



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 03:50 pm BST

PDB ID : 2R9L
Title : Polymerase Domain from Mycobacterium tuberculosis Ligase D in complex with DNA
Authors : Brissett, N.C.; Fox, G.C.; Pitcher, R.S.; Doherty, A.J.
Deposited on : 2007-09-13
Resolution : 2.40 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 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 : 2.11
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) : 2.11

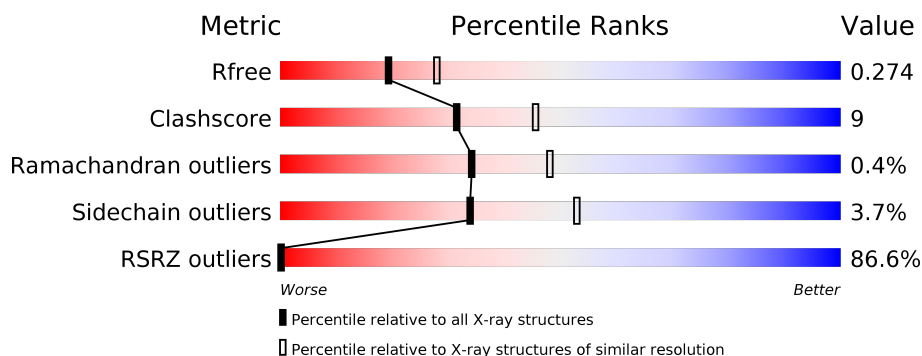
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 on 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	C	5	<div> <div>100%</div> <div> <div>60%</div> <div>40%</div> </div> </div>
1	E	5	<div> <div>100%</div> <div> <div>60%</div> <div>20%</div> <div>20%</div> </div> </div>
2	D	11	<div> <div>73%</div> <div> <div>73%</div> <div>27%</div> </div> </div>
3	F	13	<div> <div>92%</div> <div> <div>54%</div> <div>46%</div> </div> </div>
4	A	303	<div> <div>80%</div> <div> <div>76%</div> <div>18%</div> <div>• 5%</div> </div> </div>
4	B	303	<div> <div>83%</div> <div> <div>76%</div> <div>14%</div> <div>• 7%</div> </div> </div>

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
5	EDO	B	293	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5169 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 DNA chain called DNA (5'-D(P*DGP*DCP*DGP*DGP*DC)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	5	Total	C	N	O	P	0	0	0
			105	48	21	31	5			
1	E	5	Total	C	N	O	P	0	0	0
			105	48	21	31	5			

- Molecule 2 is a DNA chain called DNA (5'-D(*DGP*DCP*DCP*DGP*DCP*DAP*DAP*DCP*DGP*DCP*DA)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	11	Total	C	N	O	P	0	0	0
			221	105	45	61	10			

- Molecule 3 is a DNA chain called DNA (5'-D(*DGP*DCP*DCP*DGP*DCP*DAP*DAP*DCP*DGP*DCP*DAP*DCP*DG)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	13	Total	C	N	O	P	0	0	0
			262	124	53	73	12			

- Molecule 4 is a protein called Putative DNA ligase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	287	Total	C	N	O	S	19	0	0
			2193	1385	390	413	5			
4	B	282	Total	C	N	O	S	24	0	0
			2155	1363	384	403	5			

There are 6 discrepancies between the modelled and reference sequences:

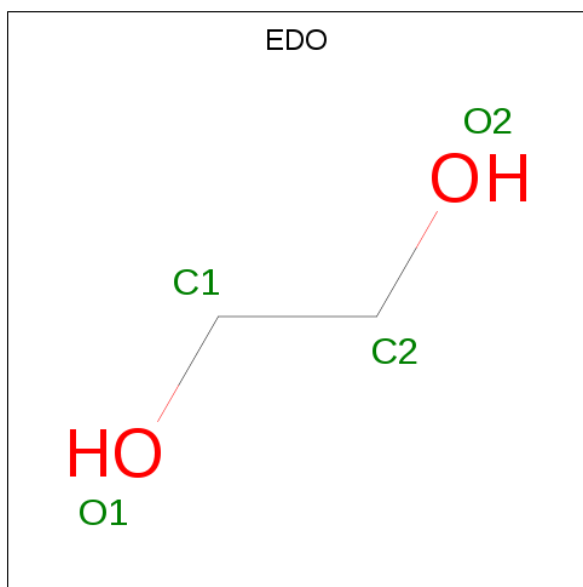
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP P71571
A	-1	SER	-	EXPRESSION TAG	UNP P71571

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	EXPRESSION TAG	UNP P71571
B	-2	GLY	-	EXPRESSION TAG	UNP P71571
B	-1	SER	-	EXPRESSION TAG	UNP P71571
B	0	HIS	-	EXPRESSION TAG	UNP P71571

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

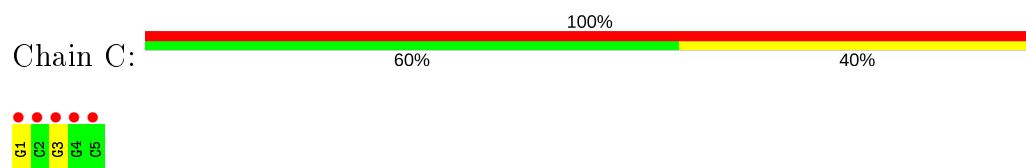
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	3	Total	O	0	0
			3	3		
7	D	5	Total	O	0	0
			5	5		
7	E	3	Total	O	0	0
			3	3		
7	F	3	Total	O	0	0
			3	3		
7	A	53	Total	O	0	0
			53	53		
7	B	30	Total	O	0	0
			30	30		

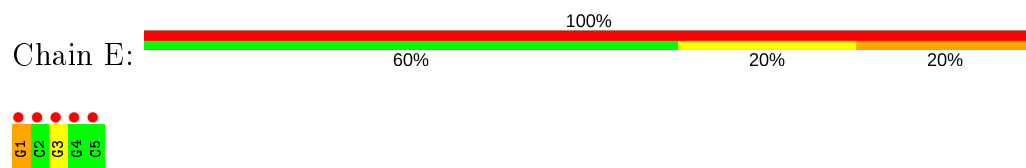
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

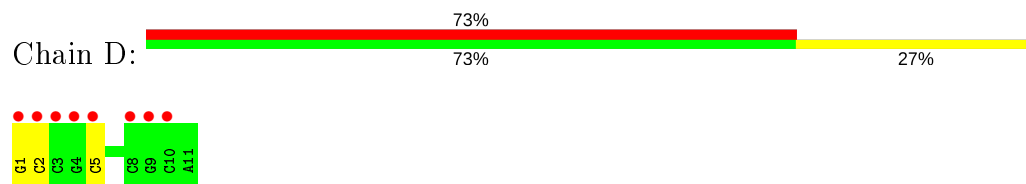
- Molecule 1: DNA (5'-D(P*DGP*DCP*DGP*DGP*DC)-3')



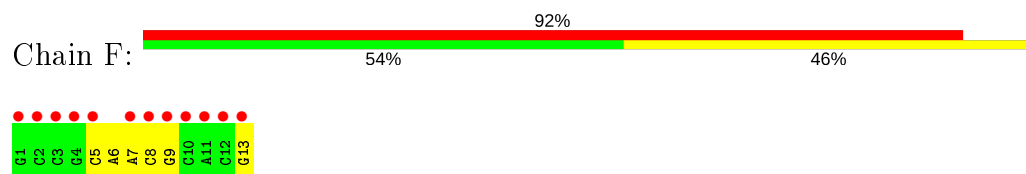
- Molecule 1: DNA (5'-D(P*DGP*DCP*DGP*DGP*DC)-3')



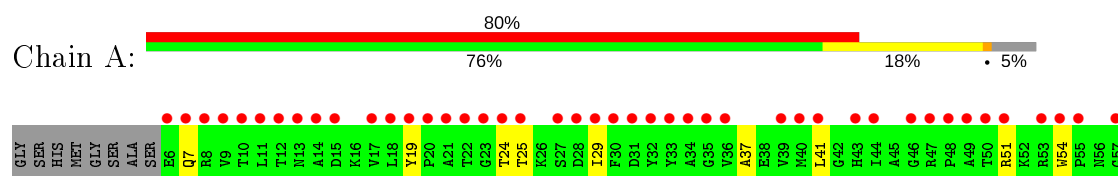
- Molecule 2: DNA (5'-D(*DGP*DCP*DCP*DGP*DCP*DAP*DAP*DCP*DGP*DCP*DA)-3')

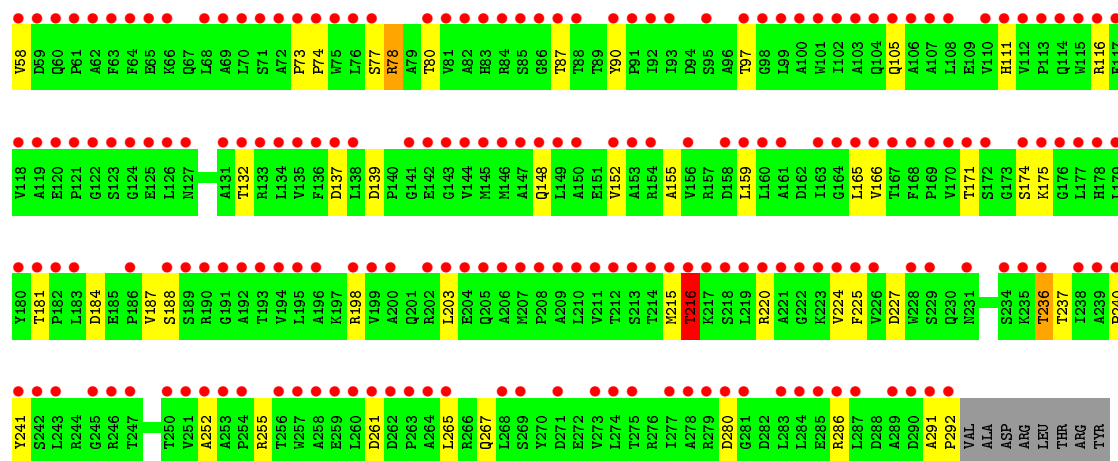


- Molecule 3: DNA (5'-D(*DGP*DCP*DCP*DGP*DCP*DAP*DAP*DCP*DGP*DCP*DAP*DCP*DG)-3')

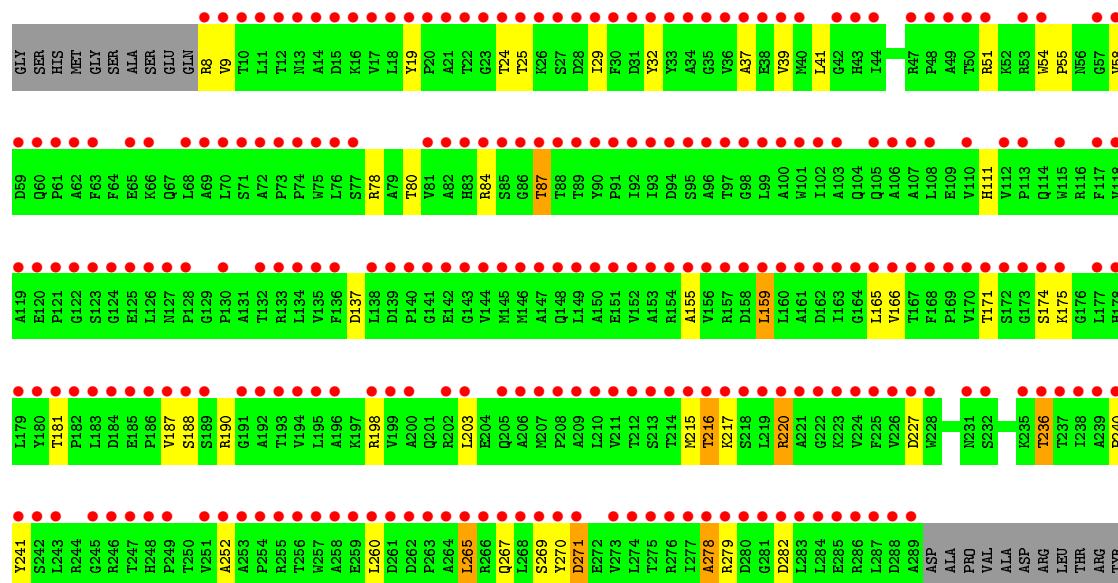
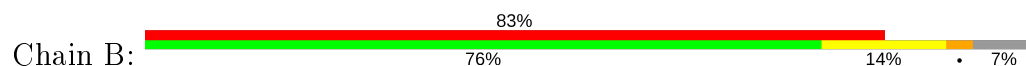


- Molecule 4: Putative DNA ligase-like protein





• Molecule 4: Putative DNA ligase-like protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.53Å 111.79Å 139.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.12 – 2.40 21.13 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.8 (21.12-2.40) 97.0 (21.13-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 2.41Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.227 , 0.272 0.231 , 0.274	Depositor DCC
R_{free} test set	1502 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	0.834	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 99.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5169	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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: PEG, EDO

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	C	1.12	1/117 (0.9%)	1.40	2/177 (1.1%)
1	E	1.16	1/117 (0.9%)	1.34	2/177 (1.1%)
2	D	0.59	0/248	1.11	1/380 (0.3%)
3	F	0.58	0/294	1.15	3/451 (0.7%)
4	A	0.38	0/2244	0.53	0/3066
4	B	0.40	2/2205 (0.1%)	0.52	2/3012 (0.1%)
All	All	0.47	4/5225 (0.1%)	0.69	10/7263 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	1	DG	OP3-P	-11.18	1.47	1.61
1	C	1	DG	OP3-P	-10.07	1.49	1.61
4	B	279	ARG	CZ-NH1	7.57	1.42	1.33
4	B	278	ALA	C-O	6.56	1.35	1.23

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1	DG	OP1-P-OP2	-7.81	107.89	119.60
1	C	1	DG	OP1-P-OP2	-7.63	108.15	119.60
1	C	1	DG	O4'-C1'-N9	-7.28	102.91	108.00
2	D	5	DC	O4'-C1'-N1	7.17	113.02	108.00
3	F	9	DG	O4'-C1'-N9	-6.58	103.40	108.00
4	B	279	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	E	1	DG	O4'-C1'-N9	-6.06	103.76	108.00
3	F	5	DC	C1'-O4'-C4'	-5.72	104.38	110.10
3	F	8	DC	C1'-O4'-C4'	-5.55	104.55	110.10
4	B	278	ALA	O-C-N	5.18	131.00	122.70

There are no chirality outliers.

There are no planarity outliers.

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	C	105	0	56	1	0
1	E	105	0	56	2	0
2	D	221	0	123	1	0
3	F	262	0	145	2	0
4	A	2193	0	2194	48	1
4	B	2155	0	2164	35	1
5	A	16	0	24	2	0
5	B	8	0	12	2	0
6	A	7	0	10	3	0
7	A	53	0	0	2	0
7	B	30	0	0	2	0
7	C	3	0	0	1	0
7	D	5	0	0	0	0
7	E	3	0	0	1	0
7	F	3	0	0	0	0
All	All	5169	0	4784	88	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 9.

All (88) 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)
4:A:116:ARG:NH2	4:A:291:ALA:HA	1.38	1.37
4:A:116:ARG:NH2	4:A:292:PRO:HD3	1.66	1.08
4:A:116:ARG:HH21	4:A:292:PRO:HD3	0.94	1.07
4:A:116:ARG:HH22	4:A:291:ALA:CA	1.75	0.97
4:A:198:ARG:NH2	6:A:297:PEG:O1	2.00	0.94
4:A:116:ARG:HH21	4:A:292:PRO:CD	1.82	0.92
4:A:116:ARG:HH22	4:A:291:ALA:HA	0.86	0.84
4:A:198:ARG:HH22	6:A:297:PEG:HO1	1.19	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:237:THR:HA	5:A:295:EDO:H12	1.61	0.82
4:A:116:ARG:NH2	4:A:291:ALA:CA	2.34	0.80
1:C:3:DG:OP2	7:C:16:HOH:O	2.05	0.74
4:B:159:LEU:HD22	4:B:203:LEU:HD13	1.72	0.72
4:B:165:LEU:HB3	4:B:181:THR:HG21	1.71	0.72
4:A:155:ALA:HB1	4:A:203:LEU:HD11	1.73	0.71
4:A:139:ASP:OD2	4:A:220:ARG:NH2	2.27	0.67
4:B:8:ARG:CG	4:B:9:VAL:N	2.56	0.67
4:A:166:VAL:HG11	4:A:286:ARG:HH12	1.58	0.67
4:A:165:LEU:HB3	4:A:181:THR:HG21	1.77	0.67
4:B:111:HIS:HB3	4:B:236:THR:HG23	1.77	0.66
4:B:8:ARG:HG2	4:B:9:VAL:N	2.08	0.66
4:B:166:VAL:O	4:B:181:THR:HG23	1.96	0.66
4:B:8:ARG:CG	4:B:9:VAL:H	2.11	0.64
4:B:278:ALA:O	7:B:315:HOH:O	2.14	0.64
4:B:165:LEU:HB3	4:B:181:THR:CG2	2.28	0.63
4:A:166:VAL:O	4:A:181:THR:HG23	1.98	0.63
4:A:165:LEU:HB3	4:A:181:THR:CG2	2.28	0.62
4:A:7:GLN:HB3	4:A:97:THR:HG21	1.82	0.62
4:B:155:ALA:HB1	4:B:203:LEU:HD11	1.80	0.61
1:E:3:DG:O6	7:E:31:HOH:O	2.15	0.60
4:A:148:GLN:O	4:A:152:VAL:HG23	2.02	0.59
4:A:155:ALA:CB	4:A:203:LEU:HD11	2.31	0.59
4:A:111:HIS:HB3	4:A:236:THR:HG23	1.87	0.57
4:B:271:ASP:N	4:B:271:ASP:OD1	2.33	0.56
4:A:220:ARG:NH1	4:A:220:ARG:HB3	2.21	0.55
4:A:25:THR:O	4:A:29:ILE:HG12	2.05	0.55
4:A:166:VAL:HG11	4:A:286:ARG:NH1	2.22	0.55
4:A:37:ALA:O	4:A:41:LEU:HG	2.07	0.54
4:A:220:ARG:HB3	4:A:220:ARG:HH11	1.72	0.54
4:B:240:PRO:O	4:B:241:TYR:HB2	2.08	0.54
4:B:187:VAL:HG22	4:B:188:SER:N	2.25	0.52
4:B:236:THR:O	5:B:293:EDO:H21	2.09	0.52
4:B:260:LEU:HA	4:B:265:LEU:HD13	1.93	0.51
4:B:19:TYR:HB2	4:B:24:THR:HB	1.94	0.50
4:B:25:THR:O	4:B:29:ILE:HG12	2.11	0.50
4:A:187:VAL:HG22	4:A:188:SER:N	2.26	0.49
4:B:190:ARG:NH2	7:B:321:HOH:O	2.20	0.49
4:B:37:ALA:O	4:B:41:LEU:HG	2.12	0.49
4:A:19:TYR:HB2	4:A:24:THR:HB	1.94	0.49
2:D:1:DG:H1'	2:D:2:DC:H5'	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:240:PRO:O	4:A:241:TYR:HB2	2.13	0.48
4:A:198:ARG:NH2	6:A:297:PEG:HO1	1.96	0.48
4:A:215:MET:O	4:A:216:THR:C	2.52	0.48
4:B:137:ASP:HB3	4:B:227:ASP:HB3	1.95	0.48
4:B:8:ARG:CD	4:B:9:VAL:H	2.28	0.47
4:A:220:ARG:HD3	4:A:225:PHE:HB2	1.97	0.46
4:A:255:ARG:NH2	4:A:265:LEU:HD12	2.30	0.46
3:F:6:DA:H2''	3:F:7:DA:C8	2.50	0.46
4:A:105:GLN:NE2	7:A:335:HOH:O	2.44	0.46
4:B:54:TRP:CD1	4:B:58:VAL:HA	2.51	0.46
4:B:215:MET:O	4:B:216:THR:C	2.54	0.46
4:A:171:THR:O	4:A:252:ALA:HA	2.17	0.45
4:A:187:VAL:HG22	4:A:188:SER:H	1.81	0.45
4:A:137:ASP:HB3	4:A:227:ASP:HB3	1.99	0.45
4:B:187:VAL:HG22	4:B:188:SER:H	1.81	0.44
4:B:171:THR:O	4:B:252:ALA:HA	2.17	0.44
4:A:148:GLN:HG2	4:A:224:VAL:HG23	1.98	0.44
4:A:78:ARG:HB2	4:A:90:TYR:O	2.18	0.44
4:B:236:THR:N	5:B:293:EDO:O1	2.51	0.44
4:B:80:THR:HG23	4:B:87:THR:HG23	1.99	0.44
3:F:13:DG:N3	3:F:13:DG:H2'	2.32	0.44
4:B:215:MET:O	4:B:220:ARG:HD3	2.18	0.44
4:A:174:SER:HB3	4:A:175:LYS:H	1.60	0.44
4:B:174:SER:HB3	4:B:175:LYS:H	1.63	0.43
1:E:1:DG:C8	4:B:55:PRO:HB3	2.54	0.43
4:A:236:THR:HG22	5:A:295:EDO:O2	2.19	0.43
4:B:32:TYR:CD1	4:B:270:TYR:HB2	2.53	0.43
4:B:217:LYS:HA	4:B:220:ARG:HG3	2.00	0.43
4:A:54:TRP:CD1	4:A:58:VAL:HA	2.53	0.43
4:A:220:ARG:CD	4:A:225:PHE:HB2	2.49	0.42
4:B:39:VAL:HG12	4:B:282:ASP:HB2	2.00	0.42
4:A:261:ASP:OD1	7:A:338:HOH:O	2.22	0.42
4:A:73:PRO:HA	4:A:74:PRO:HD3	1.84	0.42
4:A:116:ARG:HD3	4:A:132:THR:HG21	2.02	0.42
4:A:80:THR:CG2	4:A:87:THR:HG23	2.49	0.42
4:A:171:THR:HB	4:A:267:GLN:OE1	2.21	0.41
4:B:39:VAL:CG1	4:B:282:ASP:HB2	2.51	0.41
4:B:171:THR:HB	4:B:267:GLN:OE1	2.21	0.41
4:A:116:ARG:NH2	4:A:292:PRO:CD	2.57	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)
4:A:184:ASP:OD2	4:B:198:ARG:NH1[3_544]	2.03	0.17

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	
4	A	285/303 (94%)	269 (94%)	15 (5%)	1 (0%)	34	48
4	B	280/303 (92%)	269 (96%)	10 (4%)	1 (0%)	34	48
All	All	565/606 (93%)	538 (95%)	25 (4%)	2 (0%)	34	48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	216	THR
4	A	216	THR

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	
4	A	230/242 (95%)	223 (97%)	7 (3%)	41	61
4	B	226/242 (93%)	216 (96%)	10 (4%)	28	45
All	All	456/484 (94%)	439 (96%)	17 (4%)	34	53

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	51	ARG
4	A	77	SER
4	A	78	ARG
4	A	159	LEU
4	A	216	THR
4	A	236	THR
4	A	280	ASP
4	B	51	ARG
4	B	78	ARG
4	B	84	ARG
4	B	87	THR
4	B	159	LEU
4	B	220	ARG
4	B	236	THR
4	B	265	LEU
4	B	269	SER
4	B	271	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	60	GLN
4	B	60	GLN
4	B	148	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

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	EDO	A	294	-	3,3,3	0.51	0	2,2,2	0.22	0
5	EDO	B	293	-	3,3,3	0.45	0	2,2,2	0.35	0
5	EDO	A	295	-	3,3,3	0.57	0	2,2,2	0.10	0
5	EDO	A	293	-	3,3,3	0.46	0	2,2,2	0.31	0
5	EDO	A	296	-	3,3,3	0.38	0	2,2,2	0.53	0
6	PEG	A	297	-	6,6,6	0.47	0	5,5,5	0.26	0
5	EDO	B	294	-	3,3,3	0.43	0	2,2,2	0.39	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
5	EDO	A	294	-	-	0/1/1/1	-
5	EDO	B	293	-	-	1/1/1/1	-
5	EDO	A	295	-	-	1/1/1/1	-
5	EDO	A	293	-	-	0/1/1/1	-
5	EDO	A	296	-	-	1/1/1/1	-
6	PEG	A	297	-	-	3/4/4/4	-
5	EDO	B	294	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	297	PEG	O2-C3-C4-O4
5	A	295	EDO	O1-C1-C2-O2
5	A	296	EDO	O1-C1-C2-O2
5	B	293	EDO	O1-C1-C2-O2
6	A	297	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
6	A	297	PEG	O1-C1-C2-O2
5	B	294	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	293	EDO	2	0
5	A	295	EDO	2	0
6	A	297	PEG	3	0

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	C	5/5 (100%)	3.16	5 (100%) 0 0	89, 89, 89, 89	0
1	E	5/5 (100%)	4.24	5 (100%) 0 0	89, 89, 89, 89	0
2	D	11/11 (100%)	2.85	8 (72%) 0 0	84, 88, 91, 91	0
3	F	13/13 (100%)	3.53	12 (92%) 0 0	83, 90, 94, 94	0
4	A	287/303 (94%)	3.63	241 (83%) 0 0	83, 89, 100, 109	6 (2%)
4	B	282/303 (93%)	4.49	251 (89%) 0 0	82, 89, 96, 102	17 (6%)
All	All	603/640 (94%)	4.02	522 (86%) 0 0	82, 89, 98, 109	23 (3%)

All (522) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	258	ALA	15.3
4	B	29	ILE	12.2
4	B	281	GLY	11.9
4	B	263	PRO	11.4
4	A	121	PRO	10.8
4	B	221	ALA	10.5
4	B	262	ASP	10.3
4	B	243	LEU	10.2
4	A	145	MET	9.8
4	B	33	TYR	9.7
4	B	273	VAL	9.7
4	B	161	ALA	9.6
4	B	265	LEU	9.5
4	B	156	VAL	9.4
4	B	147	ALA	9.4
4	B	277	ILE	9.3
4	B	18	LEU	9.0
4	B	271	ASP	8.9
4	B	209	ALA	8.5

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Mol	Chain	Res	Type	RSRZ
4	A	216	THR	8.3
4	B	289	ALA	8.3
4	A	218	SER	8.2
4	B	123	SER	8.2
4	B	108	LEU	8.2
4	A	149	LEU	8.1
4	B	275	THR	8.1
4	A	102	ILE	8.0
4	A	108	LEU	7.9
4	A	138	LEU	7.9
4	A	160	LEU	7.9
4	B	144	VAL	7.8
4	B	211	VAL	7.7
4	B	96	ALA	7.6
4	B	149	LEU	7.5
4	A	219	LEU	7.5
4	B	102	ILE	7.5
4	B	218	SER	7.4
4	B	122	GLY	7.4
4	B	19	TYR	7.4
4	B	284	LEU	7.4
4	A	203	LEU	7.3
4	A	179	LEU	7.3
4	B	210	LEU	7.3
4	B	260	LEU	7.3
4	B	177	LEU	7.2
4	A	260	LEU	7.2
4	B	179	LEU	7.2
4	B	287	LEU	7.1
4	B	164	GLY	7.1
4	B	152	VAL	7.1
4	B	8	ARG	7.0
4	A	136	PHE	7.0
4	B	36	VAL	7.0
4	A	122	GLY	7.0
4	B	261	ASP	7.0
4	A	103	ALA	6.9
4	B	97	THR	6.9
4	A	29	ILE	6.9
4	B	264	ALA	6.8
4	A	156	VAL	6.8
4	B	121	PRO	6.8

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Mol	Chain	Res	Type	RSRZ
4	B	226	VAL	6.8
4	B	274	LEU	6.7
4	A	106	ALA	6.7
4	B	103	ALA	6.7
4	B	76	LEU	6.6
4	B	134	LEU	6.6
4	A	144	VAL	6.6
4	B	9	VAL	6.6
4	B	106	ALA	6.6
4	A	196	ALA	6.5
4	B	34	ALA	6.5
4	B	280	ASP	6.5
4	B	10	THR	6.5
4	B	93	ILE	6.4
4	B	107	ALA	6.4
4	B	124	GLY	6.4
4	B	171	THR	6.4
4	B	167	THR	6.4
4	A	134	LEU	6.3
4	B	85	SER	6.3
4	A	215	MET	6.3
4	B	278	ALA	6.3
4	A	200	ALA	6.3
4	B	206	ALA	6.2
4	B	219	LEU	6.2
4	A	258	ALA	6.1
4	A	119	ALA	6.1
4	B	216	THR	6.1
4	B	184	ASP	6.1
4	A	273	VAL	6.1
4	A	19	TYR	6.1
4	B	86	GLY	6.0
4	B	15	ASP	6.0
4	B	119	ALA	6.0
4	A	262	ASP	6.0
4	A	265	LEU	6.0
4	A	146	MET	6.0
4	A	107	ALA	6.0
4	A	192	ALA	6.0
4	A	226	VAL	6.0
4	A	243	LEU	6.0
4	B	154	ARG	6.0

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Mol	Chain	Res	Type	RSRZ
4	B	143	GLY	6.0
4	B	136	PHE	6.0
4	B	205	GLN	5.9
4	A	135	VAL	5.9
4	B	183	LEU	5.9
4	B	196	ALA	5.9
4	A	21	ALA	5.8
4	B	27	SER	5.8
4	A	263	PRO	5.8
4	A	99	LEU	5.8
4	A	274	LEU	5.8
4	A	152	VAL	5.8
4	B	146	MET	5.8
4	A	110	VAL	5.7
4	B	138	LEU	5.7
4	B	120	GLU	5.7
4	A	18	LEU	5.7
4	B	200	ALA	5.7
4	A	44	ILE	5.7
4	B	160	LEU	5.6
4	B	173	GLY	5.6
4	B	40	MET	5.6
4	A	82	ALA	5.6
4	A	72	ALA	5.6
4	A	292	PRO	5.6
4	A	210	LEU	5.6
4	A	61	PRO	5.5
4	A	205	GLN	5.5
4	A	59	ASP	5.5
4	A	264	ALA	5.5
4	B	60	GLN	5.5
4	B	199	VAL	5.5
4	A	211	VAL	5.5
4	A	112	VAL	5.4
4	B	110	VAL	5.4
4	A	34	ALA	5.4
4	B	70	LEU	5.4
4	A	224	VAL	5.4
4	A	14	ALA	5.4
4	A	170	VAL	5.4
4	B	25	THR	5.4
4	A	221	ALA	5.3

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Mol	Chain	Res	Type	RSRZ
4	B	259	GLU	5.3
4	A	188	SER	5.3
4	B	282	ASP	5.3
4	A	76	LEU	5.3
4	A	33	TYR	5.3
1	E	4	DG	5.2
4	B	74	PRO	5.2
3	F	2	DC	5.2
4	A	85	SER	5.2
4	B	59	ASP	5.2
4	A	6	GLU	5.1
4	B	170	VAL	5.1
4	B	145	MET	5.1
4	A	93	ILE	5.1
4	B	256	THR	5.1
4	B	13	ASN	5.0
4	A	87	THR	5.0
4	B	22	THR	5.0
4	B	158	ASP	5.0
4	A	86	GLY	5.0
4	B	151	GLU	4.9
4	B	12	THR	4.9
4	B	72	ALA	4.9
4	B	192	ALA	4.9
4	B	220	ARG	4.9
4	B	153	ALA	4.9
4	B	215	MET	4.9
3	F	13	DG	4.9
4	A	183	LEU	4.8
4	B	181	THR	4.8
4	B	21	ALA	4.8
4	B	49	ALA	4.8
4	A	190	ARG	4.8
4	B	270	TYR	4.8
4	B	224	VAL	4.8
4	A	278	ALA	4.8
4	B	71	SER	4.8
4	B	61	PRO	4.8
4	B	35	GLY	4.7
4	A	199	VAL	4.7
4	A	279	ARG	4.7
4	A	124	GLY	4.7

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Mol	Chain	Res	Type	RSRZ
4	A	36	VAL	4.7
4	A	49	ALA	4.7
4	B	99	LEU	4.7
4	A	180	TYR	4.7
4	B	247	THR	4.7
4	B	165	LEU	4.7
4	B	217	LYS	4.6
4	B	92	ILE	4.6
4	B	248	HIS	4.6
4	A	287	LEU	4.6
3	F	1	DG	4.6
4	A	73	PRO	4.6
2	D	2	DC	4.6
4	A	147	ALA	4.6
3	F	12	DC	4.5
4	B	68	LEU	4.5
4	B	11	LEU	4.5
4	B	195	LEU	4.5
4	A	277	ILE	4.5
4	A	290	ASP	4.5
4	A	247	THR	4.5
4	A	100	ALA	4.5
4	A	291	ALA	4.5
4	A	223	LYS	4.5
4	A	261	ASP	4.4
4	A	165	LEU	4.4
1	E	2	DC	4.3
4	B	83	HIS	4.3
4	B	240	PRO	4.3
4	B	135	VAL	4.3
2	D	4	DG	4.3
4	A	177	LEU	4.3
4	A	142	GLU	4.3
4	B	58	VAL	4.3
4	B	207	MET	4.3
1	E	3	DG	4.3
4	B	39	VAL	4.3
4	B	126	LEU	4.3
4	B	28	ASP	4.2
4	B	31	ASP	4.2
4	B	193	THR	4.2
4	A	27	SER	4.2

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Mol	Chain	Res	Type	RSRZ
4	B	17	VAL	4.2
4	B	285	GLU	4.2
4	B	241	TYR	4.2
4	B	44	ILE	4.2
4	B	30	PHE	4.2
4	B	186	PRO	4.2
4	A	98	GLY	4.1
4	B	98	GLY	4.1
4	A	120	GLU	4.1
4	A	39	VAL	4.1
4	B	213	SER	4.1
4	B	163	ILE	4.1
4	A	141	GLY	4.1
4	A	212	THR	4.1
4	B	252	ALA	4.1
4	B	254	PRO	4.0
4	B	95	SER	4.0
4	B	87	THR	4.0
4	A	123	SER	4.0
4	A	167	THR	4.0
4	A	8	ARG	3.9
4	A	68	LEU	3.9
4	B	283	LEU	3.9
4	A	10	THR	3.9
4	B	159	LEU	3.9
4	A	50	THR	3.9
4	A	15	ASP	3.9
4	B	269	SER	3.9
2	D	3	DC	3.9
4	B	203	LEU	3.9
4	B	73	PRO	3.9
4	A	164	GLY	3.8
4	B	155	ALA	3.8
4	A	31	ASP	3.8
4	A	92	ILE	3.8
4	B	162	ASP	3.8
4	B	32	TYR	3.8
4	B	105	GLN	3.8
4	B	148	GLN	3.8
4	B	38	GLU	3.8
4	A	214	THR	3.8
1	C	3	DG	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	5	DC	3.8
4	A	195	LEU	3.8
4	B	127	ASN	3.8
4	A	251	VAL	3.8
4	A	23	GLY	3.8
4	A	13	ASN	3.8
1	E	1	DG	3.8
4	A	171	THR	3.8
4	A	126	LEU	3.7
4	A	271	ASP	3.7
4	A	217	LYS	3.7
4	B	286	ARG	3.7
1	C	4	DG	3.7
4	B	101	TRP	3.7
4	B	23	GLY	3.7
4	A	240	PRO	3.7
4	A	143	GLY	3.7
4	A	63	PHE	3.7
4	B	166	VAL	3.7
4	A	207	MET	3.7
4	B	222	GLY	3.7
4	B	187	VAL	3.7
4	A	83	HIS	3.7
4	B	266	ARG	3.7
4	B	288	ASP	3.7
4	A	75	TRP	3.7
4	A	257	TRP	3.7
4	A	191	GLY	3.6
4	A	284	LEU	3.6
4	B	112	VAL	3.6
4	B	194	VAL	3.6
1	E	5	DC	3.6
4	A	55	PRO	3.6
3	F	10	DC	3.6
4	B	208	PRO	3.6
4	A	153	ALA	3.6
4	B	268	LEU	3.6
4	A	40	MET	3.6
4	A	163	ILE	3.5
4	A	32	TYR	3.5
4	A	275	THR	3.5
4	A	22	THR	3.5

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Mol	Chain	Res	Type	RSRZ
4	A	181	THR	3.5
4	A	53	ARG	3.5
4	B	223	LYS	3.5
4	A	213	SER	3.5
4	B	77	SER	3.5
4	B	189	SER	3.5
4	A	105	GLN	3.5
4	A	133	ARG	3.5
4	B	117	PHE	3.4
4	A	24	THR	3.4
4	A	250	THR	3.4
4	A	252	ALA	3.4
4	A	51	ARG	3.4
4	B	75	TRP	3.4
4	B	43	HIS	3.4
2	D	1	DG	3.4
4	A	101	TRP	3.4
4	A	150	ALA	3.4
4	B	20	PRO	3.4
4	B	115	TRP	3.4
4	B	132	THR	3.4
4	B	180	TYR	3.4
4	B	16	LYS	3.4
3	F	8	DC	3.3
4	A	176	GLY	3.3
4	A	280	ASP	3.3
4	B	257	TRP	3.3
4	A	161	ALA	3.3
4	A	241	TYR	3.3
4	A	238	ILE	3.3
4	B	130	PRO	3.3
4	B	14	ALA	3.3
3	F	11	DA	3.3
4	B	185	GLU	3.3
4	B	69	ALA	3.3
4	B	89	THR	3.3
4	B	249	PRO	3.3
4	B	239	ALA	3.3
4	B	182	PRO	3.2
4	B	37	ALA	3.2
3	F	9	DG	3.2
3	F	5	DC	3.2

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Mol	Chain	Res	Type	RSRZ
4	B	150	ALA	3.2
4	B	118	VAL	3.2
4	B	125	GLU	3.2
4	B	141	GLY	3.2
4	B	53	ARG	3.2
4	B	91	PRO	3.2
4	A	231	ASN	3.2
4	B	24	THR	3.2
3	F	4	DG	3.2
4	A	209	ALA	3.2
4	A	12	THR	3.1
4	A	256	THR	3.1
4	B	255	ARG	3.1
4	B	279	ARG	3.1
2	D	10	DC	3.1
4	B	82	ALA	3.1
4	A	259	GLU	3.1
4	A	254	PRO	3.1
4	B	169	PRO	3.1
4	A	159	LEU	3.1
4	B	251	VAL	3.1
4	B	26	LYS	3.1
4	B	140	PRO	3.1
4	A	104	GLN	3.1
4	A	127	ASN	3.1
4	B	157	ARG	3.1
4	A	194	VAL	3.1
4	A	64	PHE	3.0
4	A	20	PRO	3.0
4	A	239	ALA	3.0
4	B	50	THR	3.0
4	A	169	PRO	3.0
4	A	117	PHE	3.0
4	B	48	PRO	3.0
4	B	133	ARG	2.9
4	A	115	TRP	2.9
4	A	225	PHE	2.9
4	B	100	ALA	2.9
4	B	236	THR	2.9
4	A	81	VAL	2.9
4	A	114	GLN	2.9
4	B	231	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
4	B	237	THR	2.9
4	B	245	GLY	2.8
4	B	198	ARG	2.8
4	A	54	TRP	2.8
4	B	202	ARG	2.8
4	A	245	GLY	2.8
4	A	204	GLU	2.8
4	A	47	ARG	2.8
4	A	168	PHE	2.8
4	A	289	ALA	2.8
4	A	148	GLN	2.8
4	B	267	GLN	2.8
4	B	174	SER	2.8
4	A	242	SER	2.7
4	A	7	GLN	2.7
4	A	90	TYR	2.7
4	B	238	ILE	2.7
4	B	242	SER	2.7
4	A	9	VAL	2.7
4	A	88	THR	2.7
4	B	232	SER	2.7
4	B	225	PHE	2.7
4	A	25	THR	2.7
4	B	172	SER	2.7
4	A	202	ARG	2.7
3	F	3	DC	2.6
4	A	198	ARG	2.6
4	A	246	ARG	2.6
4	B	188	SER	2.6
4	A	116	ARG	2.6
4	A	46	GLY	2.6
4	A	166	VAL	2.6
4	B	62	ALA	2.6
4	A	220	ARG	2.6
4	A	74	PRO	2.6
4	A	91	PRO	2.6
4	A	206	ALA	2.6
4	A	236	THR	2.6
4	A	234	SER	2.6
4	B	81	VAL	2.5
4	A	285	GLU	2.5
4	A	131	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
4	B	253	ALA	2.5
4	B	51	ARG	2.5
3	F	7	DA	2.5
4	A	118	VAL	2.5
4	A	30	PHE	2.5
4	A	66	LYS	2.5
4	A	132	THR	2.5
4	B	90	TYR	2.5
4	A	58	VAL	2.5
4	A	111	HIS	2.5
4	A	222	GLY	2.5
4	A	154	ARG	2.5
2	D	9	DG	2.5
4	A	235	LYS	2.5
4	A	113	PRO	2.5
4	A	253	ALA	2.5
4	A	193	THR	2.5
4	A	175	LYS	2.4
4	A	189	SER	2.4
4	B	139	ASP	2.4
4	B	66	LYS	2.4
4	B	175	LYS	2.4
4	A	11	LEU	2.4
4	B	88	THR	2.4
2	D	5	DC	2.4
4	A	43	HIS	2.4
4	A	137	ASP	2.4
4	B	94	ASP	2.4
4	B	47	ARG	2.4
4	A	17	VAL	2.4
4	A	35	GLY	2.3
4	A	70	LEU	2.3
4	A	48	PRO	2.3
4	B	246	ARG	2.3
4	A	283	LEU	2.3
4	A	60	GLN	2.3
4	A	158	ASP	2.3
4	A	228	TRP	2.3
4	A	269	SER	2.3
1	C	1	DG	2.3
4	A	178	HIS	2.3
4	A	125	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
4	A	95	SER	2.2
4	A	80	THR	2.2
4	A	268	LEU	2.2
1	C	2	DC	2.2
4	A	182	PRO	2.2
4	A	28	ASP	2.2
4	A	172	SER	2.2
4	B	63	PHE	2.2
4	B	168	PHE	2.2
4	B	54	TRP	2.2
4	A	286	ARG	2.2
4	B	276	ARG	2.2
4	B	142	GLU	2.2
4	B	113	PRO	2.1
4	B	178	HIS	2.1
4	B	227	ASP	2.1
4	B	228	TRP	2.1
4	B	84	ARG	2.1
4	A	174	SER	2.1
4	A	62	ALA	2.1
4	A	97	THR	2.1
4	A	77	SER	2.1
4	A	57	GLY	2.1
4	B	65	GLU	2.1
4	A	69	ALA	2.1
4	A	84	ARG	2.1
4	A	186	PRO	2.1
4	B	128	PRO	2.1
4	B	214	THR	2.1
4	A	41	LEU	2.1
4	A	229	SER	2.1
4	B	42	GLY	2.1
4	B	191	GLY	2.0
4	B	235	LYS	2.0
4	B	57	GLY	2.0
2	D	8	DC	2.0
4	B	212	THR	2.0
4	A	71	SER	2.0
4	A	281	GLY	2.0
4	A	65	GLU	2.0
4	A	208	PRO	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 carbohydrates 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(\AA^2)	Q<0.9
6	PEG	A	297	7/7	0.55	0.30	100,107,110,111	0
5	EDO	B	293	4/4	0.68	0.42	91,96,96,103	0
5	EDO	A	294	4/4	0.73	0.24	90,92,93,97	0
5	EDO	A	295	4/4	0.76	0.28	84,86,90,91	0
5	EDO	B	294	4/4	0.89	0.34	99,100,101,101	0
5	EDO	A	293	4/4	0.93	0.22	87,90,91,92	0
5	EDO	A	296	4/4	0.93	0.15	84,84,88,92	0

6.5 Other polymers [i](#)

There are no such residues in this entry.