



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:35 PM GMT

PDB ID : 4ISZ
Title : RNA ligase RtcB in complex with GTP alphaS and Mn(II)
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Deposited on : 2013-01-17
Resolution : 2.30 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

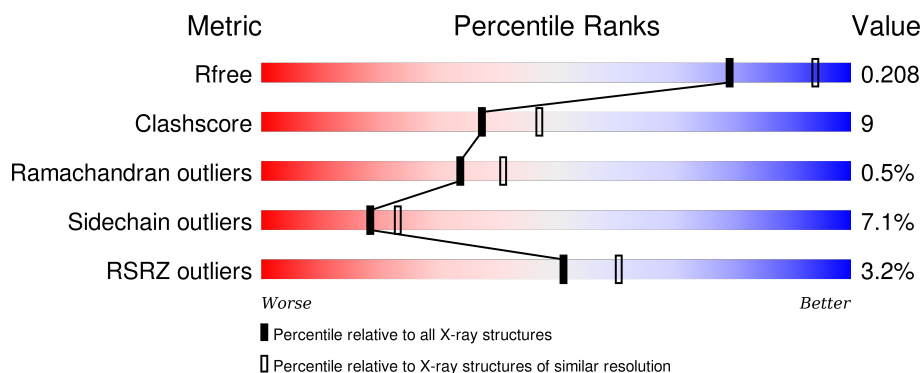
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


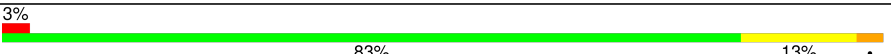
The reported resolution of this entry is 2.30 Å.

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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	481	
1	B	481	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GAV	B	501	-	-	X	X
4	SO4	A	510	-	-	-	X
4	SO4	B	512	-	-	-	X
5	SUC	B	513	-	-	-	X

2 Entry composition [i](#)

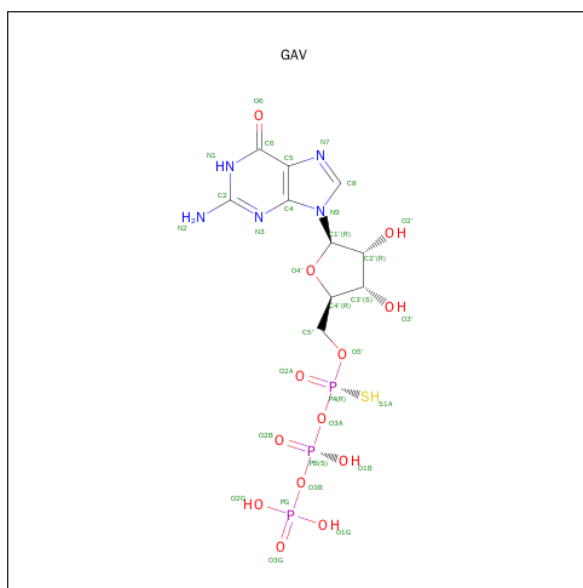
There are 6 unique types of molecules in this entry. The entry contains 15844 atoms, of which 7677 are hydrogens and 0 are deuteriums.

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 tRNA-splicing ligase RtcB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	480	Total	C	H	N	O	S	0	1	0
			7586	2380	3811	699	680	16			
1	B	480	Total	C	H	N	O	S	0	2	0
			7567	2375	3800	696	680	16			

- Molecule 2 is GUANOSINE-5'-RP-ALPHA-THIO-TRIPHOSPHATE (three-letter code: GAV) (formula: C₁₀H₁₆N₅O₁₃P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Mn	0	0
			2	2		
3	A	2	Total	Mn	0	0
			2	2		

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



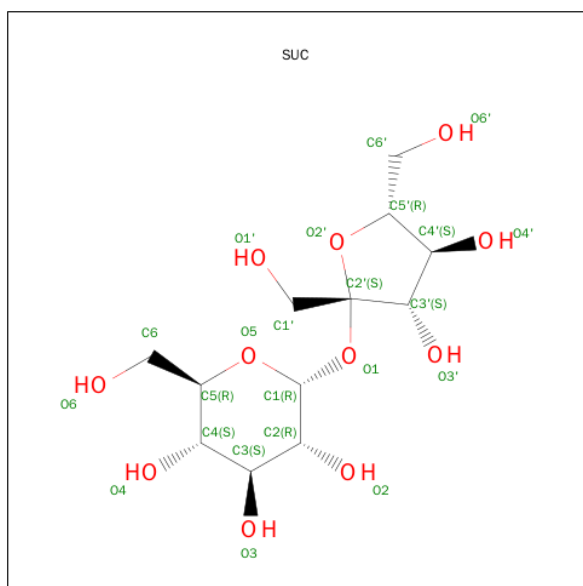
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is SUGAR (SUCROSE) (three-letter code: SUC) (formula: C₁₂H₂₂O₁₁).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			45	12	22	11		
5	A	1	Total	C	H	O	0	0
			45	12	22	11		
5	B	1	Total	C	H	O	0	0
			45	12	22	11		

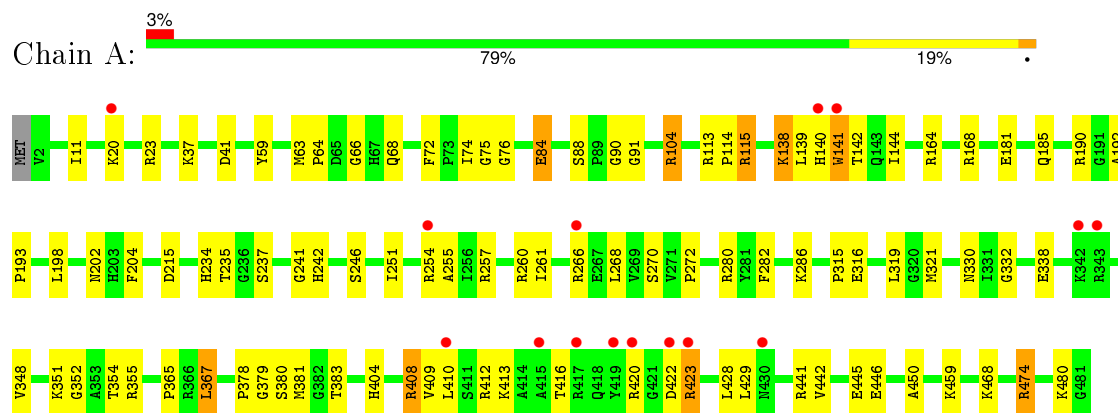
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	213	Total 213	O 213	0	0
6	B	185	Total 185	O 185	0	0

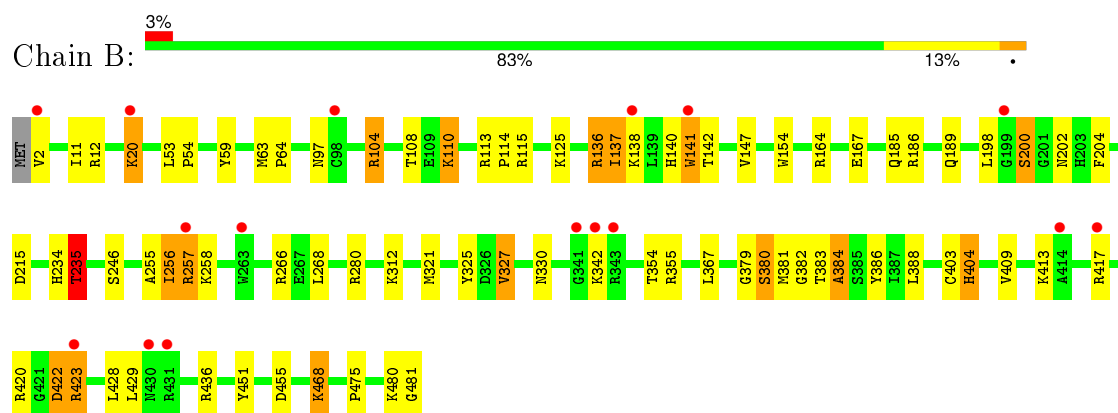
3 Residue-property plots

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: tRNA-splicing ligase RtcB



• Molecule 1: tRNA-splicing ligase RtcB



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.11Å 138.91Å 149.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.75 – 2.30 49.75 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.4 (49.75-2.30) 91.5 (49.75-2.30)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.165 , 0.205 0.178 , 0.208	Depositor DCC
R_{free} test set	2241 reflections (3.35%)	DCC
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 53.6	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	0 of 73441 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15844	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GAV, MN, SUC, 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	0.67	0/3858	0.71	1/5203 (0.0%)
1	B	0.67	0/3847	0.75	2/5189 (0.0%)
All	All	0.67	0/7705	0.73	3/10392 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	235	THR	CB-CA-C	-6.64	93.67	111.60
1	B	12	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	23	ARG	NE-CZ-NH2	-5.16	117.72	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3775	3811	3808	73	1
1	B	3767	3800	3795	71	1
2	A	32	0	13	6	0
2	B	32	0	13	25	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	45	0	0	2	0
4	B	45	0	0	0	0
5	A	46	44	44	2	0
5	B	23	22	22	0	0
6	A	213	0	0	20	0
6	B	185	0	0	9	0
All	All	8167	7677	7695	143	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 (143) 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:379:GLY:O	2:B:501:GAV:H1'	1.07	1.24
2:A:501:GAV:S1A	6:A:697:HOH:O	2.02	1.14
1:B:379:GLY:O	2:B:501:GAV:C1'	2.02	1.07
1:B:380:SER:HA	2:B:501:GAV:C4	1.86	1.06
1:B:202:ASN:HB3	2:B:501:GAV:H8	1.55	0.87
1:B:234:HIS:HE1	2:B:501:GAV:H5'1	1.50	0.75
1:B:202:ASN:OD1	1:B:451:TYR:OH	2.07	0.73
1:A:76:GLY:HA3	6:A:724:HOH:O	1.89	0.72
1:B:234:HIS:CE1	2:B:501:GAV:H5'1	2.25	0.72
1:A:408:ARG:NH2	1:A:445:GLU:O	2.24	0.71
1:B:204:PHE:CD2	2:B:501:GAV:C6	2.73	0.71
1:B:420:ARG:NH2	6:B:736:HOH:O	2.26	0.69
1:B:200:SER:OG	1:B:481:GLY:OXT	2.13	0.67
1:B:386:TYR:OH	1:B:455:ASP:OD1	2.10	0.67
1:B:380:SER:N	1:B:383:THR:OG1	2.26	0.67
1:B:379:GLY:O	2:B:501:GAV:N3	2.27	0.67
1:B:436:ARG:NH2	6:B:765:HOH:O	2.27	0.67
1:B:381:MET:N	2:B:501:GAV:C6	2.59	0.66
1:A:380:SER:HB3	1:A:383:THR:OG1	1.95	0.66
1:B:354:THR:HG21	6:B:682:HOH:O	1.97	0.65
1:A:202:ASN:OD1	1:A:412[B]:ARG:NH2	2.31	0.63
1:A:202:ASN:OD1	1:A:412[A]:ARG:NH2	2.33	0.62
1:B:202:ASN:HB3	2:B:501:GAV:C8	2.29	0.61
1:A:412[B]:ARG:NH1	1:A:446:GLU:OE2	2.34	0.60
1:B:354:THR:HG22	1:B:355:ARG:O	2.01	0.60
1:A:140:HIS:O	1:A:142:THR:N	2.34	0.60
1:B:256:ILE:CD1	6:B:701:HOH:O	2.48	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:THR:HG21	1:B:413:LYS:HD3	1.84	0.59
1:A:141:TRP:O	1:A:141:TRP:CE3	2.56	0.59
1:A:260:ARG:NH1	4:A:505:SO4:O1	2.35	0.58
1:A:412[A]:ARG:NH1	1:A:446:GLU:OE2	2.35	0.58
1:B:141:TRP:HB3	1:B:189:GLN:HA	1.85	0.58
1:B:204:PHE:CE2	2:B:501:GAV:C4	2.87	0.58
1:A:234:HIS:CE1	2:A:501:GAV:H5'1	2.38	0.58
1:B:379:GLY:O	2:B:501:GAV:C4	2.52	0.57
1:A:254:ARG:HG2	1:A:255:ALA:N	2.19	0.57
1:B:147:VAL:HG22	1:B:154:TRP:CD2	2.39	0.57
1:B:204:PHE:CD2	2:B:501:GAV:C5	2.88	0.56
5:A:514:SUC:O4	5:A:514:SUC:O6	2.12	0.56
1:A:235:THR:HB	6:A:737:HOH:O	2.05	0.56
1:A:198:LEU:HD12	1:A:235:THR:CG2	2.36	0.56
1:B:383:THR:O	1:B:384:ALA:CB	2.53	0.56
1:A:190:ARG:NH2	4:A:510:SO4:O2	2.38	0.55
1:A:168:ARG:HG3	6:A:768:HOH:O	2.06	0.55
1:A:379:GLY:O	2:A:501:GAV:H1'	2.08	0.54
1:A:198:LEU:HD12	1:A:235:THR:HG21	1.90	0.54
1:B:330:ASN:ND2	2:B:501:GAV:O2G	2.40	0.53
1:A:242:HIS:CD2	6:A:782:HOH:O	2.61	0.53
1:B:380:SER:CA	2:B:501:GAV:C4	2.74	0.53
1:B:382:GLY:HA2	1:B:475:PRO:HG3	1.92	0.52
1:B:141:TRP:CB	1:B:189:GLN:HA	2.39	0.52
1:A:192:ALA:N	1:A:193:PRO:CD	2.73	0.51
1:A:254:ARG:NH2	6:A:695:HOH:O	2.31	0.51
1:A:168:ARG:CG	6:A:768:HOH:O	2.58	0.51
1:B:136:ARG:O	1:B:137:ILE:CB	2.57	0.51
1:B:136:ARG:O	1:B:137:ILE:HB	2.11	0.51
1:A:88:SER:HB2	1:A:270:SER:HB3	1.92	0.51
1:A:215:ASP:OD2	1:A:468:LYS:HE3	2.11	0.51
1:B:380:SER:HA	2:B:501:GAV:N3	2.25	0.51
1:A:416:THR:HG21	1:B:413:LYS:CD	2.41	0.50
1:B:380:SER:CA	2:B:501:GAV:N3	2.74	0.50
1:A:115:ARG:NH2	6:A:800:HOH:O	2.45	0.50
1:A:441:ARG:NH2	6:A:788:HOH:O	2.45	0.49
1:B:204:PHE:CE2	2:B:501:GAV:C5	2.95	0.49
1:A:330:ASN:ND2	2:A:501:GAV:O2G	2.45	0.49
1:A:41:ASP:HB2	1:A:68:GLN:OE1	2.13	0.49
1:A:164:ARG:NH1	1:A:316:GLU:OE2	2.44	0.48
1:A:380:SER:HA	6:A:734:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:THR:HG22	1:A:355:ARG:N	2.28	0.48
1:B:382:GLY:HA2	1:B:475:PRO:CG	2.43	0.48
1:B:379:GLY:C	2:B:501:GAV:N3	2.67	0.48
1:A:72:PHE:CG	1:A:91:GLY:HA2	2.49	0.48
1:B:136:ARG:N	6:B:651:HOH:O	2.34	0.47
1:A:251:ILE:O	1:A:254:ARG:HG2	2.15	0.46
1:A:90:GLY:O	1:A:351:LYS:HE2	2.15	0.46
1:A:416:THR:CG2	1:B:413:LYS:HE2	2.45	0.46
1:B:202:ASN:HD22	2:B:501:GAV:PB	2.38	0.46
1:B:403:CYS:HA	6:B:707:HOH:O	2.15	0.46
1:B:380:SER:HB2	1:B:383:THR:HG21	1.97	0.46
1:A:242:HIS:HD2	6:A:782:HOH:O	1.94	0.46
1:A:202:ASN:HB2	2:A:501:GAV:O2B	2.15	0.46
1:A:104:ARG:O	1:A:321:MET:HA	2.16	0.46
1:A:168:ARG:NE	6:A:768:HOH:O	2.48	0.46
1:A:63:MET:HB3	1:A:64:PRO:HD2	1.97	0.45
1:B:204:PHE:HE2	2:B:501:GAV:C4	2.28	0.45
1:B:325:TYR:CD2	1:B:327:VAL:HG13	2.51	0.45
1:A:410:LEU:HG	1:A:450:ALA:HA	1.98	0.45
1:B:136:ARG:O	1:B:137:ILE:HG22	2.16	0.45
1:B:215:ASP:OD2	1:B:468:LYS:HE3	2.16	0.45
1:B:266:ARG:HG2	1:B:266:ARG:O	2.17	0.45
1:A:412[B]:ARG:NH1	1:A:445:GLU:OE1	2.49	0.45
1:B:164:ARG:O	1:B:167:GLU:HG2	2.17	0.45
1:B:20:LYS:CD	1:B:20:LYS:O	2.65	0.45
1:A:20:LYS:HD2	1:A:20:LYS:O	2.17	0.44
1:A:315:PRO:HA	1:A:319:LEU:HB2	1.98	0.44
5:A:514:SUC:H1'2	5:A:514:SUC:H1	1.79	0.44
1:A:237:SER:OG	1:A:241:GLY:HA3	2.17	0.44
1:A:261:ILE:CD1	1:A:272:PRO:HD3	2.48	0.44
1:A:441:ARG:CZ	6:A:788:HOH:O	2.65	0.44
1:B:255:ALA:HB2	6:B:688:HOH:O	2.18	0.44
1:A:140:HIS:C	1:A:142:THR:H	2.21	0.44
1:B:256:ILE:HD11	6:B:701:HOH:O	2.15	0.43
1:A:254:ARG:CG	1:A:255:ALA:N	2.81	0.43
1:A:261:ILE:HD11	1:A:272:PRO:HD3	2.00	0.43
1:B:198:LEU:O	1:B:235:THR:HG23	2.18	0.43
1:A:378:PRO:HD2	1:A:404:HIS:O	2.18	0.43
1:A:138:LYS:HE3	1:B:125:LYS:HG3	2.01	0.43
1:B:404:HIS:HE2	2:B:501:GAV:PA	2.41	0.43
1:A:204:PHE:HZ	1:A:378:PRO:HB3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:GLY:HA2	1:A:352:GLY:O	2.19	0.43
1:A:354:THR:HG21	6:A:659:HOH:O	2.18	0.42
1:B:140:HIS:C	1:B:142:THR:H	2.22	0.42
1:A:332:GLY:HA2	1:A:348:VAL:O	2.18	0.42
1:A:202:ASN:HB2	2:A:501:GAV:PB	2.59	0.42
1:A:354:THR:HG22	1:A:355:ARG:O	2.18	0.42
1:A:66:GLY:HA2	1:A:74:ILE:O	2.19	0.42
1:B:167:GLU:OE1	6:B:698:HOH:O	2.21	0.42
1:B:113:ARG:N	1:B:114:PRO:CD	2.82	0.42
1:A:474:ARG:HD2	6:A:646:HOH:O	2.18	0.42
1:B:422:ASP:OD1	1:B:423:ARG:N	2.53	0.41
1:A:113:ARG:N	1:A:114:PRO:HD2	2.35	0.41
1:B:2:VAL:O	1:B:2:VAL:HG12	2.19	0.41
1:A:139:LEU:HD13	1:A:144:ILE:HG22	2.02	0.41
1:B:104:ARG:O	1:B:321:MET:HA	2.21	0.41
1:A:365:PRO:HB2	1:A:367:LEU:HD12	2.01	0.41
1:A:423:ARG:NH2	6:A:754:HOH:O	2.53	0.41
1:A:446:GLU:HG3	1:A:480:LYS:HE2	2.02	0.41
1:B:379:GLY:O	2:B:501:GAV:N9	2.51	0.41
1:B:108:THR:OG1	1:B:110:LYS:HE3	2.20	0.41
1:A:280:ARG:HD3	6:A:650:HOH:O	2.20	0.41
1:A:442:VAL:O	1:A:446:GLU:HG2	2.20	0.41
1:A:282:PHE:CE2	1:A:286:LYS:HE3	2.55	0.41
1:B:53:LEU:HA	1:B:54:PRO:HD3	1.87	0.41
1:B:380:SER:HA	2:B:501:GAV:N9	2.34	0.41
1:A:254:ARG:NH1	6:A:695:HOH:O	2.53	0.41
1:B:147:VAL:HG22	1:B:154:TRP:CE2	2.56	0.41
1:B:480:LYS:HE3	1:B:480:LYS:HB2	1.81	0.41
1:B:63:MET:HB3	1:B:64:PRO:HD2	2.02	0.40
1:B:380:SER:HA	2:B:501:GAV:C5	2.47	0.40
1:B:185:GLN:HG2	1:B:186:ARG:H	1.86	0.40
1:B:97:ASN:OD1	1:B:97:ASN:O	2.39	0.40
1:A:260:ARG:CZ	6:A:776:HOH:O	2.68	0.40
1:A:168:ARG:CZ	6:A:768:HOH:O	2.69	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:A:84:GLU:OE2	1:B:257:ARG:NE[1_455]	2.19	0.01

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	480/481 (100%)	461 (96%)	17 (4%)	2 (0%)	39	48
1	B	479/481 (100%)	463 (97%)	13 (3%)	3 (1%)	30	36
All	All	959/962 (100%)	924 (96%)	30 (3%)	5 (0%)	34	41

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	384	ALA
1	A	141	TRP
1	A	381	MET
1	B	137	ILE
1	B	141	TRP

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	391/390 (100%)	366 (94%)	25 (6%)	22	28
1	B	390/390 (100%)	360 (92%)	30 (8%)	16	20
All	All	781/780 (100%)	726 (93%)	55 (7%)	18	23

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ILE

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Mol	Chain	Res	Type
1	A	37	LYS
1	A	59	TYR
1	A	84	GLU
1	A	104	ARG
1	A	115	ARG
1	A	138	LYS
1	A	181	GLU
1	A	185	GLN
1	A	246	SER
1	A	257	ARG
1	A	266	ARG
1	A	268	LEU
1	A	338	GLU
1	A	367	LEU
1	A	408	ARG
1	A	409	VAL
1	A	413	LYS
1	A	420	ARG
1	A	422	ASP
1	A	423	ARG
1	A	428	LEU
1	A	429	LEU
1	A	459	LYS
1	A	474	ARG
1	B	11	ILE
1	B	20	LYS
1	B	59	TYR
1	B	104	ARG
1	B	110	LYS
1	B	115	ARG
1	B	136	ARG
1	B	138	LYS
1	B	200	SER
1	B	235	THR
1	B	246	SER
1	B	256	ILE
1	B	257	ARG
1	B	258	LYS
1	B	268	LEU
1	B	280	ARG
1	B	312	LYS
1	B	327	VAL

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Mol	Chain	Res	Type
1	B	342	LYS
1	B	367	LEU
1	B	380	SER
1	B	388	LEU
1	B	404	HIS
1	B	409	VAL
1	B	417	ARG
1	B	422	ASP
1	B	423	ARG
1	B	428	LEU
1	B	429	LEU
1	B	468	LYS

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

Mol	Chain	Res	Type
1	A	67	HIS
1	B	140	HIS
1	B	242	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 4 are monoatomic - leaving 23 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
2	GAV	A	501	3	23,34,34	2.91	7 (30%)	32,54,54	2.20	11 (34%)
4	SO4	A	504	-	4,4,4	0.34	0	6,6,6	0.24	0
4	SO4	A	505	-	4,4,4	0.19	0	6,6,6	0.31	0
4	SO4	A	506	-	4,4,4	0.27	0	6,6,6	0.74	0
4	SO4	A	507	-	4,4,4	0.18	0	6,6,6	0.54	0
4	SO4	A	508	-	4,4,4	0.29	0	6,6,6	0.53	0
4	SO4	A	509	-	4,4,4	0.26	0	6,6,6	0.49	0
4	SO4	A	510	-	4,4,4	0.36	0	6,6,6	0.64	0
4	SO4	A	511	-	4,4,4	0.37	0	6,6,6	0.41	0
4	SO4	A	512	-	4,4,4	0.35	0	6,6,6	0.53	0
5	SUC	A	513	-	24,24,24	1.09	1 (4%)	36,36,36	2.09	9 (25%)
5	SUC	A	514	-	24,24,24	1.16	2 (8%)	36,36,36	2.38	11 (30%)
2	GAV	B	501	3	23,34,34	3.30	9 (39%)	32,54,54	2.70	13 (40%)
4	SO4	B	504	-	4,4,4	0.30	0	6,6,6	0.50	0
4	SO4	B	505	-	4,4,4	0.13	0	6,6,6	0.52	0
4	SO4	B	506	-	4,4,4	0.11	0	6,6,6	0.61	0
4	SO4	B	507	-	4,4,4	0.21	0	6,6,6	0.41	0
4	SO4	B	508	-	4,4,4	0.21	0	6,6,6	0.35	0
4	SO4	B	509	-	4,4,4	0.23	0	6,6,6	0.33	0
4	SO4	B	510	-	4,4,4	0.30	0	6,6,6	0.54	0
4	SO4	B	511	-	4,4,4	0.23	0	6,6,6	0.41	0
4	SO4	B	512	-	4,4,4	0.33	0	6,6,6	0.19	0
5	SUC	B	513	-	24,24,24	0.91	1 (4%)	36,36,36	2.15	10 (27%)

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
2	GAV	A	501	3	-	0/13/38/38	0/3/3/3
4	SO4	A	504	-	-	0/0/0/0	0/0/0/0
4	SO4	A	505	-	-	0/0/0/0	0/0/0/0
4	SO4	A	506	-	-	0/0/0/0	0/0/0/0
4	SO4	A	507	-	-	0/0/0/0	0/0/0/0
4	SO4	A	508	-	-	0/0/0/0	0/0/0/0
4	SO4	A	509	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	A	510	-	-	0/0/0/0	0/0/0/0
4	SO4	A	511	-	-	0/0/0/0	0/0/0/0
4	SO4	A	512	-	-	0/0/0/0	0/0/0/0
5	SUC	A	513	-	-	0/12/51/51	0/2/2/2
5	SUC	A	514	-	-	0/12/51/51	0/2/2/2
2	GAV	B	501	3	-	0/13/38/38	0/3/3/3
4	SO4	B	504	-	-	0/0/0/0	0/0/0/0
4	SO4	B	505	-	-	0/0/0/0	0/0/0/0
4	SO4	B	506	-	-	0/0/0/0	0/0/0/0
4	SO4	B	507	-	-	0/0/0/0	0/0/0/0
4	SO4	B	508	-	-	0/0/0/0	0/0/0/0
4	SO4	B	509	-	-	0/0/0/0	0/0/0/0
4	SO4	B	510	-	-	0/0/0/0	0/0/0/0
4	SO4	B	511	-	-	0/0/0/0	0/0/0/0
4	SO4	B	512	-	-	0/0/0/0	0/0/0/0
5	SUC	B	513	-	-	0/12/51/51	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	GAV	PA-O5'	-3.03	1.53	1.58
2	A	501	GAV	O2'-C2'	-2.53	1.36	1.43
2	B	501	GAV	C3'-C2'	-2.34	1.47	1.53
5	A	513	SUC	O4-C4	-2.30	1.37	1.43
5	A	514	SUC	O4-C4	-2.26	1.37	1.43
5	A	514	SUC	O4'-C4'	-2.23	1.37	1.43
2	B	501	GAV	O2'-C2'	-2.15	1.37	1.43
5	B	513	SUC	O4-C4	-2.06	1.38	1.43
2	A	501	GAV	C6-C5	2.25	1.45	1.41
2	A	501	GAV	C6-N1	3.87	1.40	1.33
2	B	501	GAV	C6-C5	4.15	1.49	1.41
2	B	501	GAV	O4'-C1'	4.47	1.46	1.41
2	B	501	GAV	C6-N1	4.49	1.41	1.33
2	A	501	GAV	O4'-C1'	5.18	1.47	1.41
2	A	501	GAV	C2-N1	5.35	1.44	1.35
2	B	501	GAV	C2-N1	5.81	1.45	1.35
2	A	501	GAV	C2-N2	6.36	1.47	1.34
2	B	501	GAV	C2-N2	6.68	1.47	1.34
2	A	501	GAV	C4-N3	7.77	1.47	1.35
2	B	501	GAV	C4-N3	9.06	1.49	1.35

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	514	SUC	O1-C2'-C1'	-6.08	90.19	109.69
5	B	513	SUC	O1-C2'-C1'	-5.99	90.50	109.69
2	B	501	GAV	N3-C2-N1	-5.78	118.64	127.44
5	A	514	SUC	O1-C2'-O2'	-5.29	93.71	110.52
5	A	513	SUC	O1-C2'-O2'	-5.18	94.05	110.52
2	A	501	GAV	N3-C2-N1	-5.03	119.79	127.44
5	B	513	SUC	O1-C2'-O2'	-4.67	95.69	110.52
5	A	514	SUC	O1-C2'-C3'	-4.65	91.84	108.04
5	A	513	SUC	O1-C2'-C1'	-4.56	95.07	109.69
2	B	501	GAV	C4'-O4'-C1'	-4.51	104.77	109.72
5	B	513	SUC	O1-C2'-C3'	-4.22	93.33	108.04
2	B	501	GAV	C4-C5-N7	-3.89	105.90	109.48
2	B	501	GAV	PB-O3A-PA	-3.79	120.11	133.44
2	A	501	GAV	C1'-N9-C4	-3.40	121.81	126.94
2	A	501	GAV	C5-C6-N1	-3.40	118.94	123.59
5	A	513	SUC	O1-C2'-C3'	-3.32	96.47	108.04
5	A	514	SUC	C1-O5-C5	-3.09	107.74	113.75
5	A	514	SUC	C3-C4-C5	-2.97	105.03	110.20
2	A	501	GAV	PB-O3B-PG	-2.69	123.64	132.67
2	B	501	GAV	PB-O3B-PG	-2.67	123.71	132.67
2	A	501	GAV	C6-C5-C4	-2.66	117.72	120.90
5	A	513	SUC	C6-C5-C4	-2.62	106.54	113.02
2	B	501	GAV	C6-C5-C4	-2.58	117.81	120.90
5	B	513	SUC	O3-C3-C4	-2.31	105.14	110.34
2	A	501	GAV	C4'-O4'-C1'	-2.29	107.20	109.72
2	B	501	GAV	C5-C6-N1	-2.16	120.64	123.59
5	A	513	SUC	C2'-O2'-C5'	-2.15	102.22	108.44
5	A	514	SUC	O1'-C1'-C2'	-2.05	105.34	111.91
2	B	501	GAV	C5'-C4'-C3'	-2.05	107.08	115.21
2	A	501	GAV	PB-O3A-PA	-2.04	126.27	133.44
2	A	501	GAV	O3A-PA-O5'	2.00	108.95	101.47
5	B	513	SUC	O2'-C5'-C6'	2.01	114.65	108.57
5	A	513	SUC	O3-C3-C2	2.14	115.15	110.34
5	B	513	SUC	O3-C3-C2	2.29	115.50	110.34
5	B	513	SUC	O5-C5-C4	2.35	114.09	109.68
5	A	514	SUC	C1'-C2'-C3'	2.37	122.49	114.49
2	B	501	GAV	N2-C2-N1	2.47	121.29	117.20
5	B	513	SUC	C1'-C2'-C3'	2.64	123.40	114.49
5	B	513	SUC	O2'-C2'-C3'	2.77	111.87	105.58
5	A	514	SUC	C1-C2-C3	2.93	115.74	109.97
2	A	501	GAV	O4'-C4'-C3'	3.08	111.35	105.15
5	A	514	SUC	O2'-C2'-C3'	3.20	112.87	105.58
5	A	513	SUC	O5-C5-C6	3.28	114.66	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	513	SUC	O2'-C2'-C3'	3.42	113.35	105.58
5	A	514	SUC	O5-C5-C6	3.61	115.48	106.36
2	B	501	GAV	C6-N1-C2	3.78	121.18	115.94
2	B	501	GAV	O4'-C1'-N9	4.54	117.61	108.10
2	B	501	GAV	O4'-C4'-C3'	4.57	114.35	105.15
2	A	501	GAV	C6-N1-C2	4.76	122.55	115.94
2	A	501	GAV	C2'-C1'-N9	4.80	121.62	114.29
5	B	513	SUC	O2'-C2'-C1'	5.84	123.86	107.98
5	A	514	SUC	O2'-C2'-C1'	6.01	124.33	107.98
5	A	513	SUC	O2'-C2'-C1'	6.02	124.36	107.98
2	B	501	GAV	C2'-C1'-N9	6.66	124.47	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	GAV	6	0
4	A	505	SO4	1	0
4	A	510	SO4	1	0
5	A	514	SUC	2	0
2	B	501	GAV	25	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	480/481 (99%)	-0.04	15 (3%)	52	62	14, 27, 60, 91	0
1	B	480/481 (99%)	0.00	16 (3%)	50	59	16, 28, 55, 83	1 (0%)
All	All	960/962 (99%)	-0.02	31 (3%)	51	60	14, 27, 57, 91	1 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	140	HIS	4.5
1	B	263	TRP	4.0
1	A	417	ARG	3.9
1	B	257	ARG	3.9
1	B	2	VAL	3.8
1	A	423	ARG	3.8
1	A	141	TRP	3.6
1	A	410	LEU	3.3
1	B	141	TRP	3.2
1	B	138	LYS	3.1
1	A	342	LYS	3.0
1	A	415	ALA	2.9
1	A	20	LYS	2.9
1	A	420	ARG	2.7
1	B	343	ARG	2.6
1	B	417	ARG	2.6
1	B	341	GLY	2.6
1	A	430	ASN	2.6
1	B	98	CYS	2.5
1	B	430	ASN	2.5
1	A	266	ARG	2.4
1	A	254	ARG	2.4
1	B	431	ARG	2.4
1	B	342	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	419	TYR	2.3
1	A	422	ASP	2.3
1	B	423	ARG	2.2
1	A	343	ARG	2.2
1	B	199	GLY	2.1
1	B	20	LYS	2.0
1	B	414	ALA	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. 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	512	5/5	0.91	0.33	4.69	30,34,51,73	5
2	GAV	B	501	32/32	0.80	0.39	4.63	30,49,66,71	32
4	SO4	A	510	5/5	0.88	0.23	2.81	35,35,49,51	5
5	SUC	B	513	23/23	0.93	0.23	2.60	31,48,62,74	0
4	SO4	B	510	5/5	0.89	0.24	1.92	8,39,55,62	5
5	SUC	A	513	23/23	0.95	0.20	1.69	28,46,60,72	0
2	GAV	A	501	32/32	0.86	0.23	1.67	30,49,66,71	32
5	SUC	A	514	23/23	0.90	0.26	1.43	23,44,54,62	45
4	SO4	A	504	5/5	0.99	0.21	1.35	23,33,37,50	5
4	SO4	A	505	5/5	0.92	0.23	0.94	45,47,54,61	5
4	SO4	B	504	5/5	0.98	0.21	0.44	37,38,42,43	0
4	SO4	B	511	5/5	0.91	0.11	-0.54	44,51,64,75	5
4	SO4	A	512	5/5	0.87	0.17	-0.59	55,56,61,91	0
3	MN	B	503	1/1	0.96	0.19	-0.70	45,45,45,45	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	SO4	A	506	5/5	0.99	0.10	-1.12	19,39,52,61	0
4	SO4	B	508	5/5	0.93	0.11	-1.57	44,46,49,57	5
3	MN	B	502	1/1	0.99	0.15	-1.87	40,40,40,40	1
3	MN	A	503	1/1	0.97	0.12	-2.41	36,36,36,36	1
3	MN	A	502	1/1	0.99	0.14	-3.22	37,37,37,37	1
4	SO4	A	508	5/5	0.95	0.15	-	41,41,45,50	5
4	SO4	A	507	5/5	0.96	0.10	-	39,47,63,68	0
4	SO4	B	507	5/5	0.95	0.18	-	36,45,50,51	5
4	SO4	B	505	5/5	0.89	0.22	-	42,42,55,61	5
4	SO4	B	509	5/5	0.83	0.26	-	51,53,66,75	5
4	SO4	A	511	5/5	0.91	0.34	-	46,48,53,61	5
4	SO4	A	509	5/5	0.94	0.13	-	44,46,50,58	5
4	SO4	B	506	5/5	0.94	0.31	-	39,45,53,58	5

6.5 Other polymers [i](#)

There are no such residues in this entry.