2	1.58	0.43
1:L:274:PRO:HA	1:L:275:PRO:HD3	1.90	0.43
1:B:342:THR:HG22	1:B:348:PRO:HG3	2.01	0.43
1:E:122:THR:HG23	1:E:141:ILE:HD11	2.00	0.43
1:L:704:LYS:HD2	4:O:5:DA:H5"	2.00	0.43
1:L:543:ILE:HA	1:L:546:PHE:HB2	1.99	0.42
1:B:265:SER:O	1:B:265:SER:OG	2.33	0.42
1:B:846:TYR:HA	1:B:849:PHE:CE2	2.54	0.42
1:E:402:LEU:HD12	1:E:402:LEU:HA	1.88	0.42
1:L:846:TYR:HA	1:L:849:PHE:CE2	2.54	0.42
1:B:463:HIS:HE1	8:B:1011:HOH:O	2.02	0.42
1:B:796:VAL:O	1:B:800:GLU:HG3	2.20	0.42
1:E:817:ILE:HD12	1:E:819:ALA:H	1.83	0.42
2:A:14:DG:H2'	2:A:15:DC:C6	2.54	0.42
1:I:559:VAL:HG13	1:I:561:LEU:HG	2.00	0.42
2:M:13:DC:H2'	2:M:14:DG:H8	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:468:ALA:HA	1:E:505:GLN:HB3	2.02	0.42
1:I:532:LEU:HD12	1:I:533:PRO:HD2	2.01	0.42
1:B:739:TYR:OH	2:A:12:DT:OP1	2.32	0.42
4:H:4:DG:H2''	4:H:5:DA:H5'	2.01	0.42
1:I:589:GLY:HA3	1:I:614:LYS:HD2	2.02	0.42
1:L:303:LYS:HD2	1:L:303:LYS:HA	1.77	0.42
1:B:60:LYS:HE3	1:B:60:LYS:HB2	1.79	0.42
1:I:859:ASP:HB2	1:I:860:LYS:HE2	2.02	0.42
1:L:718:ILE:O	1:L:718:ILE:HD12	2.20	0.42
1:B:582:LEU:HD22	1:B:617:ALA:HA	2.00	0.42
1:B:721:LYS:HD2	1:B:722:ARG:N	2.34	0.42
1:E:659:ILE:HG13	1:E:664:GLY:HA3	2.02	0.42
1:I:110:LYS:NZ	1:I:155:ARG:HH12	2.18	0.42
1:L:546:PHE:CE2	1:L:696:MET:HE2	2.54	0.42
1:E:163:LYS:HA	1:E:166:VAL:HG12	2.02	0.42
1:I:631:LYS:O	1:I:635:MET:HG2	2.20	0.42
1:E:572:GLY:O	1:E:576:LYS:HG2	2.20	0.41
1:B:274:PRO:HA	1:B:275:PRO:HD3	1.93	0.41
1:B:281:ILE:HD13	1:B:281:ILE:HA	1.86	0.41
1:B:576:LYS:O	1:B:580:GLU:HG3	2.20	0.41
1:L:223:SER:OG	1:L:224:THR:N	2.52	0.41
1:L:504:GLU:H	1:L:504:GLU:HG2	1.60	0.41
1:E:454:LYS:HE2	1:E:454:LYS:HB3	1.89	0.41
2:F:4:DA:N6	4:H:6:DT:O4	2.53	0.41
1:I:571:TYR:CZ	1:I:635:MET:HE2	2.54	0.41
1:L:298:ARG:HE	1:L:419:ASN:HB3	1.85	0.41
1:L:330:ILE:HD13	1:L:330:ILE:HA	1.85	0.41
1:I:215:ARG:O	1:I:219:MET:HG3	2.20	0.41
1:I:452:ILE:HG12	1:I:457:TYR:HB2	2.02	0.41
1:L:534:LEU:HD11	1:L:818:PRO:HB3	2.02	0.41
1:I:169:GLN:H	1:I:169:GLN:CD	2.28	0.41
1:I:471:ASP:OD1	1:I:471:ASP:N	2.53	0.41
1:L:782:PHE:O	1:L:786:GLN:HG2	2.20	0.41
1:E:110:LYS:HD2	1:E:110:LYS:HA	1.89	0.41
1:I:175:GLY:O	1:I:179:LYS:HG2	2.21	0.41
1:L:21:PHE:HZ	1:L:30:GLU:HG3	1.85	0.41
1:L:315:GLU:O	1:L:793:LYS:NZ	2.52	0.41
1:L:879:ASP:OD2	1:L:879:ASP:N	2.54	0.41
1:B:663:LYS:HD3	1:B:664:GLY:H	1.85	0.41
1:E:291:ARG:H	1:E:291:ARG:HG3	1.64	0.41
1:E:846:TYR:HA	1:E:849:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:342:THR:HG21	1:L:402:LEU:HD11	2.03	0.41
1:E:473:VAL:HG22	1:E:474:PRO:HD2	2.03	0.41
1:E:631:LYS:O	1:E:635:MET:HG3	2.21	0.41
1:I:82:ILE:HD12	1:I:83:ALA:H	1.85	0.41
1:I:552:ASP:HB2	1:I:691:ALA:HB3	2.03	0.41
1:L:810:ILE:HB	1:L:813:SER:HB3	2.02	0.41
1:E:141:ILE:HG22	1:E:145:ILE:HD11	2.02	0.40
1:I:19:ILE:H	1:I:19:ILE:HG13	1.63	0.40
1:I:551:ARG:HA	1:I:870:LEU:HD23	2.01	0.40
1:I:229:LEU:HD12	1:I:229:LEU:HA	1.90	0.40
1:I:550:LEU:HD12	1:I:691:ALA:HB1	2.03	0.40
1:I:553:GLU:O	1:I:557:ARG:HG3	2.22	0.40
1:B:106:LEU:HD23	1:B:106:LEU:HA	1.91	0.40
1:E:150:ARG:HB2	1:E:201:TRP:HB3	2.02	0.40
1:E:193:LYS:HA	1:E:193:LYS:HD2	1.79	0.40
1:L:341:ILE:HG13	1:L:348:PRO:HB3	2.03	0.40
1:B:517:GLU:HG3	1:B:532:LEU:HB2	2.03	0.40
2:F:11:DA:H2'	2:F:12:DT:C6	2.57	0.40
1:I:201:TRP:O	1:I:204:TRP:HB2	2.22	0.40
1:E:207:GLU:H	1:E:207:GLU:HG3	1.65	0.40
1:L:246:LEU:H	1:L:246:LEU:HG	1.53	0.40
1:L:578:VAL:HG23	1:L:680:LEU:HB3	2.02	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)
1:I:31:ARG:NH2	1:I:194:GLY:O[1_655]	2.16	0.04

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	B	847/883 (96%)	830 (98%)	17 (2%)	0	100	100
1	E	773/883 (88%)	757 (98%)	16 (2%)	0	100	100
1	I	811/883 (92%)	791 (98%)	20 (2%)	0	100	100
1	L	684/883 (78%)	666 (97%)	18 (3%)	0	100	100
All	All	3115/3532 (88%)	3044 (98%)	71 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	698/729 (96%)	675 (97%)	23 (3%)	33	55
1	E	628/729 (86%)	599 (95%)	29 (5%)	24	41
1	I	673/729 (92%)	637 (95%)	36 (5%)	20	35
1	L	528/729 (72%)	502 (95%)	26 (5%)	22	38
All	All	2527/2916 (87%)	2413 (96%)	114 (4%)	24	42

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3	THR
1	B	19	ILE
1	B	109	ILE
1	B	133	THR
1	B	157	LEU
1	B	174	VAL
1	B	202	SER
1	B	228	SER
1	B	243	THR
1	B	454	LYS
1	B	477	GLU
1	B	565	GLU
1	B	578	VAL

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Mol	Chain	Res	Type
1	B	596	THR
1	B	598	THR
1	B	634	VAL
1	B	641	SER
1	B	687	VAL
1	B	720	ARG
1	B	735	VAL
1	B	745	THR
1	B	749	LEU
1	B	783	VAL
1	E	27	HIS
1	E	74	ILE
1	E	120	LYS
1	E	121	THR
1	E	153	ARG
1	E	154	ILE
1	E	186	VAL
1	E	193	LYS
1	E	208	ASP
1	E	325	ASN
1	E	426	VAL
1	E	454	LYS
1	E	473	VAL
1	E	495	SER
1	E	553	GLU
1	E	594	VAL
1	E	606	SER
1	E	609	VAL
1	E	627	ARG
1	E	665	LEU
1	E	710	VAL
1	E	714	LYS
1	E	715	THR
1	E	735	VAL
1	E	745	THR
1	E	783	VAL
1	E	810	ILE
1	E	811	HIS
1	E	876	LEU
1	I	64	VAL
1	I	73	LEU
1	I	91	GLU

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Mol	Chain	Res	Type
1	I	106	LEU
1	I	109	ILE
1	I	110	LYS
1	I	114	VAL
1	I	120	LYS
1	I	132	THR
1	I	163	LYS
1	I	206	LYS
1	I	296	LEU
1	I	379	ARG
1	I	393	SER
1	I	395	ARG
1	I	402	LEU
1	I	473	VAL
1	I	541	SER
1	I	553	GLU
1	I	569	ASP
1	I	593	GLU
1	I	594	VAL
1	I	598	THR
1	I	600	GLU
1	I	605	ILE
1	I	693	VAL
1	I	706	LEU
1	I	752	LEU
1	I	778	ILE
1	I	795	VAL
1	I	810	ILE
1	I	841	VAL
1	I	855	GLU
1	I	859	ASP
1	I	870	LEU
1	I	877	GLU
1	L	9	ASN
1	L	37	LEU
1	L	220	LEU
1	L	246	LEU
1	L	282	THR
1	L	337	VAL
1	L	396	ILE
1	L	471	ASP
1	L	495	SER

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Mol	Chain	Res	Type
1	L	504	GLU
1	L	527	SER
1	L	585	ASP
1	L	591	ASP
1	L	651	LEU
1	L	665	LEU
1	L	680	LEU
1	L	687	VAL
1	L	689	VAL
1	L	710	VAL
1	L	718	ILE
1	L	776	SER
1	L	811	HIS
1	L	833	VAL
1	L	839	CYS
1	L	841	VAL
1	L	876	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	5	ASN
1	B	135	GLN
1	B	233	ASN
1	B	346	HIS
1	B	404	GLN
1	B	463	HIS
1	B	499	ASN
1	B	583	GLN
1	B	648	GLN
1	B	772	HIS
1	B	857	GLN
1	E	27	HIS
1	E	165	ASN
1	E	529	ASN
1	E	799	HIS
1	E	869	ASN
1	I	161	HIS
1	I	169	GLN
1	I	289	ASN
1	I	404	GLN
1	I	410	ASN

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Mol	Chain	Res	Type
1	I	523	HIS
1	I	524	HIS
1	I	671	ASN
1	I	737	GLN
1	I	744	GLN
1	L	588	ASN
1	L	649	GLN
1	L	786	GLN
1	L	799	HIS
1	L	871	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	7/12 (58%)	0	0
3	G	7/12 (58%)	0	0
3	K	7/12 (58%)	0	0
3	N	7/12 (58%)	0	0
All	All	28/48 (58%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\# Z > 2$
5	GOL	B	901	-	5,5,5	1.10	0	5,5,5	1.05	0
5	GOL	C	101	-	5,5,5	0.96	0	5,5,5	1.10	0
5	GOL	I	901	-	5,5,5	1.06	0	5,5,5	0.99	0
6	S8L	B	902	7	27,29,29	4.41	12 (44%)	38,45,45	1.22	7 (18%)

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
5	GOL	B	901	-	-	0/4/4/4	-
5	GOL	C	101	-	-	2/4/4/4	-
5	GOL	I	901	-	-	0/4/4/4	-
6	S8L	B	902	7	-	12/24/40/40	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	902	S8L	O27-C19	10.76	1.66	1.42
6	B	902	S8L	P01-O04	8.09	1.68	1.59
6	B	902	S8L	O27-C15	-7.88	1.27	1.45
6	B	902	S8L	P05-O08	7.69	1.67	1.59
6	B	902	S8L	C17-C19	-7.55	1.29	1.53
6	B	902	S8L	P05-O04	7.02	1.67	1.59
6	B	902	S8L	P09-O10	5.24	1.66	1.50
6	B	902	S8L	C22-C21	4.60	1.53	1.44
6	B	902	S8L	O28-C16	-4.43	1.32	1.43
6	B	902	S8L	O18-C17	4.17	1.53	1.43
6	B	902	S8L	P09-O11	-2.65	1.44	1.54
6	B	902	S8L	P09-O12	-2.49	1.45	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	902	S8L	C15-O27-C19	-2.72	103.47	109.47
6	B	902	S8L	C16-C17-C19	2.53	106.25	101.46
6	B	902	S8L	O23-C22-C21	-2.37	121.17	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	902	S8L	O07-P05-O06	-2.20	102.23	112.44
6	B	902	S8L	C26-N20-C21	-2.14	107.83	109.18
6	B	902	S8L	O12-P09-O08	2.08	111.61	104.64
6	B	902	S8L	O11-P09-O08	2.04	111.46	104.64

There are no chirality outliers.

All (14) torsion outliers are listed below:

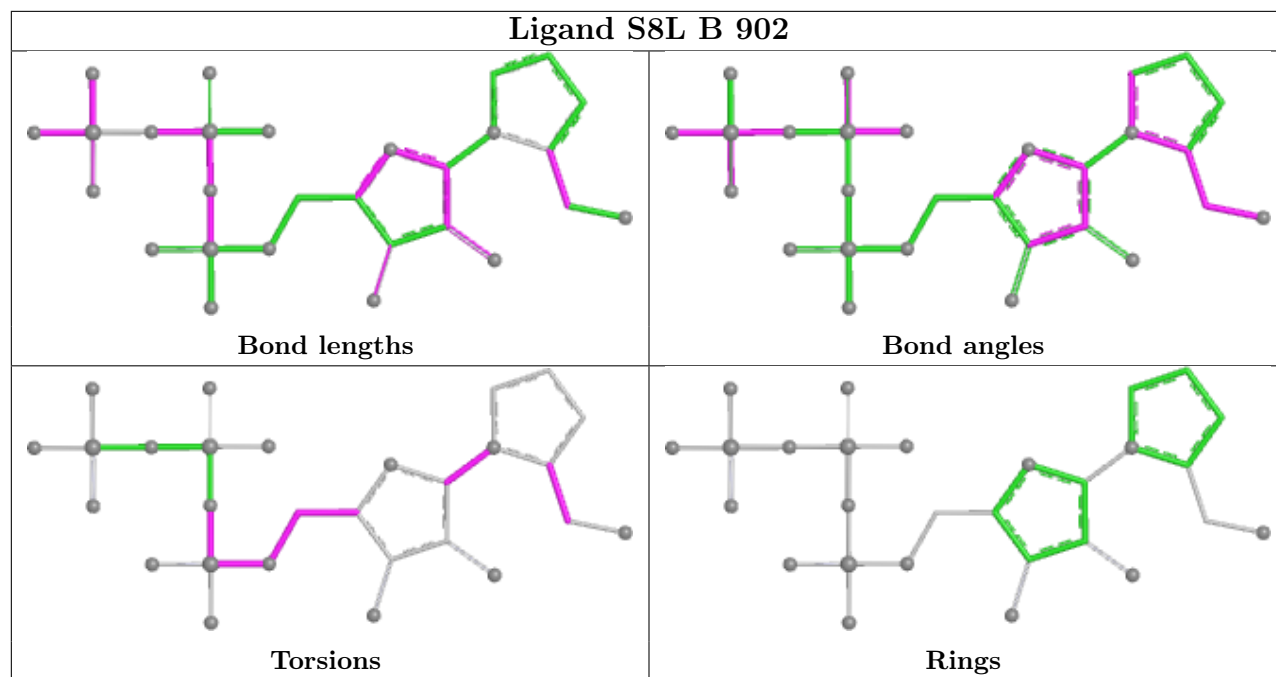
Mol	Chain	Res	Type	Atoms
5	C	101	GOL	C1-C2-C3-O3
6	B	902	S8L	C15-C14-O13-P01
6	B	902	S8L	C24-C21-C22-O23
6	B	902	S8L	N20-C21-C22-O23
6	B	902	S8L	O13-C14-C15-C16
5	C	101	GOL	O2-C2-C3-O3
6	B	902	S8L	O13-C14-C15-O27
6	B	902	S8L	C17-C19-N20-C26
6	B	902	S8L	C14-O13-P01-O02
6	B	902	S8L	C14-O13-P01-O03
6	B	902	S8L	C14-O13-P01-O04
6	B	902	S8L	P05-O04-P01-O03
6	B	902	S8L	O27-C19-N20-C26
6	B	902	S8L	P05-O04-P01-O02

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	902	S8L	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.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	B	855/883 (96%)	0.20	32 (3%)	45	37	39, 68, 134, 215	0
1	E	785/883 (88%)	0.39	46 (5%)	28	21	45, 76, 169, 252	0
1	I	825/883 (93%)	0.70	64 (7%)	19	14	59, 104, 167, 218	0
1	L	702/883 (79%)	0.74	48 (6%)	23	17	69, 114, 171, 267	0
2	A	15/18 (83%)	0.01	0	100	100	52, 71, 237, 239	0
2	F	16/18 (88%)	0.03	0	100	100	62, 110, 248, 259	0
2	J	11/18 (61%)	-0.01	0	100	100	70, 79, 176, 202	0
2	M	13/18 (72%)	0.23	0	100	100	90, 107, 176, 182	0
3	C	8/12 (66%)	-0.33	0	100	100	52, 63, 72, 83	0
3	G	8/12 (66%)	-0.57	0	100	100	59, 77, 119, 140	0
3	K	8/12 (66%)	-0.01	0	100	100	77, 94, 120, 141	0
3	N	8/12 (66%)	0.08	0	100	100	88, 107, 161, 177	0
4	D	6/9 (66%)	0.82	0	100	100	211, 225, 229, 241	0
4	H	8/9 (88%)	0.93	1 (12%)	8	6	182, 197, 224, 234	0
4	O	5/9 (55%)	0.98	0	100	100	204, 210, 212, 223	0
All	All	3273/3679 (88%)	0.48	191 (5%)	29	22	39, 93, 168, 267	0

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	752	LEU	6.9
1	E	752	LEU	6.1
1	L	125	CYS	5.5
1	I	883	ALA	5.0
1	E	195	LEU	4.8
1	I	17	ALA	4.5
1	B	2	ASN	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	752	LEU	4.4
1	I	196	LEU	4.4
1	B	244	ILE	4.1
1	I	542	GLY	4.0
1	E	119	ILE	4.0
1	I	20	PRO	3.9
1	I	120	LYS	3.9
1	B	122	THR	3.9
1	I	753	GLY	3.8
1	E	753	GLY	3.6
1	L	377	TRP	3.5
1	E	182	PHE	3.5
1	B	641	SER	3.4
1	L	558	ALA	3.4
1	B	6	ILE	3.3
1	I	385	TYR	3.3
1	I	100	PRO	3.3
1	B	374	LEU	3.3
1	L	113	ALA	3.2
1	E	246	LEU	3.2
1	I	558	ALA	3.2
1	L	246	LEU	3.2
1	B	158	GLU	3.2
1	I	605	ILE	3.2
1	L	882	PHE	3.2
1	L	630	THR	3.1
1	E	212	VAL	3.1
1	I	747	LEU	3.1
1	L	225	GLY	3.1
1	E	883	ALA	3.1
1	B	7	ALA	3.0
1	B	746	ARG	3.0
1	I	142	GLY	3.0
1	B	126	LEU	3.0
1	E	20	PRO	3.0
1	I	748	ASN	3.0
1	E	536	PHE	3.0
1	I	755	PHE	2.9
1	I	85	ILE	2.9
1	I	651	LEU	2.9
1	I	882	PHE	2.9
1	L	825	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	L	20	PRO	2.9
1	B	215	ARG	2.9
1	E	19	ILE	2.9
1	I	19	ILE	2.9
1	I	195	LEU	2.9
1	I	543	ILE	2.9
1	I	102	ALA	2.9
1	E	882	PHE	2.9
1	I	559	VAL	2.9
1	E	190	MET	2.8
1	L	542	GLY	2.8
1	B	113	ALA	2.8
1	E	165	ASN	2.8
1	E	244	ILE	2.8
1	E	258	ALA	2.8
1	I	880	PHE	2.8
1	L	220	LEU	2.7
1	B	3	THR	2.7
1	L	16	LEU	2.7
1	L	676	TYR	2.7
1	I	570	ILE	2.7
1	E	166	VAL	2.7
1	I	116	TYR	2.7
1	L	824	LEU	2.6
1	I	21	PHE	2.6
1	I	159	ALA	2.6
1	I	393	SER	2.6
1	E	355	ILE	2.6
1	I	109	ILE	2.6
1	L	845	PHE	2.6
1	E	751	PHE	2.6
1	I	201	TRP	2.5
1	L	677	MET	2.5
1	L	116	TYR	2.5
1	E	169	GLN	2.5
1	E	186	VAL	2.5
1	I	595	VAL	2.5
1	L	440	THR	2.5
1	L	4	ILE	2.5
1	L	441	LYS	2.5
1	L	17	ALA	2.5
1	I	572	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	691	ALA	2.5
1	I	479	ILE	2.4
1	E	18	ALA	2.4
1	L	814	PHE	2.4
1	L	821	ALA	2.4
1	I	246	LEU	2.4
1	I	226	MET	2.4
1	B	608	LYS	2.4
1	E	754	GLN	2.4
1	L	689	VAL	2.4
1	B	536	PHE	2.4
1	B	131	ASN	2.4
1	I	848	GLN	2.4
1	E	393	SER	2.4
1	I	204	TRP	2.4
1	B	753	GLY	2.4
1	L	667	PHE	2.4
1	E	162	PHE	2.3
1	E	354	ALA	2.3
1	I	827	ALA	2.3
1	L	221	ILE	2.3
1	B	243	THR	2.3
1	I	717	GLU	2.3
1	I	456	GLY	2.3
1	L	340	VAL	2.3
1	B	157	LEU	2.3
1	L	829	ARG	2.3
1	E	723	CYS	2.3
1	B	882	PHE	2.3
1	I	73	LEU	2.3
1	I	77	LEU	2.3
1	L	117	ILE	2.3
1	E	54	MET	2.3
1	I	472	LYS	2.3
1	I	654	THR	2.3
1	I	745	THR	2.3
1	I	250	TYR	2.3
1	I	829	ARG	2.3
1	I	197	GLY	2.3
1	L	875	ILE	2.2
1	E	211	HIS	2.2
1	B	160	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	750	MET	2.2
1	E	168	GLU	2.2
1	L	675	GLY	2.2
1	E	254	ILE	2.2
1	B	133	THR	2.2
1	I	471	ASP	2.2
1	I	603	GLY	2.2
1	L	126	LEU	2.2
1	E	200	ALA	2.2
1	L	822	ALA	2.2
1	E	116	TYR	2.2
1	L	528	TYR	2.2
1	B	377	TRP	2.2
1	E	65	ALA	2.2
1	E	45	GLU	2.2
1	E	158	GLU	2.2
1	L	419	ASN	2.2
1	L	860	LYS	2.2
1	B	59	LEU	2.2
1	I	635	MET	2.2
1	I	671	ASN	2.1
1	E	261	LEU	2.1
1	E	749	LEU	2.1
1	L	637	LEU	2.1
1	I	538	GLY	2.1
1	L	591	ASP	2.1
1	E	140	ALA	2.1
1	L	771	ALA	2.1
1	E	419	ASN	2.1
1	E	174	VAL	2.1
1	L	687	VAL	2.1
1	E	113	ALA	2.1
1	B	8	LYS	2.1
1	E	24	LEU	2.1
1	I	810	ILE	2.1
1	L	349	VAL	2.1
1	B	10	ASP	2.1
1	B	755	PHE	2.1
1	I	162	PHE	2.1
1	I	184	GLN	2.1
1	I	697	ASN	2.1
1	L	690	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	262	ALA	2.0
1	L	638	ALA	2.0
1	L	881	ALA	2.0
1	B	127	THR	2.0
1	I	123	LEU	2.0
1	L	59	LEU	2.0
1	L	545	HIS	2.0
1	B	238	GLY	2.0
1	B	134	VAL	2.0
1	E	69	ALA	2.0
4	H	2	DT	2.0
1	B	16	LEU	2.0
1	E	194	GLY	2.0
1	I	349	VAL	2.0
1	I	746	ARG	2.0
1	L	214	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

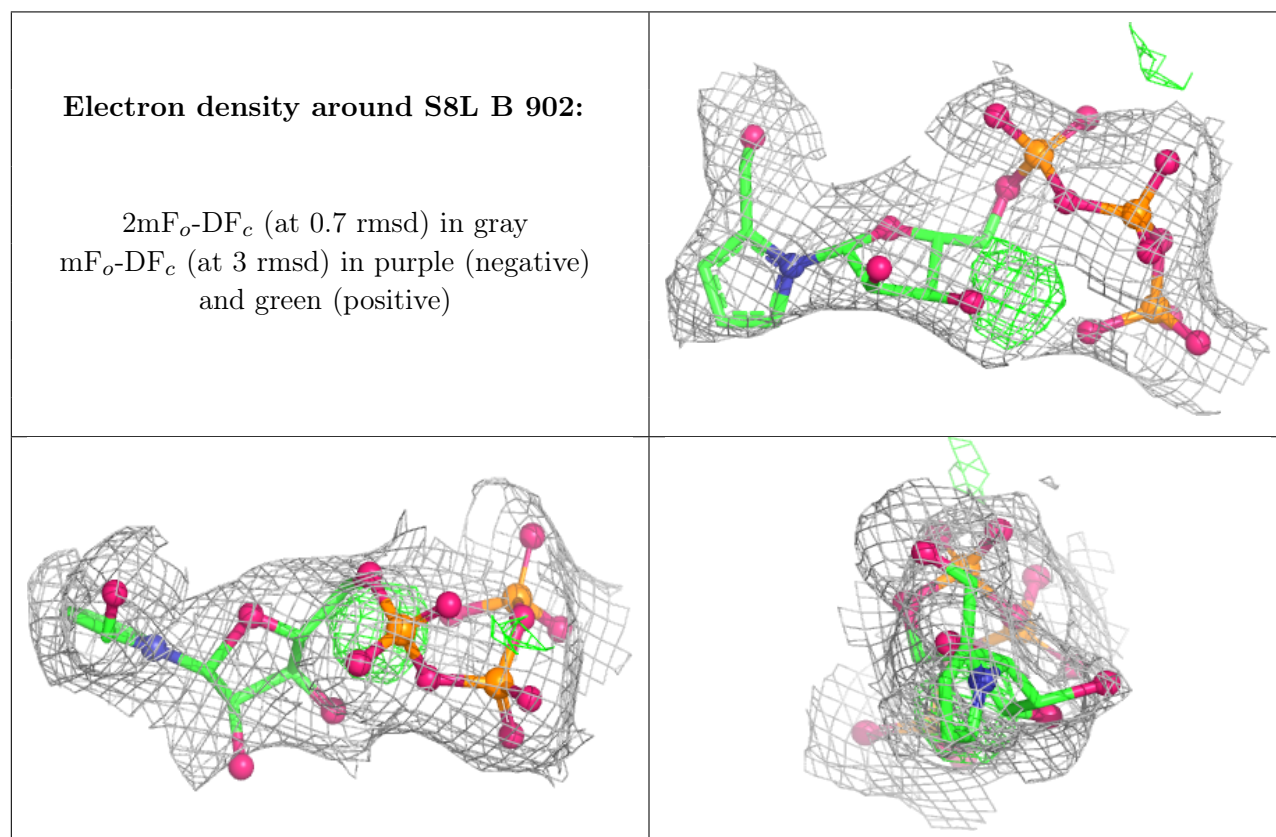
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	MG	B	903	1/1	0.79	0.15	97,97,97,97	0
5	GOL	C	101	6/6	0.83	0.11	60,69,73,77	0
5	GOL	I	901	6/6	0.84	0.12	84,85,98,105	0
7	MG	C	102	1/1	0.85	0.42	143,143,143,143	0
6	S8L	B	902	28/28	0.86	0.13	68,104,128,150	0
5	GOL	B	901	6/6	0.95	0.08	51,60,74,75	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.