



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:14 PM UTC

PDB ID : 3U02 / pdb_00003u02
Title : Crystal Structure of the tRNA modifier TiaS from *Pyrococcus furiosus*, Northeast Structural Genomics Consortium Target PfR225
Authors : Kuzin, A.; Lew, S.; Seetharaman, J.; Sahdev, S.; Xiao, R.; Ciccocanti, C.; Wang, H.; Everett, J.K.; Nair, R.; Acton, T.B.; Rost, B.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2011-09-28
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

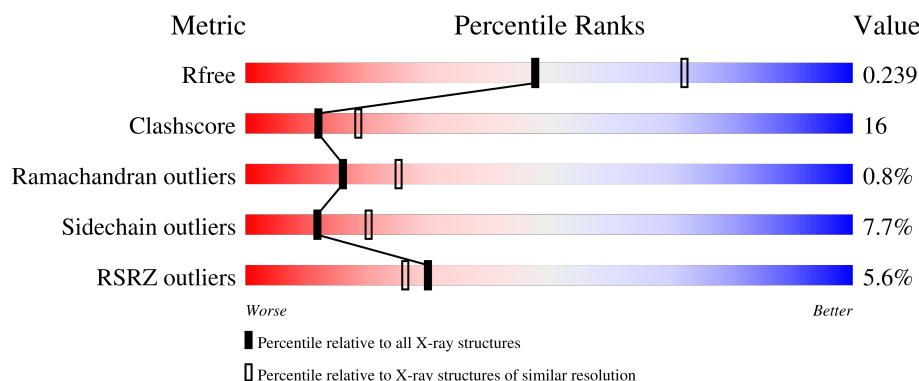
1 Overall quality at a glance

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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	252	4% 68% 23% 5% 5%
1	B	252	7% 62% 28% 6% .
1	C	252	5% 58% 27% . 10%
1	D	252	4% 62% 25% . 12%

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	SO4	A	253	-	-	X	-
2	SO4	B	254	-	-	X	-

2 Entry composition [i](#)

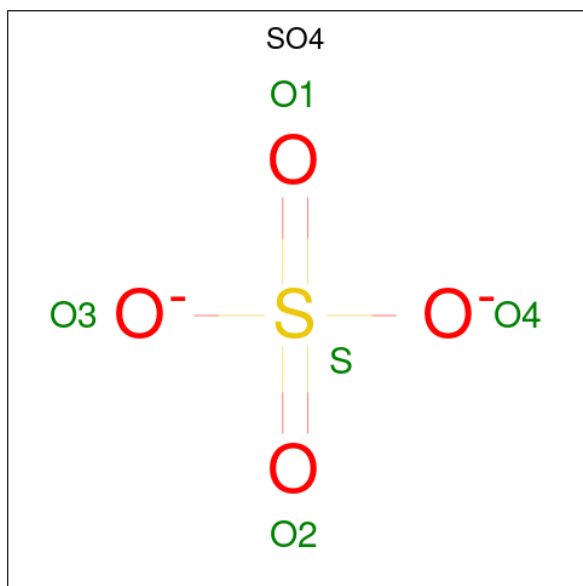
There are 6 unique types of molecules in this entry. The entry contains 8052 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Putative transcription-associated protein TFIIS.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	P	S	Se	0	0	0
			1952	1267	324	355	1	1	4			
1	B	244	Total	C	N	O	P	S	Se	0	1	0
			2011	1304	339	362	1	1	4			
1	C	226	Total	C	N	O	P	S	Se	0	1	0
			1857	1207	310	334	1	1	4			
1	D	223	Total	C	N	O	P	S	Se	0	1	0
			1836	1198	303	328	1	1	5			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



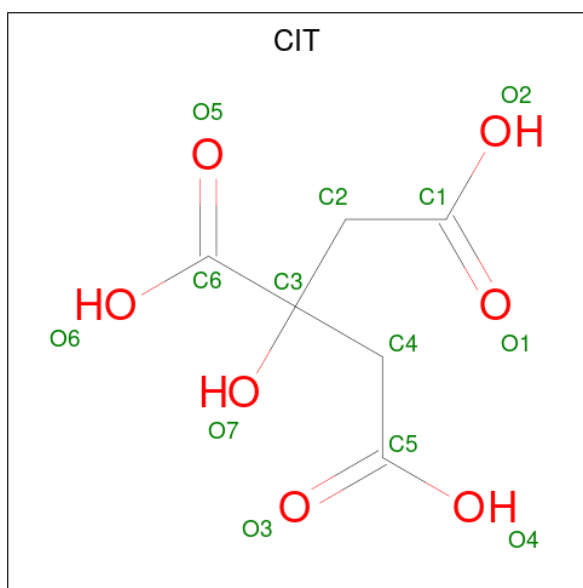
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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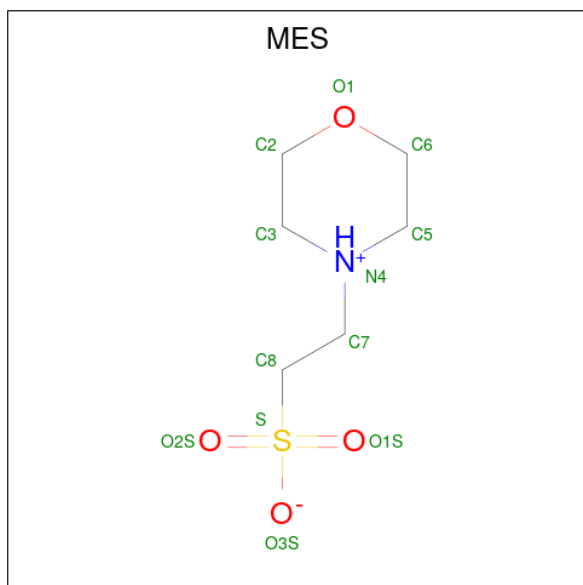
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total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

- Molecule 3 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



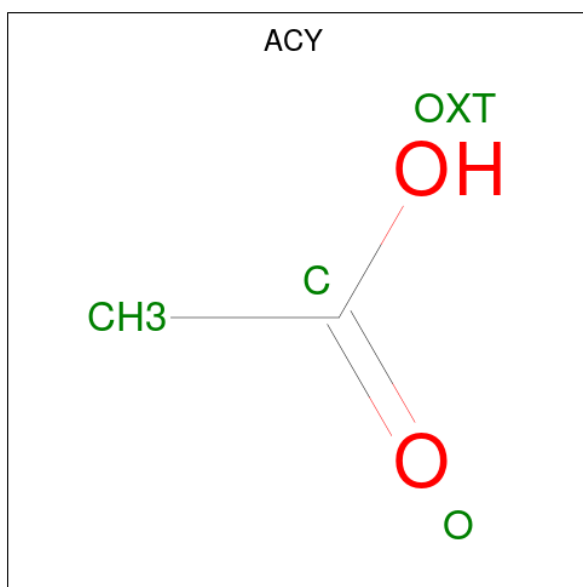
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	D	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0
			12	6	1	4	1	0

- Molecule 5 is ACETIC ACID (CCD ID: ACY) (formula: $C_2H_4O_2$).



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

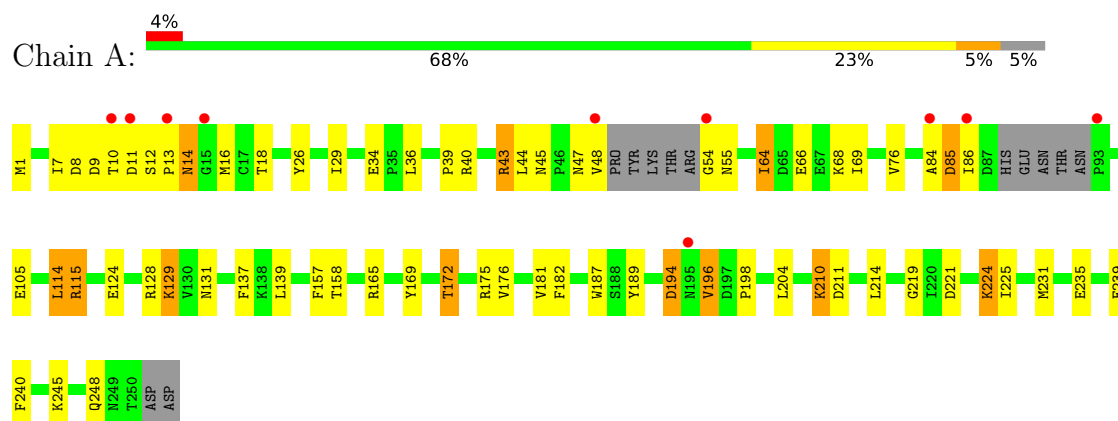
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	90	Total	O	0	0
			90	90		
6	B	81	Total	O	0	0
			81	81		
6	C	54	Total	O	0	0
			54	54		
6	D	45	Total	O	0	1
			46	46		

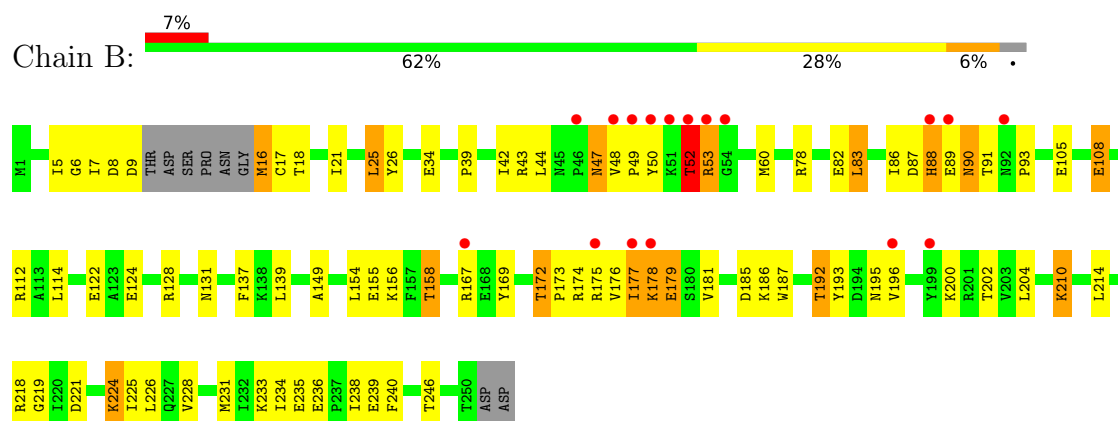
3 Residue-property plots [i](#)

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

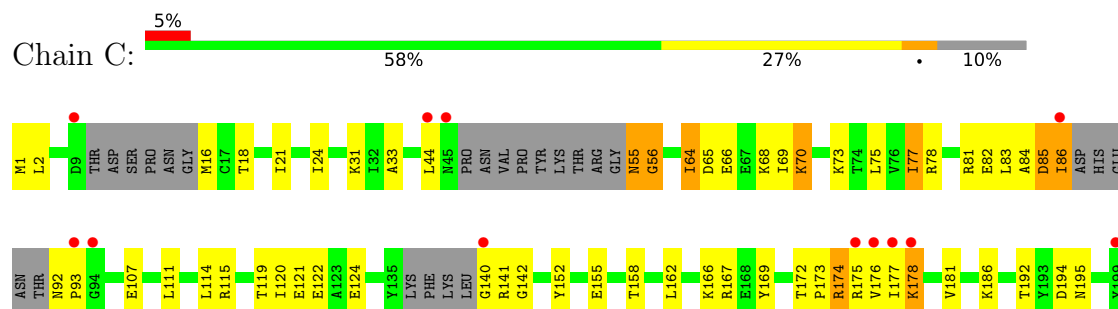
• Molecule 1: Putative transcription-associated protein TFIIS

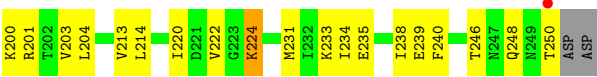


• Molecule 1: Putative transcription-associated protein TFIIS

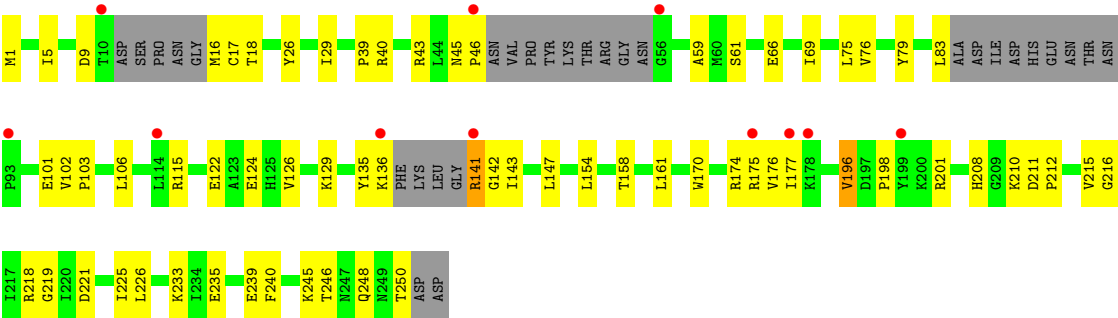


• Molecule 1: Putative transcription-associated protein TFIIS





● Molecule 1: Putative transcription-associated protein TFIIS



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.15Å 135.81Å 77.27Å 90.00° 93.76° 90.00°	Depositor
Resolution (Å)	43.90 – 2.40 43.90 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (43.90-2.40) 99.5 (43.90-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.33 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.7.1 _743	Depositor
R, R_{free}	0.179 , 0.242 0.175 , 0.239	Depositor DCC
R_{free} test set	2477 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.566	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8052	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% 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: ACY, CIT, TPO, MES, 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	0.54	0/1979	0.78	0/2667
1	B	0.54	0/2042	0.83	1/2755 (0.0%)
1	C	0.48	0/1883	0.79	0/2535
1	D	0.49	0/1863	0.79	1/2507 (0.0%)
All	All	0.51	0/7767	0.80	2/10464 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	52	THR	N-CA-C	-6.05	102.00	110.35
1	D	9	ASP	N-CA-C	5.24	116.10	108.14

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	1952	0	1988	52	0
1	B	2011	0	2049	75	0
1	C	1857	0	1897	73	0
1	D	1836	0	1885	50	0
2	A	20	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	25	0	0	3	0
2	C	10	0	0	0	0
2	D	15	0	0	1	0
3	A	13	0	5	0	0
3	B	13	0	5	1	0
3	D	13	0	5	2	0
4	A	12	0	13	2	0
5	C	4	0	3	0	0
6	A	90	0	0	4	0
6	B	81	0	0	4	0
6	C	54	0	0	4	0
6	D	46	0	0	1	0
All	All	8052	0	7850	245	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 16.

All (245) 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:C:201[B]:ARG:H	1:C:201[B]:ARG:HD3	1.26	1.01
1:C:16:MSE:HE3	1:C:167:ARG:HH12	1.27	0.96
1:C:201[B]:ARG:HH21	1:C:224:LYS:HE2	1.32	0.93
1:B:89:GLU:N	1:B:90:ASN:HA	1.87	0.88
1:B:90:ASN:O	1:B:90:ASN:ND2	2.08	0.85
1:B:181:VAL:HG21	1:B:231:MSE:HG2	1.59	0.84
1:B:25:LEU:HB3	1:B:60:MSE:HE1	1.60	0.82
1:C:181:VAL:HG21	1:C:231:MSE:HG2	1.64	0.80
1:B:43:ARG:HE	1:B:50:TYR:HB2	1.47	0.79
1:C:16:MSE:HE1	1:C:86:ILE:HG21	1.65	0.79
1:B:50:TYR:HD1	1:B:50:TYR:O	1.65	0.78
1:B:89:GLU:H	1:B:90:ASN:HA	1.45	0.78
1:C:16:MSE:HE3	1:C:167:ARG:NH1	2.00	0.77
1:A:210:LYS:H	1:A:210:LYS:HD3	1.49	0.76
1:B:8:ASP:HB3	6:B:326:HOH:O	1.88	0.72
1:C:31:LYS:NZ	6:C:308:HOH:O	2.21	0.72
1:A:124:GLU:O	1:A:128:ARG:HG3	1.90	0.72
1:A:169:TYR:O	1:A:172:THR:HB	1.91	0.71
1:A:8:ASP:OD2	1:A:10:THR:HG23	1.91	0.70
1:A:175:ARG:HB3	1:A:235:GLU:HB2	1.74	0.70
1:B:185:ASP:OD1	1:B:224:LYS:NZ	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:THR:HG23	1:C:194:ASP:OD2	1.92	0.69
1:D:141:ARG:CB	1:D:142:GLY:HA3	2.23	0.69
1:B:50:TYR:O	1:B:50:TYR:CD1	2.46	0.67
1:B:52:THR:OG1	1:B:53:ARG:HA	1.95	0.67
1:A:210:LYS:H	1:A:210:LYS:CD	2.08	0.66
1:B:124:GLU:O	1:B:128:ARG:HG3	1.95	0.66
1:C:73:LYS:O	1:C:77:ILE:HG12	1.96	0.66
1:B:48:VAL:CG1	1:B:49:PRO:HD2	2.25	0.66
1:A:10:THR:C	1:A:12:SER:H	2.03	0.65
1:D:1:MSE:HE1	1:D:66:GLU:HG3	1.77	0.65
1:C:16:MSE:CE	1:C:86:ILE:HG21	2.27	0.64
2:A:253:SO4:O1	6:A:344:HOH:O	2.12	0.64
1:B:48:VAL:HG13	1:B:49:PRO:HD2	1.80	0.64
1:C:140:GLY:C	1:C:142:GLY:H	2.06	0.63
1:D:141:ARG:HB2	1:D:142:GLY:HA3	1.80	0.63
1:D:122:GLU:O	1:D:126:VAL:HG23	1.98	0.63
1:C:92:ASN:HB2	1:C:93:PRO:HD3	1.81	0.63
1:A:10:THR:HG22	1:A:54:GLY:O	1.98	0.63
1:A:181:VAL:HG21	1:A:231:MSE:HG2	1.81	0.63
1:B:178:LYS:HD2	1:B:204:LEU:HD11	1.81	0.62
1:B:169:TYR:O	1:B:172:THR:HB	1.99	0.62
1:C:178:LYS:HD3	1:C:178:LYS:C	2.25	0.62
1:B:187:TRP:HD1	2:B:254:SO4:O1	1.82	0.61
1:B:155:GLU:OE2	1:D:198:PRO:HG2	1.99	0.61
1:B:86:ILE:HG21	1:B:167:ARG:HH12	1.66	0.61
1:D:40:ARG:NH2	1:D:61:SER:OG	2.30	0.61
1:C:21:ILE:HG12	1:C:83:LEU:HD23	1.82	0.60
1:C:201[B]:ARG:HG3	6:C:302:HOH:O	2.01	0.60
1:A:221:ASP:O	1:A:225:ILE:HG12	2.01	0.60
1:A:64:ILE:HD11	1:A:68:LYS:HB2	1.83	0.59
1:D:16[B]:MSE:HG3	1:D:17:CYS:H	1.67	0.59
1:C:231:MSE:HE2	6:C:301:HOH:O	2.03	0.59
1:C:111:LEU:O	1:C:115:ARG:HG3	2.02	0.59
1:A:43:ARG:HH12	1:A:48:VAL:HG12	1.68	0.59
1:A:210:LYS:HD3	1:A:210:LYS:N	2.17	0.59
1:A:66:GLU:HA	1:A:69:ILE:HD13	1.85	0.58
1:C:222:VAL:HG13	1:D:226:LEU:HD12	1.85	0.58
1:A:10:THR:CG2	1:A:54:GLY:O	2.51	0.58
1:C:158:THR:HG22	1:C:220:ILE:HG22	1.84	0.58
1:A:44:LEU:HA	1:A:114:LEU:HD12	1.84	0.58
1:A:29:ILE:HD11	1:A:76:VAL:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:MSE:HE2	6:A:300:HOH:O	2.02	0.58
1:C:158:THR:HG22	1:C:220:ILE:CG2	2.33	0.58
1:B:86:ILE:HG21	1:B:167:ARG:NH1	2.19	0.58
1:D:239:GLU:HG3	1:D:240:PHE:CD2	2.39	0.58
1:B:21:ILE:HG12	1:B:83:LEU:HD23	1.86	0.58
4:A:258:MES:H52	1:D:101:GLU:OE1	2.04	0.57
1:B:89:GLU:N	1:B:90:ASN:CA	2.63	0.57
1:A:224:LYS:HE2	2:A:255:SO4:O1	2.05	0.57
1:B:52:THR:HG21	1:B:53:ARG:NH2	2.20	0.57
1:B:219:GLY:HA3	1:B:225:ILE:HD11	1.85	0.56
1:D:175:ARG:HB3	1:D:235:GLU:HB2	1.88	0.56
1:B:43:ARG:NE	1:B:50:TYR:HB2	2.18	0.56
1:B:202:THR:HG21	1:B:228:VAL:HG21	1.88	0.56
1:C:70:LYS:HB2	1:C:70:LYS:NZ	2.21	0.56
1:B:16:MSE:HE2	1:B:210:LYS:HZ1	1.71	0.55
1:A:194:ASP:CG	1:A:194:ASP:O	2.48	0.55
1:B:5:ILE:HD13	1:B:60:MSE:HE3	1.88	0.55
1:A:137:PHE:CE2	1:A:139:LEU:HA	2.42	0.55
1:B:9:ASP:C	1:B:93:PRO:HB3	2.32	0.54
1:C:201[B]:ARG:HH21	1:C:224:LYS:CE	2.11	0.54
1:B:47:ASN:HA	6:B:339:HOH:O	2.08	0.54
1:D:75:LEU:HD23	1:D:79:TYR:HD2	1.73	0.53
1:A:84:ALA:C	1:A:86:ILE:H	2.15	0.53
1:B:239:GLU:HG3	1:B:240:PHE:HD2	1.72	0.53
1:B:9:ASP:OD2	1:B:53:ARG:HG3	2.08	0.53
1:C:174:ARG:NH1	1:C:213:VAL:O	2.41	0.53
1:B:52:THR:HG23	1:B:53:ARG:HB2	1.90	0.53
1:D:158:THR:HG22	1:D:248:GLN:O	2.09	0.52
1:D:135:TYR:O	1:D:136:LYS:HB2	2.10	0.52
1:D:215:VAL:HG22	1:D:216:GLY:N	2.25	0.52
1:C:201[B]:ARG:NH2	1:C:224:LYS:HE2	2.14	0.52
1:D:141:ARG:HB2	1:D:142:GLY:CA	2.39	0.52
1:D:174:ARG:HG3	1:D:174:ARG:HH11	1.74	0.52
1:B:128:ARG:HD3	6:B:276:HOH:O	2.10	0.52
1:A:1:MSE:N	4:A:258:MES:H82	2.24	0.52
1:C:194:ASP:OD2	1:C:194:ASP:N	2.41	0.51
1:D:43:ARG:NH2	3:D:256:CIT:O1	2.43	0.51
1:B:50:TYR:CD1	1:B:50:TYR:C	2.88	0.51
1:C:1:MSE:SE	1:C:69:ILE:HD11	2.60	0.51
1:D:141:ARG:HD3	1:D:141:ARG:N	2.26	0.51
1:C:64:ILE:HG13	1:C:68:LYS:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ILE:HD11	1:A:68:LYS:CB	2.41	0.51
1:C:78:ARG:O	1:C:81:ARG:HG3	2.11	0.51
1:C:234:ILE:CD1	1:C:238:ILE:HD11	2.40	0.51
1:B:175:ARG:HB3	1:B:235:GLU:HB2	1.94	0.50
1:B:177:ILE:HG23	1:B:233:LYS:HB3	1.93	0.50
1:B:78[B]:ARG:O	1:B:82:GLU:HG3	2.11	0.50
1:C:33:ALA:HB2	1:C:64:ILE:HD13	1.94	0.50
1:A:187:TRP:HD1	2:A:253:SO4:O2	1.95	0.50
1:A:10:THR:C	1:A:12:SER:N	2.69	0.50
1:C:16:MSE:HE1	1:C:86:ILE:CG2	2.40	0.50
1:C:169:TYR:O	1:C:172:THR:HB	2.12	0.49
1:B:112:ARG:HH12	1:B:122:GLU:HG2	1.77	0.49
1:B:175:ARG:HD3	1:B:236:GLU:HB3	1.95	0.49
1:C:119:THR:OG1	1:C:122:GLU:HG3	2.11	0.49
1:C:84:ALA:O	1:C:86:ILE:N	2.38	0.49
1:A:9:ASP:OD2	1:A:12:SER:HB2	2.12	0.49
1:C:140:GLY:O	1:C:142:GLY:N	2.46	0.49
1:D:170:TRP:CE2	1:D:212:PRO:HB3	2.47	0.49
1:B:89:GLU:O	1:B:89:GLU:HG3	2.12	0.49
1:B:179:GLU:CD	1:B:179:GLU:H	2.20	0.49
1:C:120:ILE:O	1:C:124:GLU:HG2	2.13	0.49
1:D:106:LEU:HD11	1:D:147:LEU:HD22	1.95	0.49
1:B:158:THR:HG21	1:B:218:ARG:HD3	1.93	0.49
1:C:44:LEU:H	1:C:55:ASN:HB2	1.78	0.49
1:A:196:VAL:HG13	1:C:107:GLU:OE2	2.13	0.48
1:B:16:MSE:HB3	1:B:17:CYS:H	1.48	0.48
1:D:158:THR:OG1	1:D:219:GLY:O	2.30	0.48
1:A:47:ASN:O	1:A:48:VAL:HG22	2.13	0.48
1:A:13:PRO:O	1:A:14:ASN:HB2	2.13	0.48
1:C:16:MSE:SE	1:C:86:ILE:HG21	2.63	0.48
1:C:231:MSE:HE3	6:C:256:HOH:O	2.13	0.48
1:D:5:ILE:O	1:D:59:ALA:HA	2.13	0.48
1:A:34:GLU:OE2	1:B:193:TYR:O	2.32	0.48
1:A:45:ASN:H	1:A:55:ASN:HD22	1.61	0.48
1:D:246:THR:OG1	1:D:248:GLN:HG3	2.13	0.48
1:B:239:GLU:HG3	1:B:240:PHE:CD2	2.48	0.48
1:B:221:ASP:O	1:B:225:ILE:HG12	2.13	0.48
1:D:221:ASP:O	1:D:225:ILE:HG12	2.14	0.48
1:C:65:ASP:OD2	1:C:68:LYS:HG3	2.14	0.48
1:D:201:ARG:O	1:D:250:THR:HG21	2.13	0.48
1:D:239:GLU:HG3	1:D:240:PHE:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:ILE:HD11	1:C:68:LYS:HD2	1.97	0.47
1:C:82:GLU:C	1:C:84:ALA:H	2.21	0.47
1:C:177:ILE:HB	1:C:233:LYS:HB3	1.97	0.47
1:D:1:MSE:CE	1:D:66:GLU:HG3	2.43	0.47
1:B:25:LEU:CB	1:B:60:MSE:HE1	2.37	0.47
1:C:33:ALA:CB	1:C:64:ILE:HD13	2.45	0.47
1:D:40:ARG:HA	1:D:245:LYS:O	2.15	0.47
3:D:256:CIT:O4	3:D:256:CIT:O7	2.33	0.47
1:B:192:THR:O	1:B:195:ASN:ND2	2.46	0.47
1:D:245:LYS:NZ	6:D:274:HOH:O	2.47	0.47
1:A:196:VAL:HG13	1:C:107:GLU:CD	2.39	0.46
1:B:174:ARG:HG3	1:B:174:ARG:HH11	1.80	0.46
1:C:81:ARG:HG3	1:C:82:GLU:N	2.31	0.46
1:D:177:ILE:HB	1:D:233:LYS:HB3	1.96	0.46
1:D:210:LYS:O	1:D:211:ASP:C	2.59	0.46
1:A:26:TYR:CE1	1:A:39:PRO:HD3	2.51	0.46
1:B:158:THR:HG22	1:B:246:THR:CG2	2.45	0.46
1:B:26:TYR:CE1	1:B:39:PRO:HD3	2.51	0.46
1:B:44:LEU:HA	1:B:114:LEU:HD22	1.98	0.46
1:A:86:ILE:HG22	1:A:86:ILE:O	2.15	0.46
1:C:174:ARG:HG2	1:C:214:LEU:HD12	1.97	0.46
1:C:172:THR:HG23	1:C:173:PRO:HD2	1.96	0.46
1:D:26:TYR:CE1	1:D:39:PRO:HD3	2.51	0.46
1:C:234:ILE:HD13	1:C:238:ILE:HD11	1.99	0.45
1:D:208:HIS:ND1	2:D:253:SO4:O4	2.27	0.45
1:A:157:PHE:CE1	1:A:245:LYS:HD2	2.52	0.45
1:A:45:ASN:O	1:A:55:ASN:ND2	2.49	0.45
1:C:92:ASN:HB2	1:C:93:PRO:CD	2.46	0.45
1:C:166:LYS:HD2	1:C:239:GLU:OE1	2.17	0.45
1:C:246:THR:HG23	1:C:248:GLN:H	1.80	0.45
1:D:75:LEU:HD23	1:D:75:LEU:C	2.42	0.45
1:A:189:TYR:HD1	2:A:256:SO4:O1	1.99	0.45
1:B:224:LYS:HE2	2:B:257:SO4:O2	2.17	0.45
1:D:1:MSE:SE	1:D:69:ILE:HD11	2.67	0.45
1:C:64:ILE:HD12	1:C:64:ILE:HA	1.71	0.45
1:C:82:GLU:HA	1:C:85:ASP:HB3	1.99	0.45
1:A:16:MSE:SE	1:A:211:ASP:HA	2.67	0.45
1:A:194:ASP:O	1:A:194:ASP:OD1	2.36	0.44
1:D:158:THR:HG21	1:D:218:ARG:HD2	1.98	0.44
1:D:29:ILE:HD11	1:D:76:VAL:HG22	1.98	0.44
1:A:239:GLU:HG3	1:A:240:PHE:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:ILE:HG13	1:B:149:ALA:HA	1.99	0.44
1:C:119:THR:HB	1:C:121:GLU:OE1	2.18	0.44
1:D:161:LEU:C	1:D:161:LEU:HD23	2.42	0.44
1:D:106:LEU:CD1	1:D:147:LEU:HD22	2.46	0.44
1:D:124:GLU:H	1:D:124:GLU:HG2	1.70	0.44
1:C:44:LEU:H	1:C:55:ASN:CB	2.30	0.44
1:C:140:GLY:C	1:C:142:GLY:N	2.72	0.44
1:B:53:ARG:HB2	1:B:53:ARG:HE	1.48	0.44
1:C:84:ALA:C	1:C:86:ILE:N	2.76	0.44
3:B:258:CIT:O2	3:B:258:CIT:C6	2.66	0.43
1:C:70:LYS:HB2	1:C:70:LYS:HZ2	1.83	0.43
1:C:77:ILE:HG12	1:C:77:ILE:H	1.56	0.43
1:B:174:ARG:HG3	1:B:174:ARG:NH1	2.33	0.43
1:B:43:ARG:HH21	1:B:50:TYR:H	1.66	0.43
1:B:231:MSE:HE3	6:B:261:HOH:O	2.18	0.43
1:D:102:VAL:HA	1:D:103:PRO:HD3	1.86	0.43
1:C:194:ASP:O	1:C:195:ASN:C	2.61	0.43
1:A:198:PRO:HG2	1:C:155:GLU:OE1	2.19	0.43
1:C:55:ASN:O	1:C:56:GLY:C	2.62	0.43
1:A:105:GLU:OE1	1:A:129:LYS:HD2	2.19	0.43
1:A:115:ARG:NH1	6:A:307:HOH:O	2.52	0.43
1:B:25:LEU:HD12	1:B:25:LEU:HA	1.81	0.43
1:C:44:LEU:HD12	1:C:44:LEU:N	2.34	0.43
1:A:158:THR:OG1	1:A:219:GLY:O	2.30	0.42
1:A:224:LYS:NZ	6:A:314:HOH:O	2.49	0.42
1:B:108:GLU:OE1	1:D:196:VAL:HG11	2.19	0.42
1:A:40:ARG:HA	1:A:245:LYS:O	2.19	0.42
1:A:165:ARG:HG2	1:A:214:LEU:HB2	2.00	0.42
1:C:24:ILE:HG13	1:C:83:LEU:HD21	2.01	0.42
1:B:16:MSE:HE2	1:B:210:LYS:NZ	2.34	0.42
1:D:79:TYR:O	1:D:83:LEU:HD12	2.20	0.42
1:A:158:THR:HG22	1:A:248:GLN:O	2.20	0.42
1:B:219:GLY:CA	1:B:225:ILE:HD11	2.49	0.42
1:D:129:LYS:HE2	1:D:129:LYS:HB3	1.76	0.42
1:B:5:ILE:CD1	1:B:60:MSE:HE3	2.50	0.42
1:B:6:GLY:C	1:B:7:ILE:HD12	2.45	0.42
1:C:200:LYS:HD3	1:C:203:VAL:HG12	2.02	0.42
1:B:16:MSE:CE	1:B:210:LYS:HG3	2.50	0.41
1:D:45:ASN:HA	1:D:46:PRO:HD3	1.93	0.41
1:A:43:ARG:NH1	1:A:48:VAL:HG12	2.33	0.41
1:A:84:ALA:C	1:A:86:ILE:N	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:ARG:NH1	1:C:235:GLU:O	2.53	0.41
1:B:172:THR:O	1:B:173:PRO:C	2.63	0.41
1:D:141:ARG:N	1:D:141:ARG:CD	2.83	0.41
1:C:66:GLU:O	1:C:69:ILE:HG12	2.20	0.41
1:B:87:ASP:O	1:B:88:HIS:C	2.64	0.41
1:C:114:LEU:HD22	1:C:152:TYR:HE1	1.85	0.41
1:D:174:ARG:HG3	1:D:174:ARG:NH1	2.34	0.41
1:B:187:TRP:CD1	2:B:254:SO4:O1	2.69	0.41
1:D:215:VAL:HG22	1:D:216:GLY:H	1.86	0.41
1:B:114:LEU:N	1:B:114:LEU:HD23	2.37	0.40
1:B:226:LEU:HD12	1:B:226:LEU:HA	1.92	0.40
1:C:81:ARG:O	1:C:85:ASP:N	2.43	0.40
1:C:239:GLU:HG3	1:C:240:PHE:HD2	1.86	0.40
1:D:115:ARG:HE	1:D:115:ARG:HB3	1.61	0.40
1:B:52:THR:CB	1:B:53:ARG:HA	2.51	0.40
1:B:234:ILE:HG22	1:B:236:GLU:O	2.21	0.40
1:B:137:PHE:CE2	1:B:139:LEU:HA	2.57	0.40
1:A:182:PHE:CD1	1:B:34:GLU:HG2	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	233/252 (92%)	219 (94%)	11 (5%)	3 (1%)	9	14
1	B	240/252 (95%)	230 (96%)	9 (4%)	1 (0%)	30	43
1	C	216/252 (86%)	208 (96%)	5 (2%)	3 (1%)	9	13
1	D	212/252 (84%)	205 (97%)	7 (3%)	0	100	100
All	All	901/1008 (89%)	862 (96%)	32 (4%)	7 (1%)	16	25

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	56	GLY
1	C	141	ARG
1	C	85	ASP
1	A	14	ASN
1	B	88	HIS
1	A	11	ASP
1	A	85	ASP

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	209/217 (96%)	193 (92%)	16 (8%)	12	20
1	B	215/217 (99%)	188 (87%)	27 (13%)	4	6
1	C	198/217 (91%)	183 (92%)	15 (8%)	12	21
1	D	197/217 (91%)	192 (98%)	5 (2%)	42	64
All	All	819/868 (94%)	756 (92%)	63 (8%)	12	20

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	36	LEU
1	A	43	ARG
1	A	64	ILE
1	A	85	ASP
1	A	114	LEU
1	A	115	ARG
1	A	129	LYS
1	A	131	ASN
1	A	172	THR
1	A	176	VAL
1	A	194	ASP
1	A	196	VAL
1	A	204	LEU
1	A	210	LYS

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Mol	Chain	Res	Type
1	A	224	LYS
1	B	16	MSE
1	B	25	LEU
1	B	47	ASN
1	B	52	THR
1	B	53	ARG
1	B	83	LEU
1	B	90	ASN
1	B	91	THR
1	B	105	GLU
1	B	108	GLU
1	B	131	ASN
1	B	154	LEU
1	B	156	LYS
1	B	158	THR
1	B	172	THR
1	B	176	VAL
1	B	177	ILE
1	B	178	LYS
1	B	179	GLU
1	B	186	LYS
1	B	192	THR
1	B	196	VAL
1	B	200	LYS
1	B	210	LYS
1	B	214	LEU
1	B	224	LYS
1	B	238	ILE
1	C	2	LEU
1	C	55	ASN
1	C	64	ILE
1	C	70	LYS
1	C	75	LEU
1	C	77	ILE
1	C	86	ILE
1	C	162	LEU
1	C	174	ARG
1	C	176	VAL
1	C	178	LYS
1	C	186	LYS
1	C	204	LEU
1	C	224	LYS

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Mol	Chain	Res	Type
1	C	250	THR
1	D	141	ARG
1	D	143	ILE
1	D	154	LEU
1	D	176	VAL
1	D	196	VAL

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

Mol	Chain	Res	Type
1	B	125	HIS
1	C	208	HIS
1	D	249	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	TPO	D	18	1	8,10,11	1.24	0	10,14,16	1.86	2 (20%)
1	TPO	C	18	1	8,10,11	1.14	0	10,14,16	1.88	2 (20%)
1	TPO	A	18	1	8,10,11	1.31	1 (12%)	10,14,16	1.52	1 (10%)
1	TPO	B	18	1	8,10,11	1.19	1 (12%)	10,14,16	2.00	1 (10%)

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
1	TPO	D	18	1	-	3/9/11/13	-
1	TPO	C	18	1	-	2/9/11/13	-
1	TPO	A	18	1	-	1/9/11/13	-
1	TPO	B	18	1	-	2/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	18	TPO	P-OG1	2.14	1.63	1.59
1	B	18	TPO	P-O3P	2.02	1.62	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	18	TPO	P-OG1-CB	-5.38	108.70	123.33
1	C	18	TPO	P-OG1-CB	-5.01	109.72	123.33
1	D	18	TPO	P-OG1-CB	-4.66	110.67	123.33
1	A	18	TPO	P-OG1-CB	-3.85	112.86	123.33
1	D	18	TPO	CG2-CB-CA	-2.43	108.52	113.26
1	C	18	TPO	CG2-CB-CA	-2.18	109.02	113.26

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	18	TPO	O-C-CA-CB
1	C	18	TPO	CB-OG1-P-O1P
1	B	18	TPO	CB-OG1-P-O3P
1	D	18	TPO	CB-OG1-P-O1P
1	A	18	TPO	O-C-CA-CB
1	B	18	TPO	O-C-CA-CB
1	D	18	TPO	C-CA-CB-CG2
1	D	18	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

19 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	$\# Z > 2$
2	SO4	A	256	-	4,4,4	0.24	0	6,6,6	0.20	0
2	SO4	A	254	-	4,4,4	0.22	0	6,6,6	0.21	0
2	SO4	B	254	-	4,4,4	0.29	0	6,6,6	0.12	0
3	CIT	A	257	-	12,12,12	1.23	0	17,17,17	1.82	5 (29%)
2	SO4	B	253	-	4,4,4	0.27	0	6,6,6	0.06	0
2	SO4	A	253	-	4,4,4	0.27	0	6,6,6	0.14	0
2	SO4	B	255	-	4,4,4	0.25	0	6,6,6	0.15	0
2	SO4	C	253	-	4,4,4	0.24	0	6,6,6	0.14	0
2	SO4	D	253	-	4,4,4	0.26	0	6,6,6	0.13	0
5	ACY	C	255	-	3,3,3	0.75	0	3,3,3	0.88	0
2	SO4	D	255	-	4,4,4	0.29	0	6,6,6	0.22	0
2	SO4	D	254	-	4,4,4	0.25	0	6,6,6	0.29	0
4	MES	A	258	-	12,12,12	1.51	2 (16%)	15,16,16	1.41	2 (13%)
2	SO4	C	254	-	4,4,4	0.24	0	6,6,6	0.06	0
2	SO4	A	255	-	4,4,4	0.27	0	6,6,6	0.34	0
3	CIT	B	258	-	12,12,12	1.12	0	17,17,17	1.60	4 (23%)
3	CIT	D	256	-	12,12,12	1.08	0	17,17,17	1.74	4 (23%)
2	SO4	B	257	-	4,4,4	0.21	0	6,6,6	0.12	0
2	SO4	B	256	-	4,4,4	0.22	0	6,6,6	0.15	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
3	CIT	B	258	-	-	3/16/16/16	-
4	MES	A	258	-	-	5/6/14/14	0/1/1/1
3	CIT	D	256	-	-	6/16/16/16	-
3	CIT	A	257	-	-	3/16/16/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	258	MES	C5-N4	-3.27	1.38	1.46
4	A	258	MES	C7-C8	-2.48	1.45	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	256	CIT	O6-C6-C3	4.20	121.20	113.14
3	A	257	CIT	O6-C6-C3	3.72	120.28	113.14
3	B	258	CIT	O6-C6-C3	3.41	119.69	113.14
3	A	257	CIT	O4-C5-O3	-3.12	115.30	123.33
3	A	257	CIT	O4-C5-C4	2.93	123.62	114.35
4	A	258	MES	C2-C3-N4	2.55	113.99	110.12
3	B	258	CIT	O2-C1-C2	2.44	122.09	114.35
4	A	258	MES	C5-N4-C3	2.42	114.04	108.84
3	D	256	CIT	O4-C5-C4	2.35	121.79	114.35
3	A	257	CIT	O6-C6-O5	-2.33	116.40	123.86
3	B	258	CIT	O2-C1-O1	-2.32	117.37	123.33
3	D	256	CIT	C3-C2-C1	-2.31	107.60	113.92
3	B	258	CIT	O4-C5-C4	2.16	121.19	114.35
3	D	256	CIT	O2-C1-C2	2.15	121.16	114.35
3	A	257	CIT	O7-C3-C6	2.03	111.84	108.96

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	257	CIT	C2-C3-C4-C5
3	A	257	CIT	O7-C3-C4-C5
3	A	257	CIT	C6-C3-C4-C5
3	D	256	CIT	C2-C3-C6-O5
3	D	256	CIT	C2-C3-C6-O6
3	D	256	CIT	O7-C3-C6-O5
3	D	256	CIT	O7-C3-C6-O6

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Mol	Chain	Res	Type	Atoms
4	A	258	MES	N4-C7-C8-S
4	A	258	MES	C7-C8-S-O3S
4	A	258	MES	C7-C8-S-O1S
4	A	258	MES	C7-C8-S-O2S
4	A	258	MES	C8-C7-N4-C3
3	D	256	CIT	C3-C4-C5-O4
3	B	258	CIT	O2-C1-C2-C3
3	B	258	CIT	O1-C1-C2-C3
3	D	256	CIT	C3-C4-C5-O3
3	B	258	CIT	C3-C4-C5-O4

There are no ring outliers.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	256	SO4	1	0
2	B	254	SO4	2	0
2	A	253	SO4	2	0
2	D	253	SO4	1	0
4	A	258	MES	2	0
2	A	255	SO4	1	0
3	B	258	CIT	1	0
3	D	256	CIT	2	0
2	B	257	SO4	1	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	235/252 (93%)	-0.10	10 (4%) 40 36	17, 30, 82, 105	0
1	B	239/252 (94%)	0.00	17 (7%) 22 18	17, 32, 89, 123	1 (0%)
1	C	221/252 (87%)	0.12	13 (5%) 28 24	19, 36, 79, 113	1 (0%)
1	D	218/252 (86%)	0.09	11 (5%) 34 30	18, 36, 75, 105	0
All	All	913/1008 (90%)	0.03	51 (5%) 30 26	17, 34, 84, 123	2 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	86	ILE	5.5
1	A	54	GLY	5.4
1	D	10	THR	4.9
1	A	48	VAL	4.8
1	D	199	TYR	4.8
1	C	93	PRO	4.4
1	B	49	PRO	4.3
1	D	46	PRO	4.3
1	A	86	ILE	4.1
1	B	177	ILE	3.7
1	C	140	GLY	3.5
1	B	52	THR	3.3
1	B	196	VAL	3.2
1	B	51	LYS	3.1
1	A	84	ALA	3.1
1	A	13	PRO	3.1
1	D	93	PRO	3.1
1	D	175	ARG	3.1
1	C	175	ARG	2.9
1	C	199	TYR	2.8
1	C	178	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	199	TYR	2.8
1	D	178	LYS	2.8
1	D	141	ARG	2.8
1	B	48	VAL	2.7
1	B	92	ASN	2.6
1	C	250	THR	2.6
1	B	88	HIS	2.6
1	D	136	LYS	2.6
1	B	50	TYR	2.5
1	B	178	LYS	2.5
1	C	177	ILE	2.5
1	B	175	ARG	2.5
1	C	45	ASN	2.5
1	B	46	PRO	2.4
1	A	15	GLY	2.4
1	A	10	THR	2.3
1	B	53	ARG	2.3
1	D	177	ILE	2.3
1	C	9	ASP	2.2
1	A	195	ASN	2.2
1	C	176	VAL	2.2
1	A	93	PRO	2.2
1	D	114	LEU	2.1
1	B	89	GLU	2.1
1	D	56	GLY	2.1
1	B	167	ARG	2.1
1	A	11	ASP	2.0
1	C	44	LEU	2.0
1	B	54	GLY	2.0
1	C	94	GLY	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	TPO	B	18	11/12	0.88	0.12	23,29,93,93	0
1	TPO	A	18	11/12	0.93	0.09	23,31,74,93	0
1	TPO	C	18	11/12	0.93	0.11	31,35,92,143	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	TPO	D	18	11/12	0.93	0.10	30,36,137,138	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	C	254	5/5	0.76	0.14	127,128,131,132	0
5	ACY	C	255	4/4	0.84	0.16	32,38,39,47	0
2	SO4	B	255	5/5	0.86	0.15	78,86,87,90	0
4	MES	A	258	12/12	0.87	0.14	26,51,68,70	0
2	SO4	A	256	5/5	0.87	0.18	71,82,88,98	0
3	CIT	D	256	13/13	0.88	0.11	50,61,68,75	0
2	SO4	D	255	5/5	0.90	0.15	63,66,72,80	0
2	SO4	D	254	5/5	0.90	0.12	49,53,59,64	0
2	SO4	C	253	5/5	0.91	0.10	75,79,88,88	0
2	SO4	B	256	5/5	0.92	0.08	58,64,65,66	0
2	SO4	B	257	5/5	0.92	0.13	53,64,68,82	0
3	CIT	A	257	13/13	0.92	0.10	30,40,52,53	0
3	CIT	B	258	13/13	0.93	0.07	35,41,55,59	0
2	SO4	D	253	5/5	0.93	0.12	59,67,70,71	0
2	SO4	B	254	5/5	0.95	0.11	46,56,59,60	0
2	SO4	A	254	5/5	0.96	0.09	45,54,62,62	0
2	SO4	B	253	5/5	0.96	0.07	38,56,64,64	0
2	SO4	A	253	5/5	0.98	0.06	30,32,40,41	0
2	SO4	A	255	5/5	0.99	0.05	31,41,45,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.