



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:37 PM GMT

PDB ID : 4PEH
Title : Dbr1 in complex with synthetic linear RNA
Authors : Montemayor, E.J.; Katolik, A.; Clark, N.E.; Taylor, A.B.; Schuermann, J.P.; Combs, D.J.; Johnsson, R.; Holloway, S.P.; Stevens, S.W.; Damha, M.J.; Hart, P.J.
Deposited on : 2014-04-23
Resolution : 2.10 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

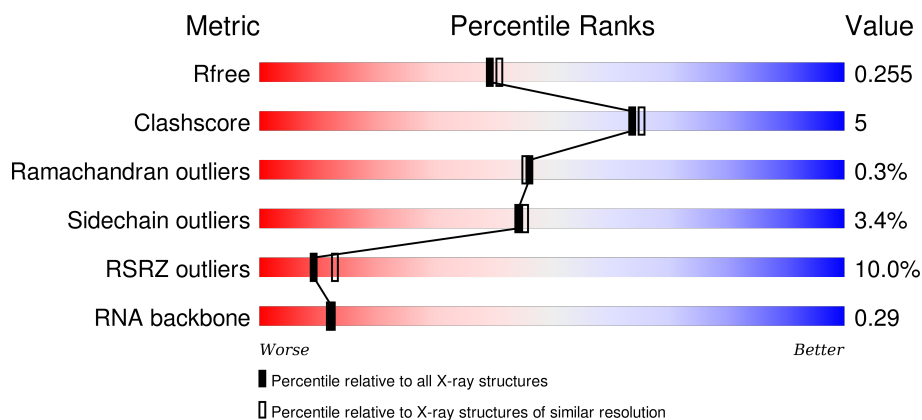
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)
RNA backbone	2183	1118 (2.80-1.40)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	356	<div> <div>10%</div> <div>85%</div> <div>12%</div> <div>..</div> </div>
1	B	356	<div> <div>9%</div> <div>83%</div> <div>15%</div> <div>..</div> </div>
1	C	356	<div> <div>6%</div> <div>87%</div> <div>10%</div> <div>..</div> </div>
1	D	356	<div> <div>10%</div> <div>85%</div> <div>12%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	E	356	
2	V	7	
2	W	7	
2	X	7	
2	Y	7	
2	Z	7	

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
4	SO4	A	402	-	-	-	X
4	SO4	B	402	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15765 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 RNA lariat debranching enzyme, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	2	0
			2872	1866	469	523	14			
1	B	349	Total	C	N	O	S	0	1	0
			2860	1859	465	522	14			
1	C	349	Total	C	N	O	S	0	2	0
			2864	1861	466	523	14			
1	D	349	Total	C	N	O	S	0	0	0
			2857	1857	465	521	14			
1	E	349	Total	C	N	O	S	0	0	0
			2857	1857	465	521	14			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP C4M1P9
A	0	ALA	-	expression tag	UNP C4M1P9
A	14	SER	CYS	engineered mutation	UNP C4M1P9
B	-1	GLY	-	expression tag	UNP C4M1P9
B	0	ALA	-	expression tag	UNP C4M1P9
B	14	SER	CYS	engineered mutation	UNP C4M1P9
C	-1	GLY	-	expression tag	UNP C4M1P9
C	0	ALA	-	expression tag	UNP C4M1P9
C	14	SER	CYS	engineered mutation	UNP C4M1P9
D	-1	GLY	-	expression tag	UNP C4M1P9
D	0	ALA	-	expression tag	UNP C4M1P9
D	14	SER	CYS	engineered mutation	UNP C4M1P9
E	-1	GLY	-	expression tag	UNP C4M1P9
E	0	ALA	-	expression tag	UNP C4M1P9
E	14	SER	CYS	engineered mutation	UNP C4M1P9

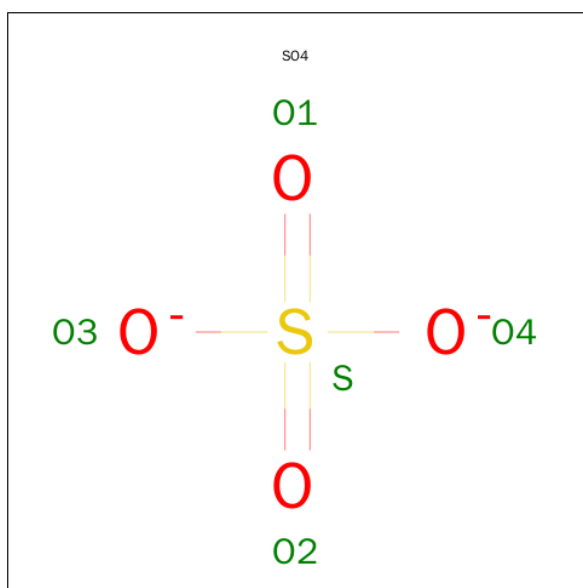
- Molecule 2 is a RNA chain called RNA (5'-R(*CP*UP*AP*(A2P)P*AP*CP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	V	4	Total	C	N	O	P	0	0	0
			69	29	13	23	4			
2	W	5	Total	C	N	O	P	0	0	1
			73	29	13	26	5			
2	X	6	Total	C	N	O	P	0	0	1
			95	39	18	32	6			
2	Y	5	Total	C	N	O	P	0	0	0
			91	39	18	29	5			
2	Z	4	Total	C	N	O	P	0	0	0
			69	29	13	23	4			

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

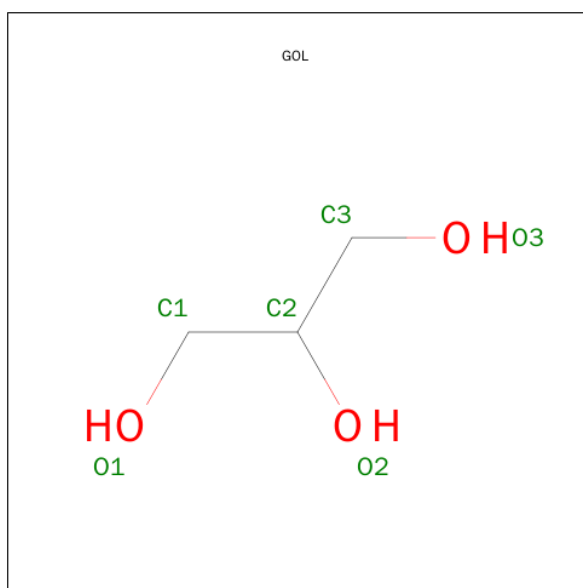
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		
3	E	1	Total	Mn	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	190	Total O 190 190	0	0

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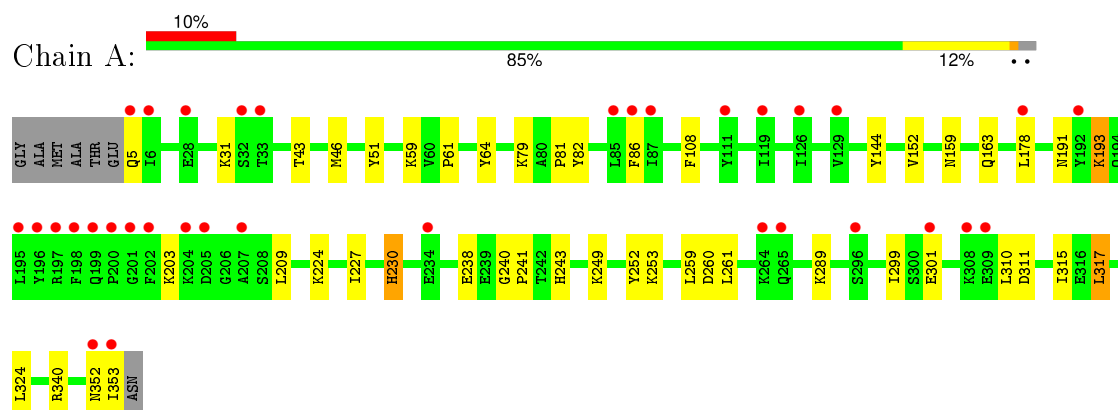
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	V	6	Total 6	O 6	0	0
6	B	208	Total 208	O 208	0	0
6	W	5	Total 5	O 5	0	0
6	C	228	Total 228	O 228	0	0
6	X	10	Total 10	O 10	0	0
6	D	191	Total 191	O 191	0	0
6	Y	2	Total 2	O 2	0	0
6	E	163	Total 163	O 163	0	0
6	Z	4	Total 4	O 4	0	0

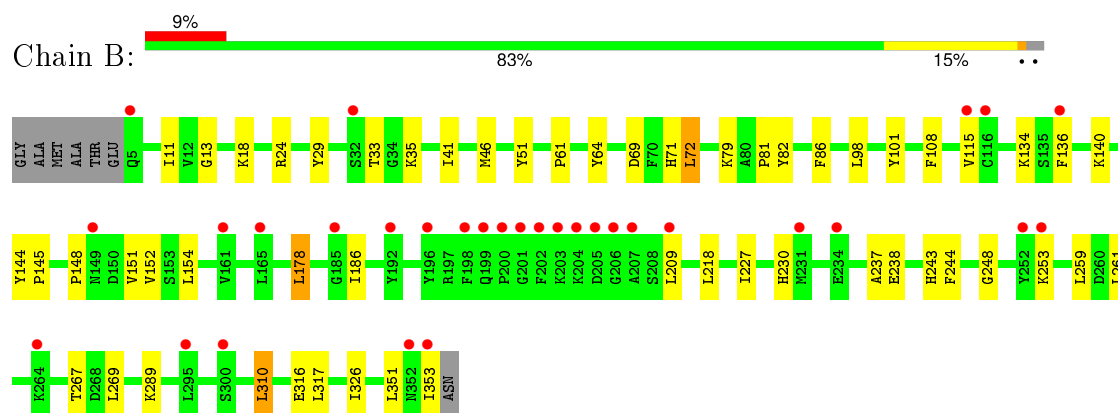
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

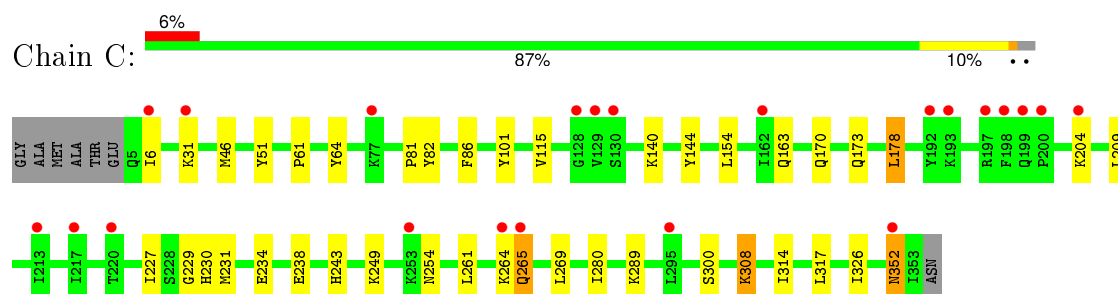
- Molecule 1: RNA lariat debranching enzyme, putative



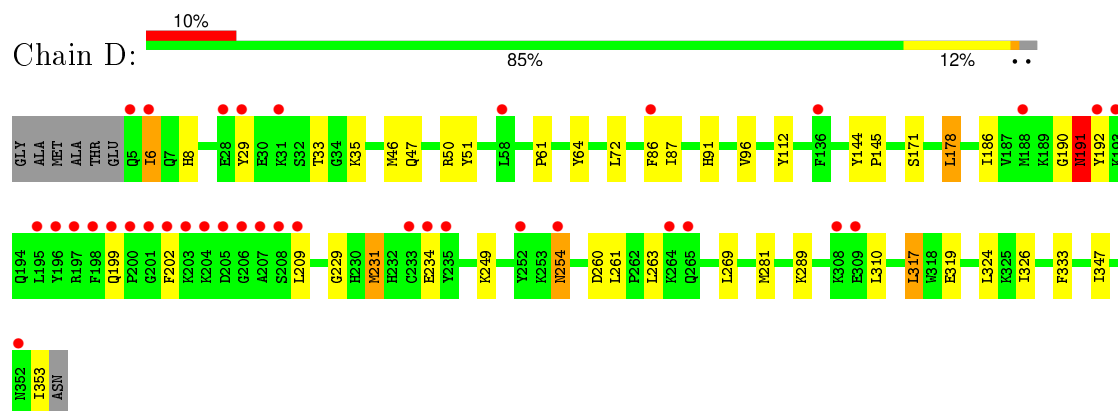
- Molecule 1: RNA lariat debranching enzyme, putative



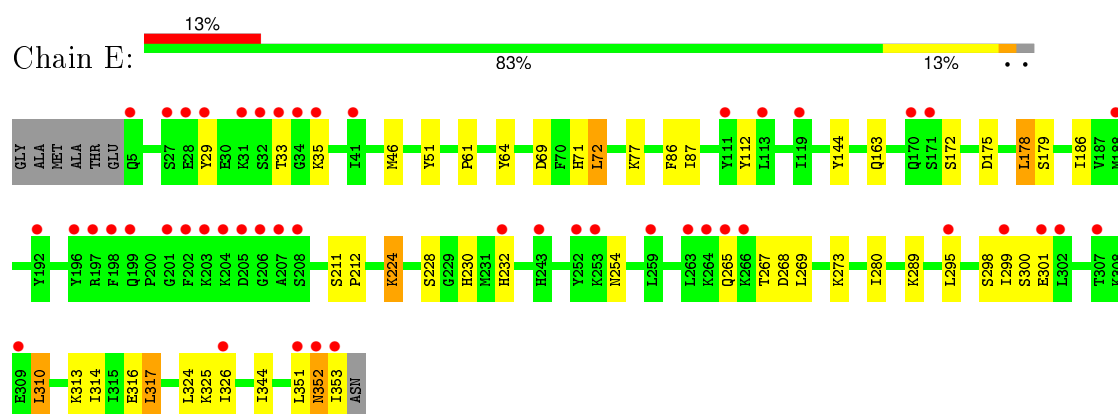
- Molecule 1: RNA lariat debranching enzyme, putative



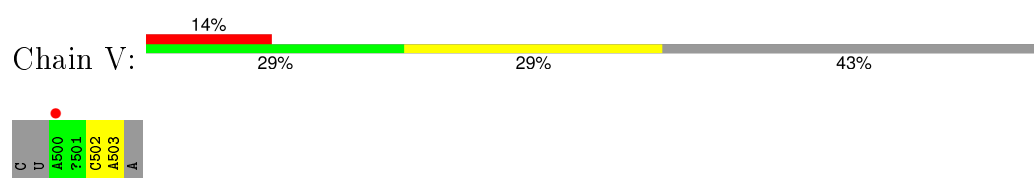
- Molecule 1: RNA lariat debranching enzyme, putative



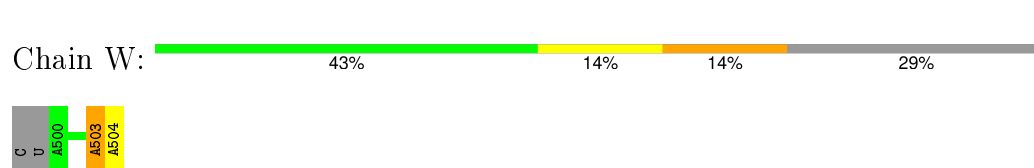
- Molecule 1: RNA lariat debranching enzyme, putative



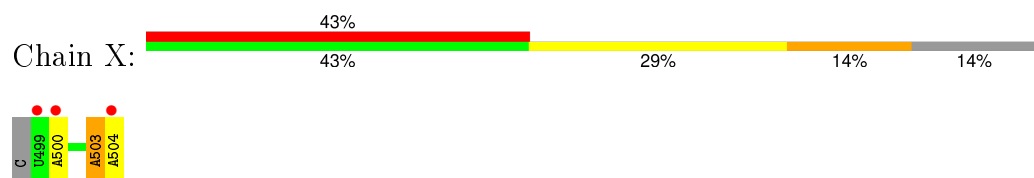
- Molecule 2: RNA (5'-R(*CP*UP*AP*(A2P)P*AP*CP*AP*A)-3')



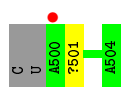
- Molecule 2: RNA (5'-R(*CP*UP*AP*(A2P)P*AP*CP*AP*A)-3')



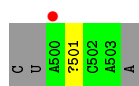
- Molecule 2: RNA (5'-R(*CP*UP*AP*(A2P)P*AP*CP*AP*A)-3')



- Molecule 2: RNA (5'-R(*CP*UP*AP*(A2P)P*AP*CP*AP*A)-3')



- Molecule 2: RNA (5'-R(*CP*UP*AP*(A2P)P*AP*CP*AP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.02Å 141.94Å 212.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.03 – 2.10 39.03 – 2.09	Depositor EDS
% Data completeness (in resolution range)	98.7 (39.03-2.10) 98.6 (39.03-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.203 , 0.247 0.211 , 0.255	Depositor DCC
R_{free} test set	6421 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 129111 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15765	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: A2P, GOL, MN, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.29	0/2954	0.46	0/3993
1	B	0.30	0/2941	0.47	0/3975
1	C	0.30	0/2945	0.47	0/3980
1	D	0.28	0/2935	0.46	0/3967
1	E	0.29	0/2935	0.46	0/3967
2	V	0.20	0/46	0.68	0/68
2	W	0.24	0/50	0.73	0/76
2	X	0.29	0/75	0.78	0/114
2	Y	0.24	0/71	0.63	0/107
2	Z	0.31	0/46	0.66	0/68
All	All	0.29	0/14998	0.47	0/20315

There are no bond length outliers.

There are no bond angle outliers.

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	A	2872	0	2844	28	0
1	B	2860	0	2837	36	0
1	C	2864	0	2839	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2857	0	2832	29	0
1	E	2857	0	2832	35	0
2	V	69	0	33	2	0
2	W	73	0	32	1	0
2	X	95	0	43	1	0
2	Y	91	0	44	1	0
2	Z	69	0	33	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	5	0	0	0	0
4	B	10	0	0	0	0
4	C	15	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
5	A	6	0	8	3	0
6	A	190	0	0	5	0
6	B	208	0	0	5	0
6	C	228	0	0	8	0
6	D	191	0	0	4	0
6	E	163	0	0	5	0
6	V	6	0	0	2	0
6	W	5	0	0	1	0
6	X	10	0	0	0	0
6	Y	2	0	0	1	0
6	Z	4	0	0	1	0
All	All	15765	0	14377	151	0

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

All (151) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:LEU:HD11	1:B:353:ILE:HD11	1.51	0.90
2:X:503:A:H4'	2:X:504:A:OP1	1.86	0.75
1:E:298:SER:HB3	1:E:301:GLU:HB2	1.69	0.74
1:B:351:LEU:HB3	1:B:353:ILE:HD12	1.70	0.72
1:A:61:PRO:HG2	1:A:64:TYR:HD2	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:PRO:O	1:B:151:VAL:HG23	1.90	0.72
1:E:33:THR:HB	1:E:35:LYS:HD3	1.74	0.70
1:D:209:LEU:HD21	1:D:231:MET:HE2	1.74	0.68
2:W:503:A:H4'	2:W:504:A:OP2	1.93	0.68
1:C:238:GLU:OE1	1:C:243:HIS:ND1	2.25	0.67
1:B:310:LEU:CD1	1:B:353:ILE:HD11	2.25	0.66
1:A:193:LYS:NZ	6:A:686:HOH:O	2.27	0.66
1:E:61:PRO:HG2	1:E:64:TYR:HD2	1.61	0.66
1:B:310:LEU:HD21	1:B:353:ILE:HD13	1.78	0.66
1:D:61:PRO:HG2	1:D:64:TYR:HD2	1.59	0.66
1:D:353:ILE:C	1:D:353:ILE:HD12	2.17	0.65
1:C:61:PRO:HG2	1:C:64:TYR:HD2	1.61	0.64
1:B:61:PRO:HG2	1:B:64:TYR:HD2	1.63	0.64
1:E:351:LEU:O	1:E:352:ASN:HB2	1.97	0.64
1:C:31:LYS:NZ	6:C:682:HOH:O	2.32	0.62
1:D:6:ILE:HA	1:D:263:LEU:H	1.65	0.61
1:E:353:ILE:O	1:E:353:ILE:HG22	2.00	0.61
1:C:249:LYS:NZ	6:C:710:HOH:O	2.34	0.60
1:A:59:LYS:NZ	2:V:503:A:OP2	2.35	0.60
1:B:353:ILE:O	1:B:353:ILE:HG22	2.02	0.59
1:A:5:GLN:NE2	6:A:662:HOH:O	2.35	0.59
1:D:47:GLN:NE2	6:D:566:HOH:O	2.29	0.59
1:C:229[A]:GLY:O	1:C:231:MET:N	2.29	0.58
1:D:87:ILE:HD13	1:D:178:LEU:HB3	1.86	0.57
1:C:170:GLN:NE2	6:C:687:HOH:O	2.35	0.57
1:A:249:LYS:HE3	1:A:252:TYR:CE2	2.39	0.57
1:A:163:GLN:HG2	5:A:403:GOL:H2	1.85	0.56
1:B:33:THR:HB	1:B:35:LYS:HD3	1.87	0.56
1:D:249:LYS:NZ	6:Y:701:HOH:O	2.37	0.56
1:B:310:LEU:HD21	1:B:353:ILE:CD1	2.36	0.55
1:B:46:MET:HG3	1:B:86:PHE:CD1	2.41	0.54
1:E:352:ASN:C	1:E:353:ILE:HG13	2.27	0.54
1:E:46:MET:HG3	1:E:86:PHE:CD1	2.42	0.54
1:D:191:ASN:ND2	6:D:666:HOH:O	2.22	0.54
1:E:268:ASP:HB2	1:E:325:LYS:HE2	1.90	0.54
1:A:230:HIS:HA	6:V:701:HOH:O	2.08	0.53
1:B:227:ILE:HD11	1:B:259:LEU:HD11	1.91	0.53
1:A:46:MET:HG3	1:A:86:PHE:CD2	2.44	0.53
1:D:254:ASN:N	1:D:254:ASN:OD1	2.40	0.52
1:A:259:LEU:HB3	1:A:261:LEU:HD13	1.92	0.52
1:E:273:LYS:NZ	6:E:588:HOH:O	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:HIS:HA	6:W:701:HOH:O	2.10	0.51
1:A:352:ASN:O	1:A:353:ILE:HG23	2.10	0.51
1:B:18:LYS:HE2	6:B:682:HOH:O	2.10	0.51
1:C:269:LEU:HG	1:C:326:ILE:HD12	1.93	0.50
1:C:46:MET:HG3	1:C:86:PHE:CD2	2.46	0.50
1:B:69:ASP:O	1:B:72:LEU:HB2	2.11	0.50
1:B:269:LEU:HG	1:B:326:ILE:HD12	1.93	0.50
1:B:41:ILE:HG23	1:B:178:LEU:HD21	1.93	0.50
1:E:87:ILE:HD13	1:E:178:LEU:HB3	1.94	0.50
1:A:203:LYS:NZ	6:A:645:HOH:O	2.42	0.49
1:E:71:HIS:CE1	1:E:72:LEU:HD13	2.47	0.49
1:C:234:GLU:HB2	1:C:254:ASN:HB2	1.95	0.49
1:A:31:LYS:HE2	6:A:660:HOH:O	2.12	0.49
1:A:340:ARG:NH1	6:A:560:HOH:O	2.35	0.49
1:C:308:LYS:NZ	6:C:646:HOH:O	2.45	0.49
1:D:33:THR:HB	1:D:35:LYS:HD3	1.95	0.48
1:C:140:LYS:NZ	6:C:596:HOH:O	2.45	0.48
1:A:193:LYS:H	1:A:193:LYS:HD3	1.79	0.48
1:E:175:ASP:OD2	6:E:594:HOH:O	2.20	0.48
1:C:264:LYS:HG2	1:C:265:GLN:HG2	1.94	0.48
1:D:46:MET:HG3	1:D:86:PHE:CD2	2.48	0.48
1:B:24:ARG:NH1	6:B:695:HOH:O	2.28	0.48
1:D:229:GLY:O	1:D:231:MET:N	2.46	0.47
1:C:280:ILE:HG13	1:C:314:ILE:HG23	1.96	0.47
1:A:79:LYS:HE2	1:A:108:PHE:CE2	2.49	0.47
1:A:59:LYS:HD3	1:A:152:VAL:HG12	1.96	0.47
1:E:273:LYS:HE3	1:E:324:LEU:HD11	1.97	0.47
1:E:232:HIS:NE2	2:Z:501:A2P:O3P	2.47	0.47
1:E:289:LYS:NZ	6:E:567:HOH:O	2.31	0.47
1:C:144:TYR:HB3	1:C:289:LYS:O	2.14	0.47
1:D:319:GLU:HG3	1:D:324:LEU:HG	1.96	0.47
1:E:280:ILE:HD13	1:E:344:ILE:HG23	1.97	0.47
1:E:77:LYS:NZ	6:E:550:HOH:O	2.48	0.46
1:A:238:GLU:OE1	1:A:243[A]:HIS:ND1	2.48	0.46
1:A:144:TYR:HB3	1:A:289:LYS:O	2.15	0.46
1:C:154:LEU:O	6:C:597:HOH:O	2.20	0.46
1:B:310:LEU:CD2	1:B:353:ILE:HD13	2.43	0.46
1:E:69:ASP:O	1:E:72:LEU:HB2	2.17	0.45
1:A:311:ASP:O	1:A:315:ILE:HG12	2.16	0.45
1:D:269:LEU:HG	1:D:326:ILE:HD12	1.98	0.45
1:D:190:GLY:O	1:D:192:TYR:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:TYR:HB3	1:D:289:LYS:O	2.15	0.45
1:E:265:GLN:CD	6:E:618:HOH:O	2.54	0.45
1:B:13:GLY:HA3	1:B:248:GLY:O	2.16	0.45
1:D:281:MET:HE3	6:D:604:HOH:O	2.16	0.45
1:B:140:LYS:O	6:B:541:HOH:O	2.21	0.45
1:E:254:ASN:N	1:E:254:ASN:OD1	2.50	0.44
1:B:98:LEU:HD22	1:B:154:LEU:HD21	1.98	0.44
1:D:86:PHE:CZ	1:D:112:TYR:HB2	2.52	0.44
1:D:353:ILE:C	1:D:353:ILE:CD1	2.85	0.44
1:E:179:SER:OG	1:E:228:SER:OG	2.34	0.44
1:B:29:TYR:OH	1:B:35:LYS:HE2	2.18	0.44
1:B:186:ILE:HD12	1:B:218:LEU:HD11	1.99	0.44
1:B:101:TYR:HB2	1:B:115:VAL:HG23	2.00	0.44
1:B:144:TYR:HB3	1:B:289:LYS:O	2.17	0.44
1:B:18:LYS:HD2	6:B:613:HOH:O	2.18	0.44
1:B:134:LYS:HB3	1:B:136:PHE:CE1	2.53	0.44
1:D:234:GLU:HB2	1:D:254:ASN:HB2	1.99	0.44
1:D:8:HIS:ND1	1:D:260:ASP:OD1	2.40	0.43
1:E:269:LEU:HG	1:E:326:ILE:HD12	1.99	0.43
1:D:96:VAL:HG13	1:D:333:PHE:CD2	2.53	0.43
1:B:238:GLU:OE1	1:B:243:HIS:ND1	2.50	0.43
1:E:352:ASN:O	1:E:353:ILE:HG13	2.19	0.43
2:V:502:C:OP1	6:V:706:HOH:O	2.21	0.43
1:D:144:TYR:CG	1:D:145:PRO:HA	2.54	0.43
1:A:43:THR:HG21	1:A:227:ILE:HG22	2.00	0.43
1:D:29:TYR:OH	1:D:35:LYS:HE2	2.18	0.43
1:A:81:PRO:HG2	1:A:82:TYR:CD2	2.54	0.43
1:B:81:PRO:HG2	1:B:82:TYR:CD2	2.54	0.42
1:E:175:ASP:O	1:E:224:LYS:HB3	2.18	0.42
1:D:6:ILE:O	6:D:587:HOH:O	2.22	0.42
1:E:144:TYR:HB3	1:E:289:LYS:O	2.18	0.42
1:A:317:LEU:HA	1:A:317:LEU:HD12	1.83	0.42
1:B:259:LEU:HB3	1:B:261:LEU:HD13	2.02	0.42
1:B:71:HIS:CE1	1:B:72:LEU:HD13	2.55	0.42
1:C:81:PRO:HG2	1:C:82:TYR:CD2	2.55	0.42
1:A:191:ASN:OD1	1:A:193:LYS:HG2	2.19	0.42
1:B:144:TYR:CG	1:B:145:PRO:HA	2.55	0.42
1:E:163:GLN:HB3	1:E:299:ILE:HB	2.02	0.42
1:A:299:ILE:N	5:A:403:GOL:H32	2.35	0.41
1:D:91:HIS:NE2	2:Y:501:A2P:O2'	2.50	0.41
1:D:199:GLN:HB2	1:D:202:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:LEU:HB3	1:D:347:ILE:HG12	2.01	0.41
1:C:101:TYR:HB2	1:C:115:VAL:HG23	2.02	0.41
1:A:249:LYS:HE3	1:A:252:TYR:HE2	1.81	0.41
1:D:50:ARG:HD3	1:D:333:PHE:CE2	2.55	0.41
1:A:324:LEU:HD23	1:A:324:LEU:HA	1.90	0.41
1:B:237:ALA:HB3	1:B:244:PHE:HB3	2.03	0.41
1:C:173:GLN:O	6:C:628:HOH:O	2.21	0.41
1:E:29:TYR:OH	1:E:35:LYS:HE2	2.20	0.41
1:C:178:LEU:HD12	1:C:227:ILE:HB	2.02	0.41
1:E:230:HIS:HA	6:Z:703:HOH:O	2.21	0.41
1:E:310:LEU:HD13	1:E:310:LEU:HA	1.89	0.41
1:E:86:PHE:CZ	1:E:112:TYR:HB2	2.56	0.41
1:B:11:ILE:HG21	1:B:227:ILE:HD13	2.02	0.41
1:E:280:ILE:HG13	1:E:314:ILE:HG23	2.03	0.41
1:E:313:LYS:O	1:E:317:LEU:HD22	2.21	0.41
1:C:170:GLN:HB3	6:C:712:HOH:O	2.19	0.41
1:A:299:ILE:H	5:A:403:GOL:H32	1.86	0.41
1:E:316:GLU:HG2	1:E:317:LEU:HD13	2.03	0.41
1:A:240:GLY:HA3	1:A:241:PRO:HD2	1.94	0.41
1:E:295:LEU:HD23	1:E:295:LEU:HA	1.80	0.40
1:E:211:SER:HA	1:E:212:PRO:HD2	1.87	0.40
1:B:316:GLU:OE1	6:B:648:HOH:O	2.22	0.40
1:B:79:LYS:HE2	1:B:108:PHE:CE2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	349/356 (98%)	342 (98%)	6 (2%)	1 (0%)	46	45
1	B	348/356 (98%)	341 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	349/356 (98%)	340 (97%)	7 (2%)	2 (1%)	30	24
1	D	347/356 (98%)	335 (96%)	10 (3%)	2 (1%)	30	24
1	E	347/356 (98%)	334 (96%)	12 (4%)	1 (0%)	46	45
All	All	1740/1780 (98%)	1692 (97%)	42 (2%)	6 (0%)	46	45

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	191	ASN
1	A	230	HIS
1	C	230	HIS
1	C	352	ASN
1	D	254	ASN
1	E	352	ASN

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	A	318/320 (99%)	307 (96%)	11 (4%)	43	44
1	B	317/320 (99%)	308 (97%)	9 (3%)	51	55
1	C	317/320 (99%)	304 (96%)	13 (4%)	37	36
1	D	316/320 (99%)	305 (96%)	11 (4%)	43	44
1	E	316/320 (99%)	306 (97%)	10 (3%)	46	48
All	All	1584/1600 (99%)	1530 (97%)	54 (3%)	44	45

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	TYR
1	A	159	ASN
1	A	178	LEU
1	A	193	LYS

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Mol	Chain	Res	Type
1	A	209	LEU
1	A	224	LYS
1	A	253	LYS
1	A	260	ASP
1	A	301	GLU
1	A	310	LEU
1	A	317	LEU
1	B	51	TYR
1	B	72	LEU
1	B	152	VAL
1	B	178	LEU
1	B	209	LEU
1	B	253	LYS
1	B	267	THR
1	B	310	LEU
1	B	317	LEU
1	C	6	ILE
1	C	51	TYR
1	C	163	GLN
1	C	178	LEU
1	C	204	LYS
1	C	209	LEU
1	C	261	LEU
1	C	265	GLN
1	C	300[A]	SER
1	C	300[B]	SER
1	C	308	LYS
1	C	317	LEU
1	C	352	ASN
1	D	6	ILE
1	D	51	TYR
1	D	72	LEU
1	D	171	SER
1	D	178	LEU
1	D	186	ILE
1	D	191	ASN
1	D	231	MET
1	D	261	LEU
1	D	310	LEU
1	D	317	LEU
1	E	51	TYR
1	E	72	LEU

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Mol	Chain	Res	Type
1	E	172	SER
1	E	178	LEU
1	E	186	ILE
1	E	224	LYS
1	E	267	THR
1	E	300	SER
1	E	310	LEU
1	E	317	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	120	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	V	0/7	-	-
2	W	2/7 (28%)	0	1 (50%)
2	X	2/7 (28%)	1 (50%)	1 (50%)
2	Y	1/7 (14%)	0	0
2	Z	0/7	-	-
All	All	5/35 (14%)	1 (20%)	2 (40%)

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	X	500	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	W	503	A
2	X	503	A

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 5 are monoatomic - leaving 9 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	$\# Z > 2$
4	SO4	A	402	-	4,4,4	0.37	0	6,6,6	0.21	0
5	GOL	A	403	-	5,5,5	0.36	0	5,5,5	0.21	0
4	SO4	B	402	-	4,4,4	0.24	0	6,6,6	0.09	0
4	SO4	B	403	-	4,4,4	0.36	0	6,6,6	0.11	0
4	SO4	C	402	-	4,4,4	0.24	0	6,6,6	0.12	0
4	SO4	C	403	-	4,4,4	0.32	0	6,6,6	0.20	0
4	SO4	C	404	-	4,4,4	0.30	0	6,6,6	0.09	0
4	SO4	D	402	-	4,4,4	0.42	0	6,6,6	0.19	0
4	SO4	E	402	-	4,4,4	0.40	0	6,6,6	0.14	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
4	SO4	A	402	-	-	0/0/0/0	0/0/0/0
5	GOL	A	403	-	-	0/4/4/4	0/0/0/0
4	SO4	B	402	-	-	0/0/0/0	0/0/0/0
4	SO4	B	403	-	-	0/0/0/0	0/0/0/0
4	SO4	C	402	-	-	0/0/0/0	0/0/0/0
4	SO4	C	403	-	-	0/0/0/0	0/0/0/0
4	SO4	C	404	-	-	0/0/0/0	0/0/0/0
4	SO4	D	402	-	-	0/0/0/0	0/0/0/0
4	SO4	E	402	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	403	GOL	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	A	349/356 (98%)	0.61	34 (9%) 10 14	24, 37, 61, 71	0
1	B	349/356 (98%)	0.71	31 (8%) 12 16	22, 36, 60, 75	0
1	C	349/356 (98%)	0.55	22 (6%) 23 31	20, 33, 52, 66	0
1	D	349/356 (98%)	0.77	36 (10%) 9 12	21, 38, 70, 87	0
1	E	349/356 (98%)	0.96	48 (13%) 4 5	21, 42, 70, 84	0
2	V	3/7 (42%)	0.49	1 (33%) 0 1	55, 55, 59, 74	0
2	W	4/7 (57%)	0.79	0 100 100	55, 70, 73, 83	1 (25%)
2	X	5/7 (71%)	2.06	3 (60%) 0 0	45, 62, 76, 102	0
2	Y	4/7 (57%)	1.82	1 (25%) 1 1	67, 78, 86, 89	0
2	Z	3/7 (42%)	1.92	1 (33%) 0 1	54, 54, 69, 86	0
All	All	1764/1815 (97%)	0.73	177 (10%) 9 13	20, 38, 66, 102	1 (0%)

All (177) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	ILE	8.4
1	E	198	PHE	8.2
1	E	204	LYS	8.0
1	B	203	LYS	7.0
1	D	206	GLY	6.8
1	D	205	ASP	6.8
1	D	202	PHE	6.5
1	D	196	TYR	6.4
1	B	204	LYS	6.1
1	B	202	PHE	5.9
1	E	253	LYS	5.9
1	D	198	PHE	5.9
1	D	203	LYS	5.6

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Mol	Chain	Res	Type	RSRZ
1	E	263	LEU	5.5
1	D	199	GLN	5.4
2	Z	500	A	5.2
1	E	196	TYR	5.0
1	E	28	GLU	5.0
1	D	195	LEU	5.0
2	X	499	U	5.0
1	C	198	PHE	4.9
1	D	200	PRO	4.9
1	A	33	THR	4.9
1	E	353	ILE	4.8
1	B	353	ILE	4.7
1	D	192	TYR	4.7
1	B	136	PHE	4.6
1	A	198	PHE	4.6
1	B	205	ASP	4.5
1	C	6	ILE	4.5
1	D	204	LYS	4.4
1	E	33	THR	4.4
1	E	32	SER	4.3
1	E	202	PHE	4.3
1	E	205	ASP	4.3
1	D	207	ALA	4.2
1	C	264	LYS	4.2
1	A	32	SER	4.2
1	E	252	TYR	4.1
1	E	29	TYR	4.0
1	D	208	SER	3.9
1	B	206	GLY	3.9
1	B	198	PHE	3.9
1	E	5	GLN	3.8
1	E	27	SER	3.8
1	E	307	THR	3.8
1	D	31	LYS	3.8
2	Y	500	A	3.8
1	A	192	TYR	3.7
1	B	352	ASN	3.7
1	A	265	GLN	3.7
1	B	207	ALA	3.7
1	E	309	GLU	3.7
1	E	171	SER	3.7
1	E	352	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	209	LEU	3.5
1	D	209	LEU	3.5
1	A	5	GLN	3.5
1	D	136	PHE	3.5
1	A	195	LEU	3.5
1	E	31	LYS	3.4
1	E	264	LYS	3.4
1	D	352	ASN	3.4
1	C	204	LYS	3.4
1	D	254	ASN	3.4
1	D	252	TYR	3.4
1	B	196	TYR	3.3
1	E	351	LEU	3.3
1	E	35	LYS	3.2
1	C	352	ASN	3.2
1	B	253	LYS	3.2
1	E	206	GLY	3.2
1	A	197	ARG	3.1
1	E	199	GLN	3.1
1	D	265	GLN	3.1
1	D	188	MET	3.1
1	E	243	HIS	3.1
1	E	207	ALA	3.0
1	C	197	ARG	3.0
1	E	197	ARG	3.0
1	A	204	LYS	3.0
1	E	326	ILE	3.0
1	E	34	GLY	2.9
1	E	192	TYR	2.9
1	E	201	GLY	2.9
1	C	253	LYS	2.9
1	C	213	ILE	2.9
1	E	203	LYS	2.9
1	A	264	LYS	2.8
1	C	192	TYR	2.8
1	B	201	GLY	2.8
1	E	232	HIS	2.8
1	A	301	GLU	2.8
1	E	266	LYS	2.7
1	C	31	LYS	2.7
1	D	234	GLU	2.7
1	B	300[A]	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	196	TYR	2.7
1	D	309	GLU	2.7
1	B	185	GLY	2.7
1	D	193	LYS	2.6
1	D	308	LYS	2.6
1	C	129	VAL	2.6
1	A	199	GLN	2.6
1	E	113	LEU	2.6
1	D	29	TYR	2.6
1	D	235	TYR	2.6
1	C	193	LYS	2.6
1	A	111	TYR	2.6
1	D	197	ARG	2.6
1	B	116	CYS	2.6
1	B	200	PRO	2.6
1	D	264	LYS	2.5
1	A	86	PHE	2.5
1	A	296	SER	2.5
1	C	77	LYS	2.5
1	A	178	LEU	2.4
1	A	126	ILE	2.4
1	A	308	LYS	2.4
1	B	231	MET	2.4
1	E	119	ILE	2.4
1	A	234	GLU	2.4
1	D	58	LEU	2.4
1	E	208	SER	2.4
1	D	86	PHE	2.4
1	E	111	TYR	2.4
1	A	87	ILE	2.3
1	D	5	GLN	2.3
1	C	162	ILE	2.3
1	C	217	ILE	2.3
1	B	5	GLN	2.3
1	A	352	ASN	2.3
1	B	149	ASN	2.3
1	E	265	GLN	2.3
1	E	259	LEU	2.3
1	E	299	ILE	2.3
1	C	220	THR	2.3
1	C	295	LEU	2.3
1	C	199	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	301	GLU	2.3
2	V	500	A	2.3
1	A	28	GLU	2.2
1	D	201	GLY	2.2
1	A	85	LEU	2.2
1	C	265	GLN	2.2
1	A	129	VAL	2.2
1	B	161	VAL	2.2
1	B	32	SER	2.2
1	B	295	LEU	2.2
1	B	192	TYR	2.2
1	D	6	ILE	2.2
1	D	233	CYS	2.2
1	B	264	LYS	2.2
2	X	500	A	2.2
1	A	201	GLY	2.2
1	B	252	TYR	2.2
2	X	504	A	2.2
1	E	295	LEU	2.1
1	A	202	PHE	2.1
1	C	130	SER	2.1
1	A	119	ILE	2.1
1	B	199	GLN	2.1
1	D	28	GLU	2.1
1	E	170	GLN	2.1
1	A	207	ALA	2.1
1	B	115	VAL	2.1
1	E	188	MET	2.1
1	A	353	ILE	2.1
1	A	200	PRO	2.1
1	A	309	GLU	2.1
1	A	205	ASP	2.1
1	E	41	ILE	2.1
1	E	302	LEU	2.0
1	C	128	GLY	2.0
1	B	165	LEU	2.0
1	B	234	GLU	2.0
1	C	200	PRO	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	SO4	B	402	5/5	0.86	0.26	10.87	56,56,67,81	0
4	SO4	A	402	5/5	0.98	0.14	2.53	42,44,53,59	0
4	SO4	C	402	5/5	0.92	0.24	1.68	57,59,60,79	0
4	SO4	C	403	5/5	0.96	0.15	1.36	47,49,52,53	0
5	GOL	A	403	6/6	0.86	0.19	1.33	48,56,58,62	0
4	SO4	E	402	5/5	0.99	0.11	-0.79	42,42,50,50	0
4	SO4	D	402	5/5	0.98	0.12	-1.34	41,41,42,47	0
3	MN	A	401	1/1	1.00	0.11	-1.53	28,28,28,28	0
4	SO4	B	403	5/5	0.98	0.10	-1.71	44,46,49,50	0
3	MN	E	401	1/1	0.99	0.11	-2.64	24,24,24,24	0
3	MN	C	401	1/1	1.00	0.07	-2.68	26,26,26,26	0
3	MN	D	401	1/1	0.99	0.08	-3.21	33,33,33,33	0
3	MN	B	401	1/1	0.99	0.06	-5.80	29,29,29,29	0
4	SO4	C	404	5/5	0.96	0.18	-	62,67,78,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.