



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 11:23 AM EDT

PDB ID : 8DH1
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

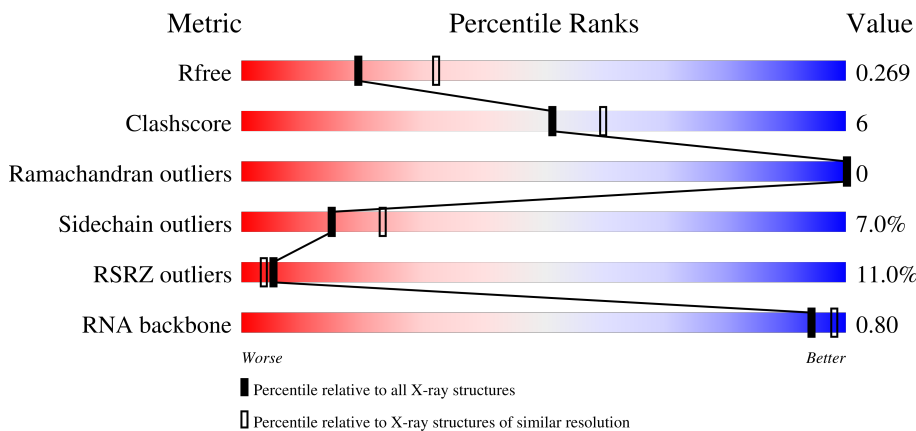
1 Overall quality at a glance i

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}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)
RNA backbone	3102	1010 (2.96-2.36)

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	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 83%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">5% 83% 14% ••</p>
1	E	883	<div style="display: flex; align-items: center;"> <div style="width: 10%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 72%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">10% 72% 16% • 11%</p>
1	I	883	<div style="display: flex; align-items: center;"> <div style="width: 10%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 72%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">10% 72% 19% • 7%</p>
1	L	883	<div style="display: flex; align-items: center;"> <div style="width: 14%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 66%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">14% 66% 12% • 20%</p>

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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 [i](#)

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

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

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

- Molecule 3 is a RNA chain called RNA.

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

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

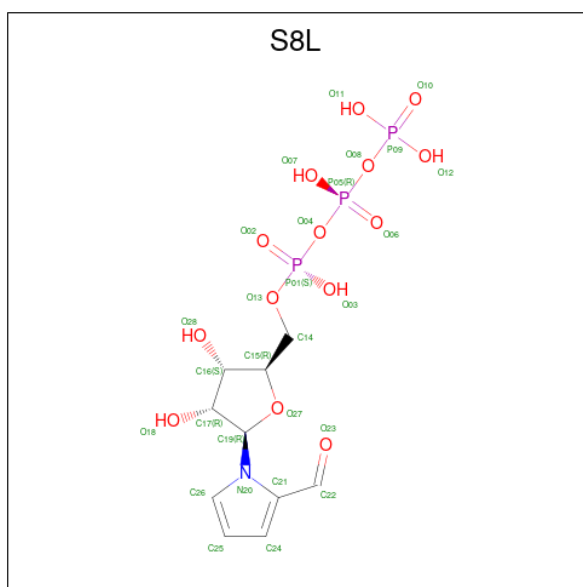
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	D	6	Total 121	C 58	N 20	O 37	P 6	0	0	0
4	H	8	Total 160	C 77	N 25	O 50	P 8	0	0	0
4	O	5	Total 102	C 49	N 17	O 31	P 5	0	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 6 is 1-{5-O-[(S)-hydroxy{[(R)-hydroxy(phosphonoxy)phosphoryl]oxy}phosphoryl]-beta-D-ribofuranosyl}-1H-pyrrole-2-carbaldehyde (three-letter code: S8L) (formula: C₁₀H₁₆NO₁₄P₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 8 is water.

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

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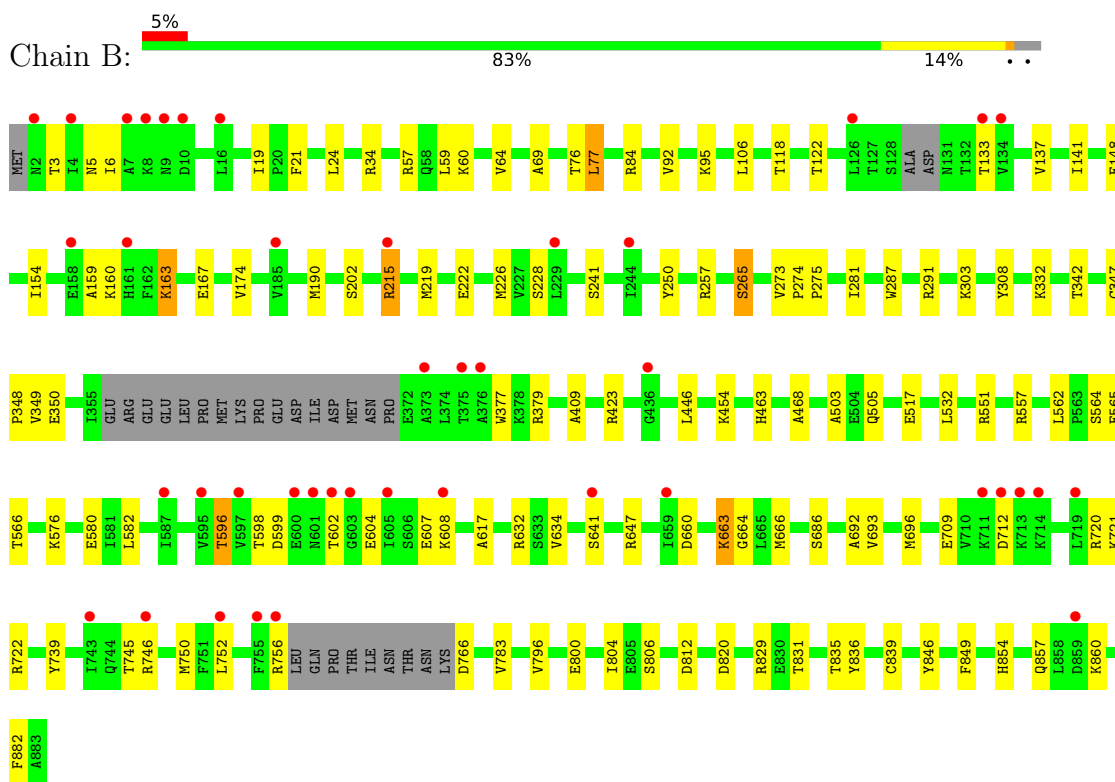
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	O	1	Total	O	0	0
			1	1		

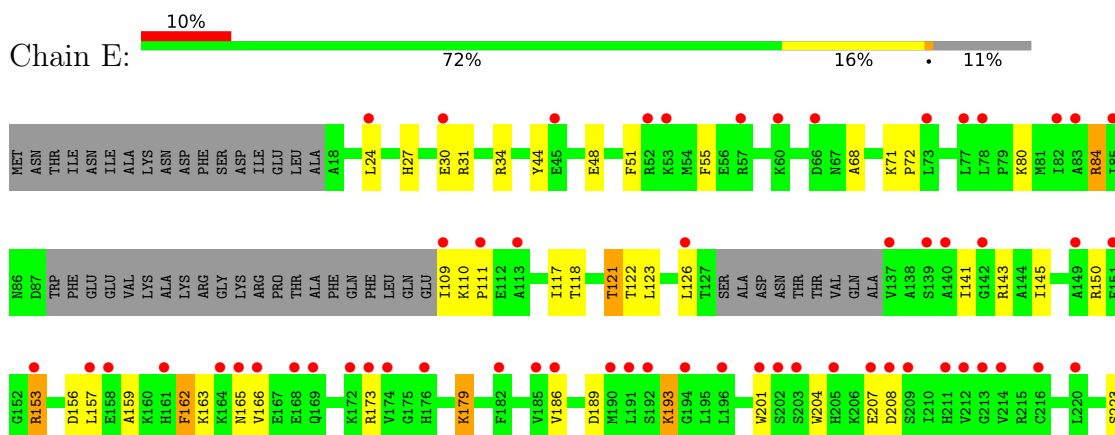
3 Residue-property plots [i](#)

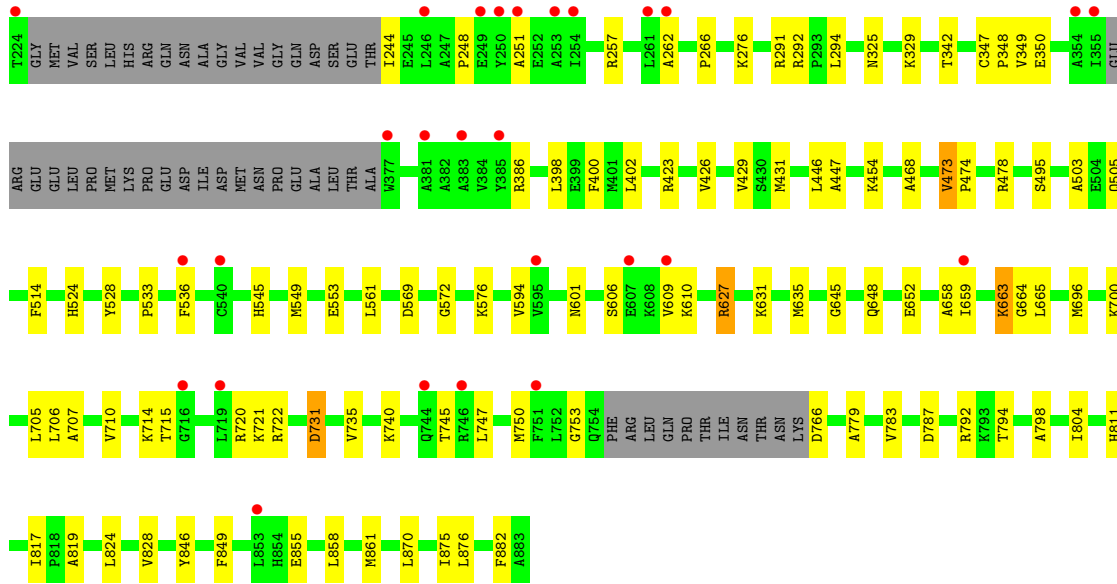
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: T7 RNA polymerase

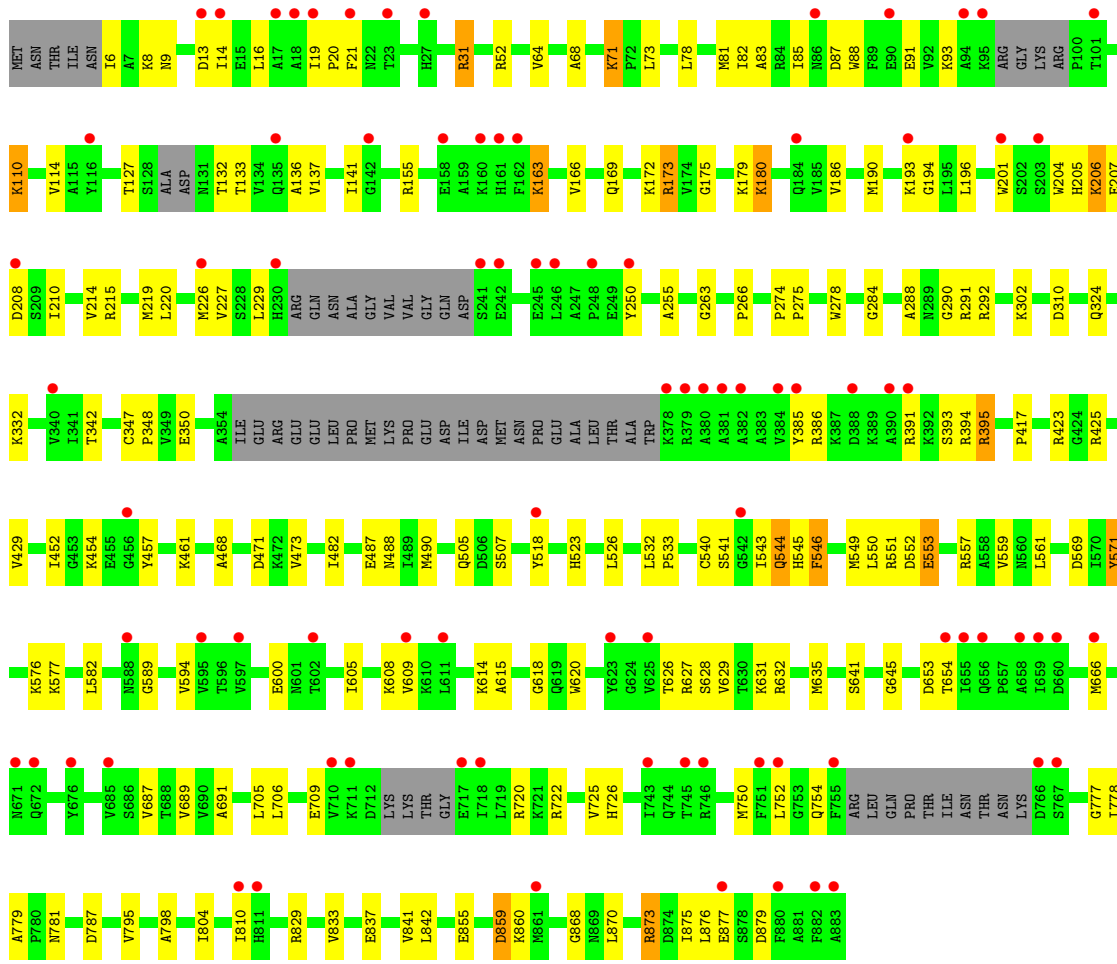


- Molecule 1: T7 RNA polymerase

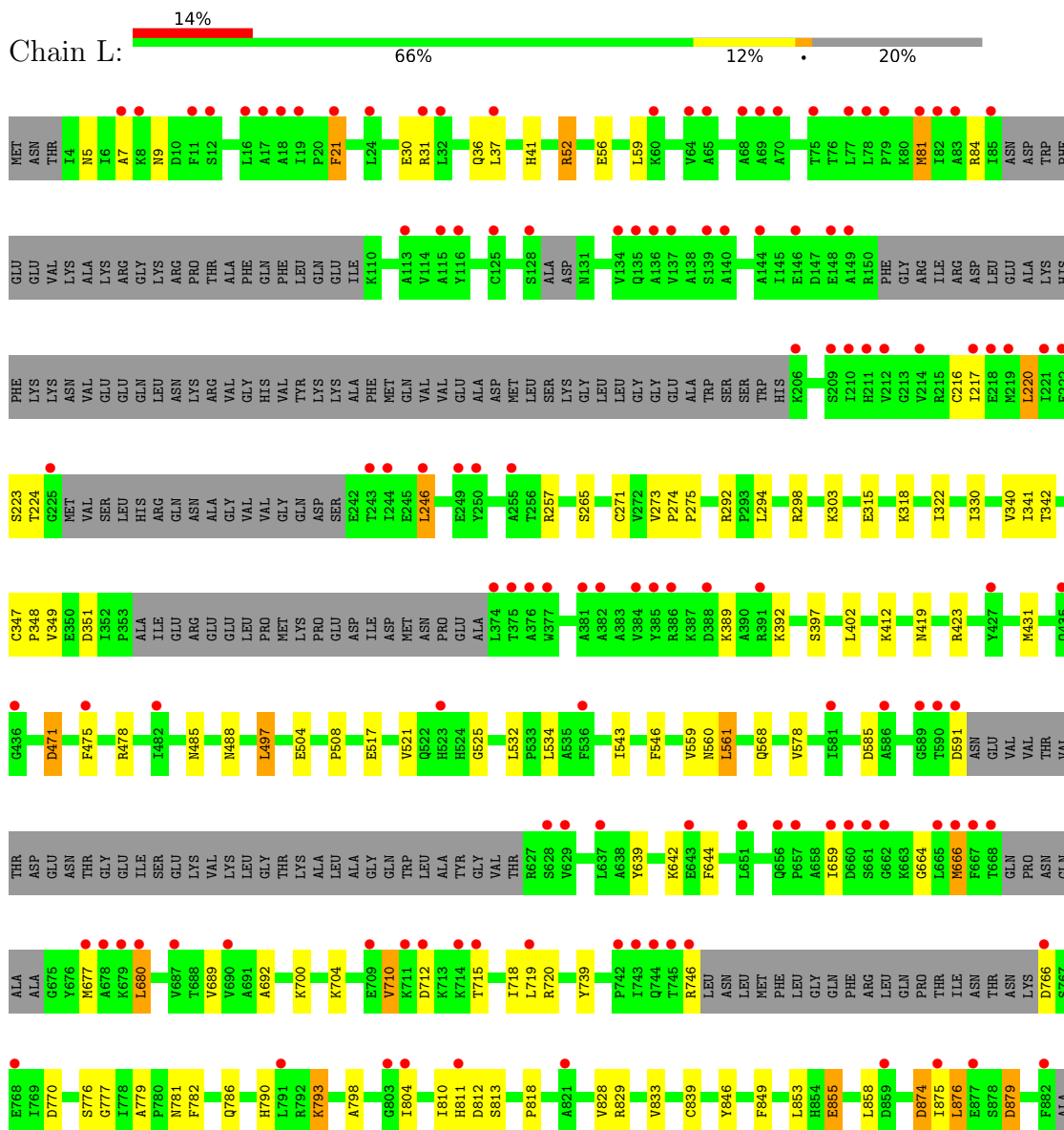




• Molecule 1: T7 RNA polymerase



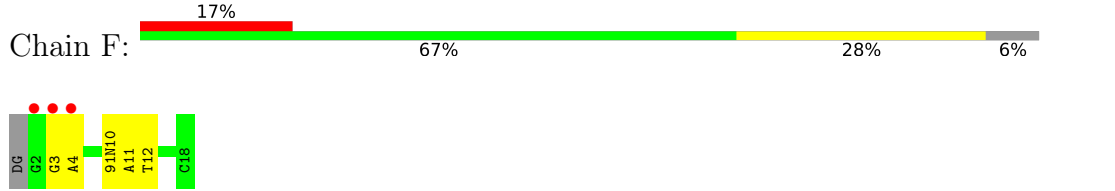
• Molecule 1: T7 RNA polymerase



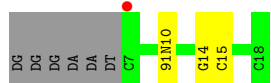
● Molecule 2: Template strand DNA



● Molecule 2: Template strand DNA



● Molecule 2: Template strand DNA



● Molecule 2: Template strand DNA



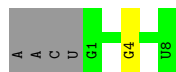
● Molecule 3: RNA



● Molecule 3: RNA



● Molecule 3: RNA



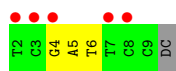
● Molecule 3: RNA



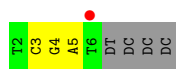
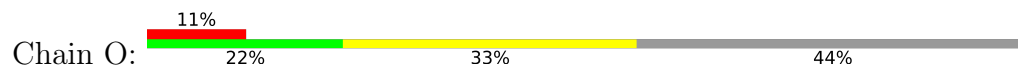
● Molecule 4: Non-template strand DNA



● 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)	Xtrriage
Refinement program	PHENIX 1.19	Depositor
R, R_{free}	0.230 , 0.272 0.227 , 0.269	Depositor DCC
R_{free} test set	6387 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	65.0	Xtrriage
Anisotropy	0.365	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 60.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

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	0.29	0/6869	0.51	1/9291 (0.0%)
1	E	0.29	0/6262	0.52	2/8472 (0.0%)
1	I	0.30	0/6623	0.52	0/8957
1	L	0.28	0/5474	0.52	1/7411 (0.0%)
2	A	0.61	0/343	0.82	0/524
2	F	0.56	0/365	0.82	0/559
2	J	0.63	0/248	0.83	0/377
2	M	0.59	0/294	0.87	0/448
3	C	0.34	0/194	0.82	0/301
3	G	0.24	0/194	0.72	0/301
3	K	0.21	0/194	0.70	0/301
3	N	0.20	0/191	0.65	0/297
4	D	0.48	0/134	0.96	0/204
4	H	0.49	0/177	0.97	0/270
4	O	0.56	0/113	1.06	0/172
All	All	0.31	0/27675	0.56	4/37885 (0.0%)

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.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	787	ASP	CB-CG-OD1	5.70	123.43	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	812	ASP	CB-CG-OD1	5.67	123.40	118.30
1	E	731	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	77	LEU	CB-CG-CD2	-5.04	102.44	111.00

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 [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	B	6719	0	6670	60	0
1	E	6125	0	6043	66	0
1	I	6478	0	6406	99	1
1	L	5358	0	5131	57	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	293	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 (293) 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: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: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:154:ILE:HG23	1:B:190:MET:HE1	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:I:6:ILE:HD11	1:I:52:ARG:CZ	2.36	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: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: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:I:461:LYS:HZ2	1:I:518:TYR:HE1	1.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:215:ARG:HH21	1:B:219:MET:HE1	1.75	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
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:HE1	1:L:220:LEU:HA	1.94	0.50
1:B:118:THR:HG22	1:B:141:ILE:HG21	1.92	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: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:E:173:ARG:O	1:E:179:LYS:NZ	2.47	0.48
1:I:490:MET:HE1	1:I:523:HIS:HE1	1.78	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:B:332:LYS:NZ	1:B:409:ALA:O	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:400:PHE:CZ	1:E:431:MET:HE2	2.49	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: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: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: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:L:874:ASP:OD2	1:L:874:ASP:N	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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:I:207:GLU:CD	1:I:207:GLU:H	2.20	0.45
1:B:281:ILE:HD11	1:B:308:TYR:HB2	1.99	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: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:790:HIS:NE2	1:L:828:VAL:O	2.44	0.44
1:B:24:LEU:HD13	1:B:287:TRP:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:L:700:LYS:HZ3	1:L:779:ALA:H	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:I:490:MET:HE1	1:I:523:HIS:CE1	2.54	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:569:ASP:CG	1:E:627:ARG:HH21	2.24	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 [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	B	698/729 (96%)	665 (95%)	33 (5%)	26	40
1	E	628/729 (86%)	581 (92%)	47 (8%)	13	21
1	I	673/729 (92%)	622 (92%)	51 (8%)	13	21
1	L	528/729 (72%)	483 (92%)	45 (8%)	10	15
All	All	2527/2916 (87%)	2351 (93%)	176 (7%)	15	23

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3	THR
1	B	5	ASN
1	B	19	ILE
1	B	57	ARG
1	B	133	THR
1	B	160	LYS
1	B	163	LYS
1	B	174	VAL
1	B	202	SER
1	B	215	ARG
1	B	228	SER
1	B	241	SER
1	B	265	SER

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Mol	Chain	Res	Type
1	B	377	TRP
1	B	423	ARG
1	B	454	LYS
1	B	565	GLU
1	B	596	THR
1	B	598	THR
1	B	608	LYS
1	B	634	VAL
1	B	641	SER
1	B	647	ARG
1	B	663	LYS
1	B	666	MET
1	B	712	ASP
1	B	720	ARG
1	B	745	THR
1	B	750	MET
1	B	752	LEU
1	B	756	ARG
1	B	766	ASP
1	B	783	VAL
1	E	27	HIS
1	E	31	ARG
1	E	80	LYS
1	E	84	ARG
1	E	121	THR
1	E	143	ARG
1	E	153	ARG
1	E	162	PHE
1	E	165	ASN
1	E	179	LYS
1	E	186	VAL
1	E	189	ASP
1	E	193	LYS
1	E	204	TRP
1	E	208	ASP
1	E	276	LYS
1	E	292	ARG
1	E	325	ASN
1	E	398	LEU
1	E	423	ARG
1	E	426	VAL
1	E	473	VAL

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Mol	Chain	Res	Type
1	E	495	SER
1	E	514	PHE
1	E	553	GLU
1	E	594	VAL
1	E	601	ASN
1	E	606	SER
1	E	609	VAL
1	E	610	LYS
1	E	627	ARG
1	E	663	LYS
1	E	665	LEU
1	E	700	LYS
1	E	710	VAL
1	E	714	LYS
1	E	715	THR
1	E	720	ARG
1	E	735	VAL
1	E	740	LYS
1	E	745	THR
1	E	750	MET
1	E	766	ASP
1	E	783	VAL
1	E	811	HIS
1	E	870	LEU
1	E	876	LEU
1	I	16	LEU
1	I	21	PHE
1	I	71	LYS
1	I	73	LEU
1	I	81	MET
1	I	91	GLU
1	I	93	LYS
1	I	110	LYS
1	I	114	VAL
1	I	132	THR
1	I	163	LYS
1	I	173	ARG
1	I	180	LYS
1	I	193	LYS
1	I	196	LEU
1	I	206	LYS
1	I	266	PRO

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Mol	Chain	Res	Type
1	I	292	ARG
1	I	302	LYS
1	I	385	TYR
1	I	391	ARG
1	I	393	SER
1	I	394	ARG
1	I	395	ARG
1	I	423	ARG
1	I	473	VAL
1	I	487	GLU
1	I	488	ASN
1	I	507	SER
1	I	541	SER
1	I	544	GLN
1	I	546	PHE
1	I	553	GLU
1	I	569	ASP
1	I	571	TYR
1	I	600	GLU
1	I	605	ILE
1	I	627	ARG
1	I	641	SER
1	I	666	MET
1	I	726	HIS
1	I	750	MET
1	I	752	LEU
1	I	795	VAL
1	I	810	ILE
1	I	841	VAL
1	I	855	GLU
1	I	859	ASP
1	I	873	ARG
1	I	877	GLU
1	I	879	ASP
1	L	5	ASN
1	L	9	ASN
1	L	21	PHE
1	L	31	ARG
1	L	37	LEU
1	L	41	HIS
1	L	52	ARG
1	L	81	MET

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Mol	Chain	Res	Type
1	L	84	ARG
1	L	216	CYS
1	L	220	LEU
1	L	246	LEU
1	L	257	ARG
1	L	265	SER
1	L	347	CYS
1	L	351	ASP
1	L	392	LYS
1	L	397	SER
1	L	412	LYS
1	L	423	ARG
1	L	471	ASP
1	L	475	PHE
1	L	497	LEU
1	L	561	LEU
1	L	585	ASP
1	L	591	ASP
1	L	642	LYS
1	L	644	PHE
1	L	666	MET
1	L	677	MET
1	L	680	LEU
1	L	710	VAL
1	L	720	ARG
1	L	746	ARG
1	L	766	ASP
1	L	776	SER
1	L	793	LYS
1	L	811	HIS
1	L	833	VAL
1	L	839	CYS
1	L	853	LEU
1	L	855	GLU
1	L	874	ASP
1	L	876	LEU
1	L	879	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	232	GLN

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Mol	Chain	Res	Type
1	B	583	GLN
1	B	857	GLN
1	E	404	GLN
1	E	869	ASN
1	I	161	HIS
1	I	169	GLN
1	I	523	HIS
1	L	486	HIS
1	L	588	ASN
1	L	649	GLN

5.3.3 RNA [i](#)

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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
6	S8L	B	902	7	23,29,29	5.70	8 (34%)	29,45,45	1.43	7 (24%)
5	GOL	B	901	-	5,5,5	1.07	0	5,5,5	0.98	0
5	GOL	C	101	-	5,5,5	0.94	0	5,5,5	1.02	0
5	GOL	I	901	-	5,5,5	1.02	0	5,5,5	0.92	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
6	S8L	B	902	7	-	7/18/40/40	0/2/2/2
5	GOL	B	901	-	-	0/4/4/4	-
5	GOL	C	101	-	-	2/4/4/4	-
5	GOL	I	901	-	-	0/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	902	S8L	O27-C19	18.48	1.66	1.41
6	B	902	S8L	C17-C19	-15.83	1.29	1.53
6	B	902	S8L	O27-C15	-7.84	1.27	1.45
6	B	902	S8L	P09-O10	5.03	1.66	1.50
6	B	902	S8L	O28-C16	-4.66	1.32	1.43
6	B	902	S8L	O18-C17	4.38	1.53	1.43
6	B	902	S8L	P09-O11	-2.57	1.44	1.54
6	B	902	S8L	P09-O12	-2.41	1.45	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	902	S8L	C16-C17-C19	3.50	106.25	100.98
6	B	902	S8L	P05-O04-P01	-3.05	122.36	132.83
6	B	902	S8L	P05-O08-P09	-2.58	123.98	132.83
6	B	902	S8L	O23-C22-C21	-2.12	121.17	124.17
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
6	B	902	S8L	O07-P05-O06	-2.03	102.23	112.24

There are no chirality outliers.

All (9) torsion outliers are listed below:

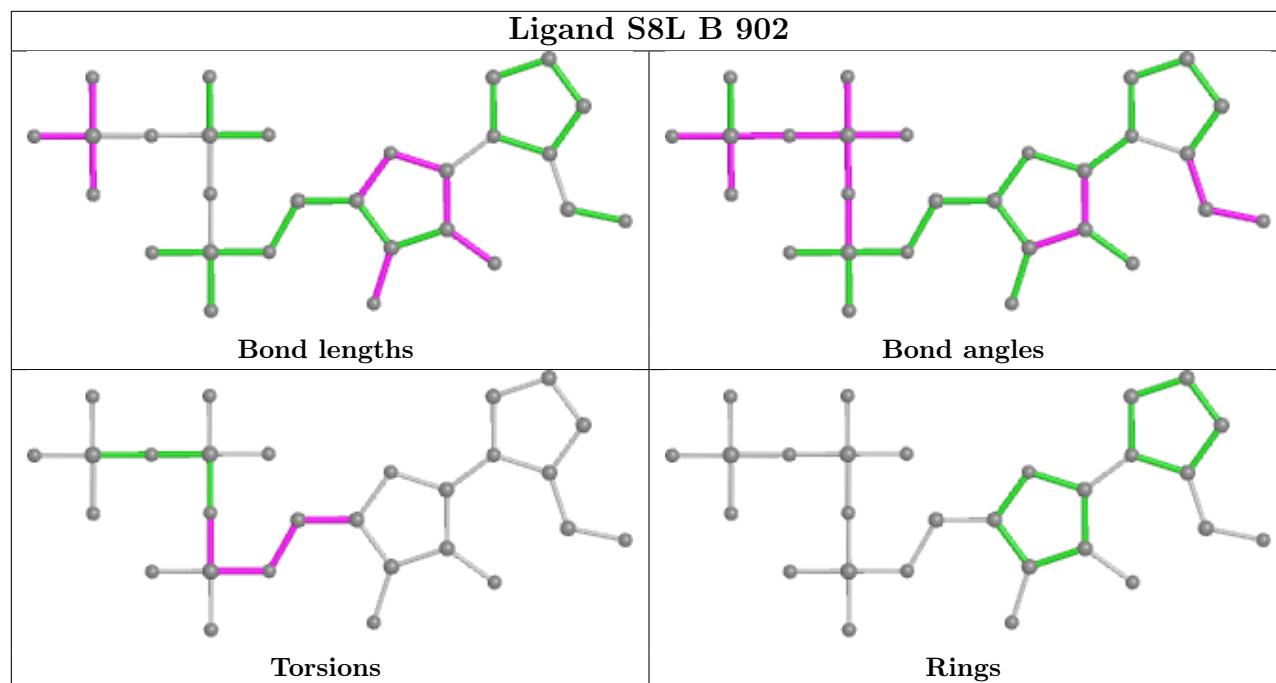
Mol	Chain	Res	Type	Atoms
5	C	101	GOL	C1-C2-C3-O3
6	B	902	S8L	C15-C14-O13-P01
6	B	902	S8L	C14-O13-P01-O04
6	B	902	S8L	O13-C14-C15-C16
5	C	101	GOL	O2-C2-C3-O3
6	B	902	S8L	O13-C14-C15-O27
6	B	902	S8L	C14-O13-P01-O02
6	B	902	S8L	C14-O13-P01-O03
6	B	902	S8L	P05-O04-P01-O03

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 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	B	855/883 (96%)	0.37	42 (4%) 29 26	39, 68, 134, 215	0
1	E	785/883 (88%)	0.62	85 (10%) 5 4	45, 76, 169, 252	0
1	I	825/883 (93%)	0.75	85 (10%) 6 4	59, 104, 167, 218	0
1	L	702/883 (79%)	0.96	126 (17%) 1 1	69, 114, 171, 267	0
2	A	15/18 (83%)	0.95	4 (26%) 0 0	52, 71, 237, 239	0
2	F	16/18 (88%)	0.71	3 (18%) 1 1	62, 110, 248, 259	0
2	J	11/18 (61%)	0.73	1 (9%) 9 7	70, 79, 176, 202	0
2	M	13/18 (72%)	0.68	1 (7%) 13 10	90, 107, 176, 182	0
3	C	8/12 (66%)	0.48	0 100 100	52, 63, 72, 83	0
3	G	8/12 (66%)	-0.02	0 100 100	59, 77, 119, 140	0
3	K	8/12 (66%)	0.22	0 100 100	77, 94, 120, 141	0
3	N	8/12 (66%)	0.56	1 (12%) 3 2	88, 107, 161, 177	0
4	D	6/9 (66%)	3.24	5 (83%) 0 0	211, 225, 229, 241	0
4	H	8/9 (88%)	2.44	5 (62%) 0 0	182, 197, 224, 234	0
4	O	5/9 (55%)	1.39	1 (20%) 1 1	204, 210, 212, 223	0
All	All	3273/3679 (88%)	0.67	359 (10%) 5 4	39, 93, 168, 267	0

All (359) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	17	ALA	9.0
1	L	113	ALA	6.8
1	L	21	PHE	6.0
1	L	16	LEU	5.5
1	L	744	GLN	5.2
1	L	384	VAL	5.0
1	E	205	HIS	5.0

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Mol	Chain	Res	Type	RSRZ
1	L	65	ALA	5.0
1	I	101	THR	5.0
1	I	142	GLY	5.0
1	E	140	ALA	5.0
1	E	168	GLU	4.9
1	L	214	VAL	4.9
1	I	746	ARG	4.9
1	I	717	GLU	4.8
1	E	196	LEU	4.7
1	E	246	LEU	4.7
1	L	882	PHE	4.7
1	L	82	ILE	4.7
1	I	658	ALA	4.6
1	L	81	MET	4.5
4	H	3	DC	4.5
1	E	212	VAL	4.3
1	I	242	GLU	4.3
2	J	7	DC	4.3
1	E	254	ILE	4.3
1	I	203	SER	4.3
1	L	667	PHE	4.2
1	I	193	LYS	4.2
1	L	719	LEU	4.2
1	I	390	ALA	4.2
4	D	8	DC	4.2
1	E	249	GLU	4.2
1	E	137	VAL	4.2
1	I	380	ALA	4.1
1	E	158	GLU	4.1
1	L	78	LEU	4.1
1	L	116	TYR	4.1
1	I	384	VAL	4.1
1	E	208	ASP	4.0
1	L	219	MET	3.9
1	E	201	TRP	3.9
1	I	767	SER	3.9
1	E	216	CYS	3.9
1	B	600	GLU	3.9
1	B	244	ILE	3.9
1	I	743	ILE	3.9
2	A	3	DG	3.9
1	I	654	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	L	746	ARG	3.8
1	L	79	PRO	3.8
1	L	11	PHE	3.8
1	L	586	ALA	3.8
1	I	95	LYS	3.8
1	E	194	GLY	3.8
1	E	377	TRP	3.8
1	L	374	LEU	3.8
4	H	4	DG	3.8
1	B	719	LEU	3.7
1	L	766	ASP	3.7
1	E	73	LEU	3.7
1	E	157	LEU	3.7
1	E	164	LYS	3.7
1	B	755	PHE	3.7
1	L	377	TRP	3.7
1	I	19	ILE	3.7
1	B	10	ASP	3.7
1	L	24	LEU	3.7
1	E	153	ARG	3.6
1	I	161	HIS	3.6
1	E	52	ARG	3.6
4	D	7	DT	3.6
1	B	597	VAL	3.6
1	L	536	PHE	3.6
1	L	69	ALA	3.6
1	E	744	GLN	3.6
1	E	173	ARG	3.6
1	B	714	LYS	3.6
1	I	710	VAL	3.5
1	L	743	ILE	3.5
1	B	601	ASN	3.5
1	E	186	VAL	3.5
1	L	125	CYS	3.5
1	E	191	LEU	3.4
1	L	382	ALA	3.4
1	I	671	ASN	3.4
1	L	657	PRO	3.4
1	B	16	LEU	3.4
1	L	375	THR	3.4
1	L	715	THR	3.4
2	F	3	DG	3.4

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Mol	Chain	Res	Type	RSRZ
4	D	3	DC	3.4
1	I	245	GLU	3.4
1	L	712	ASP	3.4
1	B	713	LYS	3.4
1	L	64	VAL	3.4
1	L	255	ALA	3.4
1	L	381	ALA	3.4
1	E	109	ILE	3.4
4	O	6	DT	3.4
1	B	859	ASP	3.4
1	E	355	ILE	3.3
4	D	5	DA	3.3
1	E	746	ARG	3.3
1	I	752	LEU	3.3
1	E	190	MET	3.3
2	F	2	DG	3.3
1	E	354	ALA	3.3
1	L	436	GLY	3.3
1	B	608	LYS	3.3
1	I	880	PHE	3.2
1	L	659	ILE	3.2
1	I	17	ALA	3.2
1	L	221	ILE	3.2
1	I	660	ASP	3.2
1	I	388	ASP	3.2
1	L	85	ILE	3.2
1	E	751	PHE	3.2
1	L	218	GLU	3.2
1	I	162	PHE	3.1
1	L	77	LEU	3.1
1	L	803	GLY	3.1
1	I	226	MET	3.1
1	E	202	SER	3.1
1	L	136	ALA	3.1
1	E	224	THR	3.1
1	L	75	THR	3.1
1	E	82	ILE	3.1
1	L	628	SER	3.1
1	L	742	PRO	3.1
1	E	250	TYR	3.1
1	B	7	ALA	3.1
1	I	385	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	174	VAL	3.0
1	E	83	ALA	3.0
1	I	755	PHE	3.0
1	L	386	ARG	3.0
1	E	261	LEU	3.0
1	L	70	ALA	3.0
1	L	875	ILE	3.0
1	L	591	ASP	3.0
1	I	625	VAL	3.0
1	B	756	ARG	3.0
1	I	751	PHE	3.0
1	L	385	TYR	3.0
1	E	220	LEU	3.0
1	L	665	LEU	2.9
1	L	680	LEU	2.9
1	I	241	SER	2.9
1	I	250	TYR	2.9
1	I	86	ASN	2.9
1	L	222	GLU	2.9
1	B	752	LEU	2.9
4	D	6	DT	2.9
1	L	768	GLU	2.9
1	B	376	ALA	2.9
1	L	217	ILE	2.9
1	L	662	GLY	2.9
1	I	160	LYS	2.9
1	I	248	PRO	2.9
1	E	176	HIS	2.9
1	L	18	ALA	2.9
1	E	24	LEU	2.8
2	F	4	DA	2.8
1	B	8	LYS	2.8
1	L	651	LEU	2.8
1	L	243	THR	2.8
1	E	169	GLN	2.8
1	B	373	ALA	2.8
1	L	668	THR	2.8
1	I	391	ARG	2.8
1	B	712	ASP	2.8
1	E	853	LEU	2.8
1	I	659	ILE	2.8
1	E	165	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	213	GLY	2.8
2	A	5	DA	2.8
1	L	482	ILE	2.8
1	I	378	LYS	2.7
1	I	745	THR	2.7
1	I	381	ALA	2.7
1	I	246	LEU	2.7
1	I	14	ILE	2.7
1	L	144	ALA	2.7
1	I	861	MET	2.7
1	E	607	GLU	2.7
1	I	184	GLN	2.7
1	B	602	THR	2.7
1	B	158	GLU	2.7
1	I	883	ALA	2.7
1	I	766	ASP	2.7
1	I	94	ALA	2.7
1	L	149	ALA	2.7
1	E	609	VAL	2.7
1	L	212	VAL	2.7
1	E	139	SER	2.7
1	L	714	LYS	2.7
2	A	4	DA	2.7
1	E	111	PRO	2.6
1	E	161	HIS	2.6
1	I	882	PHE	2.6
1	L	249	GLU	2.6
1	L	8	LYS	2.6
1	L	139	SER	2.6
1	E	53	LYS	2.6
1	I	676	TYR	2.6
1	E	30	GLU	2.6
1	E	45	GLU	2.6
1	I	595	VAL	2.6
1	I	597	VAL	2.6
1	L	391	ARG	2.6
1	L	677	MET	2.6
1	L	666	MET	2.6
1	E	182	PHE	2.6
1	I	208	ASP	2.6
1	E	659	ILE	2.6
1	L	37	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
4	H	2	DT	2.6
1	L	148	GLU	2.6
1	E	57	ARG	2.6
1	E	253	ALA	2.5
1	L	643	GLU	2.5
1	L	225	GLY	2.5
1	E	85	ILE	2.5
1	I	655	ILE	2.5
1	E	126	LEU	2.5
2	M	18	DC	2.5
1	E	172	LYS	2.5
1	L	206	LYS	2.5
1	L	877	GLU	2.5
1	B	659	ILE	2.5
1	E	166	VAL	2.5
1	L	656	GLN	2.5
1	B	4	ILE	2.5
1	I	201	TRP	2.5
1	B	229	LEU	2.5
1	B	595	VAL	2.5
1	I	666	MET	2.5
1	E	149	ALA	2.5
1	I	718	ILE	2.5
1	B	603	GLY	2.4
1	L	83	ALA	2.4
1	B	743	ILE	2.4
1	I	685	VAL	2.4
1	L	687	VAL	2.4
1	L	679	LYS	2.4
1	I	588	ASN	2.4
1	E	262	ALA	2.4
1	L	115	ALA	2.4
1	L	246	LEU	2.4
1	I	13	ASP	2.4
1	L	678	ALA	2.4
1	L	146	GLU	2.4
1	B	746	ARG	2.4
1	L	804	ILE	2.4
1	I	518	TYR	2.4
1	L	709	GLU	2.4
1	L	745	THR	2.4
1	L	388	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	142	GLY	2.4
1	E	716	GLY	2.4
1	E	211	HIS	2.4
1	L	135	GLN	2.4
1	E	251	ALA	2.4
1	L	244	ILE	2.4
1	L	581	ILE	2.4
1	I	602	THR	2.3
1	L	859	ASP	2.3
1	B	2	ASN	2.3
1	E	214	VAL	2.3
1	I	340	VAL	2.3
1	E	66	ASP	2.3
1	I	623	TYR	2.3
1	L	821	ALA	2.3
1	B	215	ARG	2.3
1	L	523	HIS	2.3
1	E	78	LEU	2.3
1	B	711	LYS	2.3
1	E	151	PHE	2.3
1	L	128	SER	2.3
1	L	250	TYR	2.3
1	L	690	VAL	2.3
1	E	77	LEU	2.3
1	L	12	SER	2.3
1	B	134	VAL	2.3
1	L	637	LEU	2.3
1	B	133	THR	2.3
1	I	877	GLU	2.3
1	L	427	TYR	2.3
2	A	6	DT	2.3
1	E	203	SER	2.2
1	L	209	SER	2.2
1	L	211	HIS	2.2
1	I	135	GLN	2.2
1	L	60	LYS	2.2
3	N	8	U	2.2
1	E	113	ALA	2.2
1	L	140	ALA	2.2
1	L	19	ILE	2.2
1	I	379	ARG	2.2
1	I	18	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	711	LYS	2.2
1	B	126	LEU	2.2
1	I	230	HIS	2.2
1	I	611	LEU	2.2
1	L	811	HIS	2.2
1	I	382	ALA	2.2
1	I	456	GLY	2.2
1	I	542	GLY	2.2
1	B	587	ILE	2.2
1	E	192	SER	2.2
1	I	27	HIS	2.2
1	I	90	GLU	2.2
1	I	656	GLN	2.2
1	I	672	GLN	2.2
1	B	9	ASN	2.2
1	E	595	VAL	2.2
1	B	161	HIS	2.2
1	B	375	THR	2.2
1	E	185	VAL	2.1
1	I	810	ILE	2.1
1	E	540	CYS	2.1
1	B	641	SER	2.1
1	E	207	GLU	2.1
1	L	661	SER	2.1
1	I	609	VAL	2.1
1	L	210	ILE	2.1
1	L	31	ARG	2.1
1	E	381	ALA	2.1
1	E	383	ALA	2.1
1	E	209	SER	2.1
1	I	116	TYR	2.1
1	E	719	LEU	2.1
1	I	811	HIS	2.1
1	L	589	GLY	2.1
1	L	376	ALA	2.1
1	I	21	PHE	2.1
4	H	8	DC	2.1
1	I	711	LYS	2.1
1	E	385	TYR	2.1
4	H	7	DT	2.1
1	L	32	LEU	2.1
1	L	7	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	435	GLN	2.0
1	L	660	ASP	2.0
1	E	60	LYS	2.0
1	E	536	PHE	2.0
1	L	475	PHE	2.0
1	B	185	VAL	2.0
1	L	134	VAL	2.0
1	L	629	VAL	2.0
1	B	605	ILE	2.0
1	I	158	GLU	2.0
1	L	590	THR	2.0
1	B	436	GLY	2.0
1	L	68	ALA	2.0
1	I	23	THR	2.0
1	L	791	LEU	2.0
1	L	137	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](#)

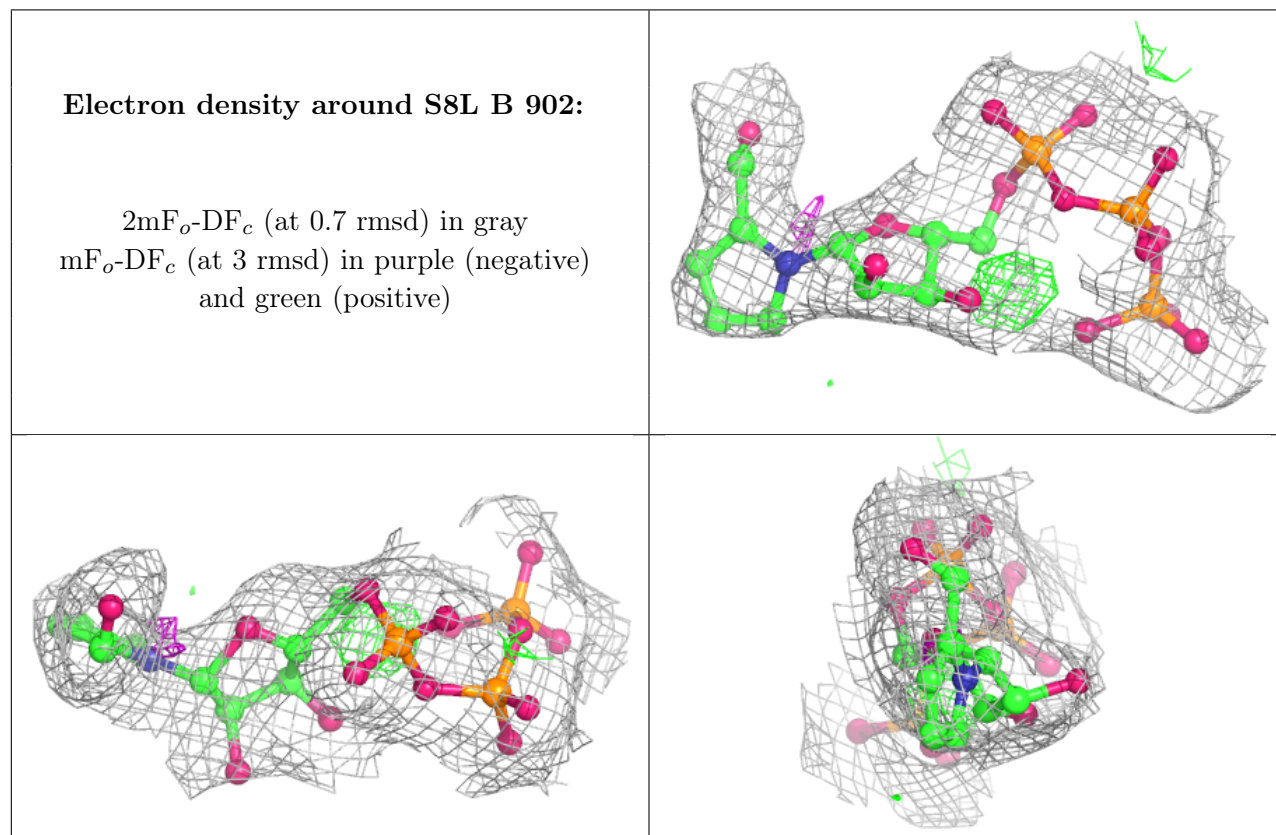
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	I	901	6/6	0.82	0.21	84,85,98,105	0
6	S8L	B	902	28/28	0.90	0.20	68,104,128,150	0
5	GOL	C	101	6/6	0.91	0.20	60,69,73,77	0
7	MG	B	903	1/1	0.92	0.37	97,97,97,97	0
5	GOL	B	901	6/6	0.95	0.24	51,60,74,75	0
7	MG	C	102	1/1	0.95	0.44	143,143,143,143	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.