Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2023 – 04:18 AM EDT

PDB ID	:	3AF6
Title	:	The crystal structure of an archaeal CPSF subunit, PH1404 from Pyrococcus horikoshii complexed with RNA-analog
Authors	:	Nishida, Y.; Ishikawa, H.; Nakagawa, N.; Masui, R.; Kuramitsu, S.
Deposited on	:	2010-02-24
Resolution	:	2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

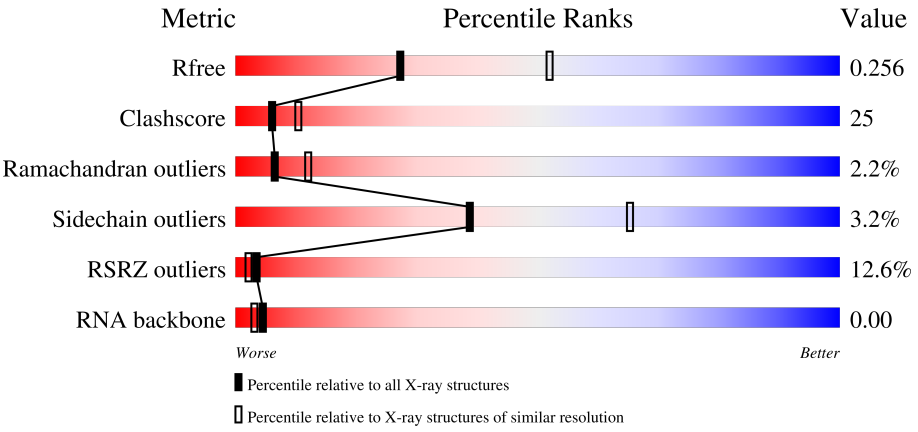
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)
RNA backbone	3102	1040 (2.90-2.30)

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 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 <=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	651	12%, 58%, 37%, . .
2	B	6	17%, 67%, 17%
2	C	6	17%, 17%, 67%

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	SSU	C	1	-	-	-	X
3	SO4	A	652	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5269 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.

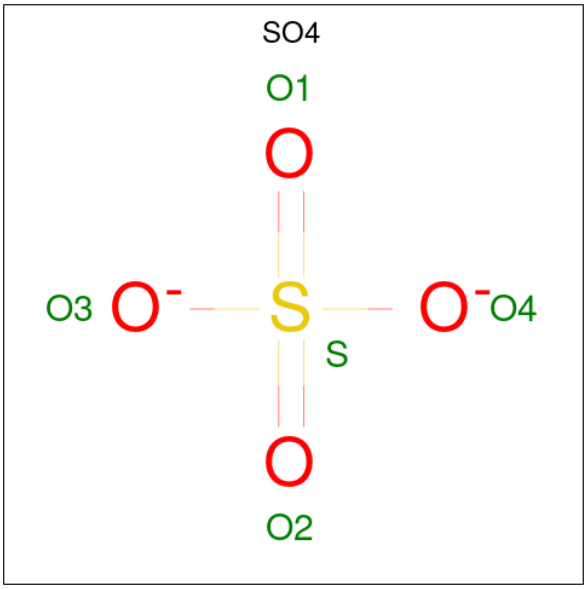
- Molecule 1 is a protein called Putative uncharacterized protein PH1404.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	637	5099	3257	897	929	16	0	0	0

- Molecule 2 is a RNA chain called 5'-R(*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU))-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
2	B	6	85	36	8	31	5	5	0	0	1
			Total	C	N	O	P	S			
2	C	2	21	9	2	8	1	1	0	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Zn 2 2	0	0

- Molecule 5 is water.

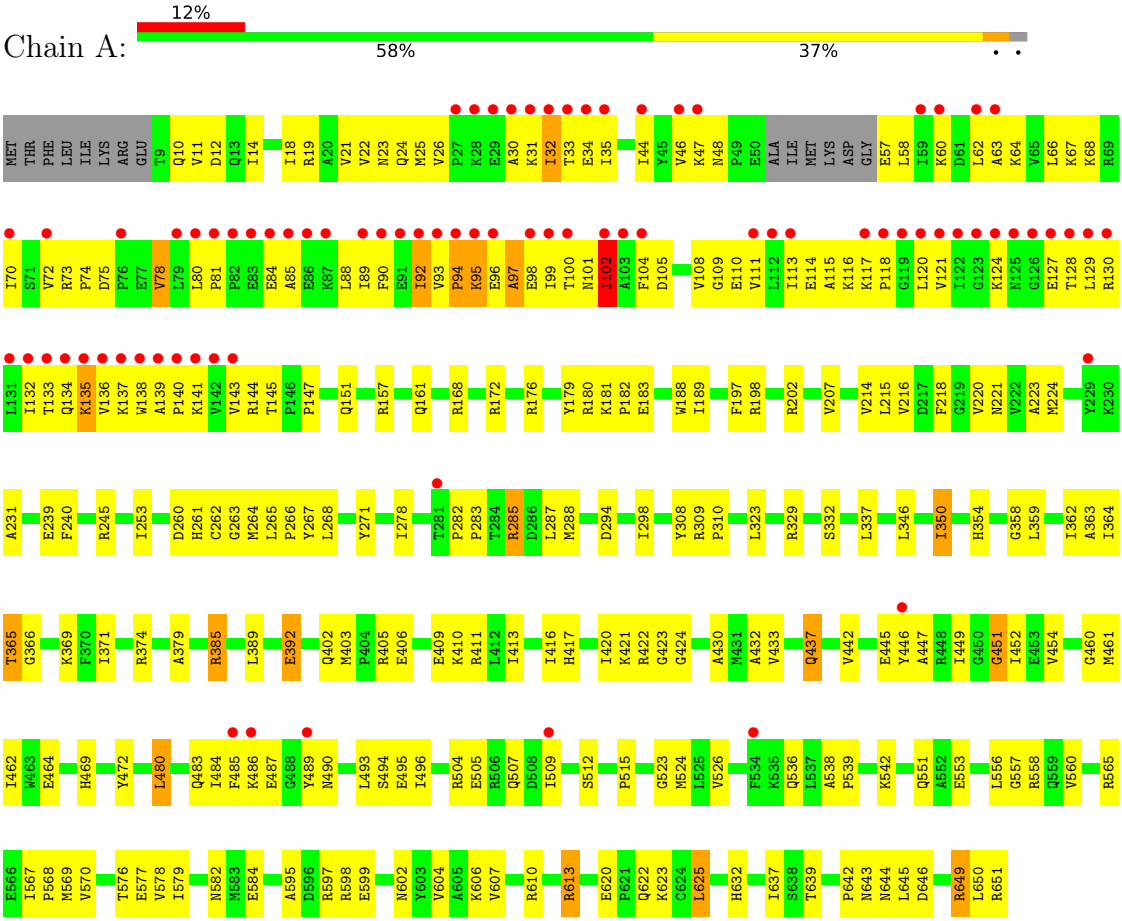
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	36	Total O 36 36	0	0
5	C	1	Total O 1 1	0	0

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.

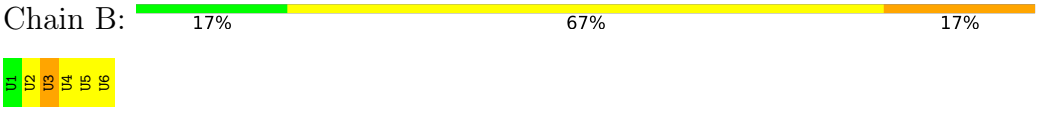
• Molecule 1: Putative uncharacterized protein PH1404

Chain A:



• Molecule 2: 5'-R(*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU))-3'

Chain B:



• Molecule 2: 5'-R(*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU)P*(SSU))-3'

Chain C:


U1
U2
SSU
SSU
SSU
SSU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	86.44Å 86.44Å 237.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.59 – 2.60 42.59 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.2 (42.59-2.60) 98.1 (42.59-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 2.61Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.220 , 0.258 0.221 , 0.256	Depositor DCC
R_{free} test set	5199 reflections (9.85%)	wwPDB-VP
Wilson B-factor (Å^2)	49.8	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5269	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: ZN, SSU, 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	0.35	0/5205	0.63	1/7048 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	350	ILE	N-CA-C	-5.03	97.41	111.00

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	5099	0	5211	254	0
2	B	85	0	40	13	0
2	C	21	0	10	6	0
3	A	25	0	0	2	0
4	A	2	0	0	0	0
5	A	36	0	0	3	0
5	C	1	0	0	0	0
All	All	5269	0	5261	259	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 25.

All (259) 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:A:417:HIS:HB3	5:A:677:HOH:O	1.57	1.02
1:A:26:VAL:HG22	1:A:58:LEU:HD21	1.52	0.90
1:A:553:GLU:HG2	1:A:558:ARG:NH1	1.92	0.85
1:A:67:LYS:HE3	2:B:4:SSU:H4'	1.60	0.83
1:A:285:ARG:HG2	1:A:285:ARG:HH21	1.43	0.83
1:A:62:LEU:HD22	1:A:70:ILE:HD13	1.61	0.82
2:B:5:SSU:H4'	2:B:6:SSU:OP2	1.79	0.81
1:A:639:THR:O	2:C:1:SSU:H6	1.82	0.79
1:A:632:HIS:CG	2:C:1:SSU:H1'	2.18	0.79
1:A:610:ARG:HD2	5:A:665:HOH:O	1.84	0.77
1:A:294:ASP:O	1:A:298:ILE:HG12	1.85	0.77
1:A:147:PRO:HG3	1:A:490:ASN:ND2	2.01	0.76
1:A:30:ALA:HA	1:A:48:ASN:HD21	1.49	0.75
1:A:21:VAL:HG22	1:A:25:MET:HE1	1.69	0.74
1:A:323:LEU:HD11	1:A:329:ARG:HG3	1.70	0.73
1:A:88:LEU:HD21	1:A:135:LYS:HB3	1.71	0.72
1:A:285:ARG:HG2	1:A:285:ARG:NH2	2.01	0.72
1:A:524:MET:HB2	1:A:526:VAL:HG23	1.71	0.72
1:A:480:LEU:O	1:A:484:ILE:HG12	1.89	0.72
1:A:110:GLU:OE1	1:A:141:LYS:HG3	1.89	0.71
1:A:19:ARG:HA	1:A:22:VAL:HG12	1.71	0.70
1:A:385:ARG:HH21	1:A:385:ARG:HB3	1.55	0.70
1:A:63:ALA:HB3	2:B:2:SSU:O2'	1.92	0.70
1:A:359:LEU:HG	1:A:651:ARG:HD3	1.74	0.69
1:A:539:PRO:O	1:A:582:ASN:HB2	1.92	0.69
1:A:11:VAL:HG13	1:A:12:ASP:H	1.58	0.69
1:A:172:ARG:O	1:A:176:ARG:HG3	1.92	0.68
1:A:92:ILE:HG12	1:A:92:ILE:O	1.94	0.67
1:A:21:VAL:HG11	1:A:66:LEU:HD21	1.78	0.66
1:A:551:GLN:HE21	1:A:557:GLY:HA3	1.61	0.66
1:A:30:ALA:HA	1:A:48:ASN:ND2	2.11	0.65
1:A:81:PRO:HG2	1:A:84:GLU:HB3	1.77	0.65
1:A:68:LYS:HE3	1:A:179:TYR:CE1	2.32	0.65
1:A:130:ARG:O	1:A:133:THR:HG22	1.96	0.65
1:A:329:ARG:HA	2:B:3:SSU:O4	1.98	0.64
1:A:358:GLY:HA2	2:B:5:SSU:H1'	1.79	0.64
1:A:403:MET:CE	1:A:411:ARG:HH21	2.11	0.64
1:A:485:PHE:CE1	1:A:486:LYS:HG2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:VAL:HG13	1:A:12:ASP:N	2.12	0.64
1:A:102:ILE:HG23	1:A:102:ILE:O	1.98	0.64
1:A:416:ILE:O	1:A:420:ILE:HG12	1.98	0.63
1:A:88:LEU:HD23	1:A:88:LEU:O	1.99	0.63
1:A:19:ARG:HA	1:A:22:VAL:CG1	2.29	0.63
1:A:168:ARG:CD	1:A:172:ARG:HH22	2.12	0.62
1:A:67:LYS:HA	2:B:3:SSU:H1'	1.81	0.62
1:A:168:ARG:HD2	1:A:172:ARG:HH22	1.63	0.61
1:A:282:PRO:HB2	1:A:283:PRO:HD3	1.82	0.61
1:A:198:ARG:HD2	1:A:643:ASN:OD1	1.99	0.61
1:A:80:LEU:HD12	1:A:136:VAL:HA	1.80	0.61
1:A:130:ARG:HG3	1:A:130:ARG:HH11	1.65	0.61
1:A:602:ASN:HD21	1:A:606:LYS:NZ	1.98	0.61
1:A:649:ARG:HE	1:A:651:ARG:C	2.03	0.61
1:A:220:VAL:HB	1:A:264:MET:HG2	1.83	0.61
1:A:403:MET:HE2	1:A:411:ARG:HH21	1.65	0.61
1:A:73:ARG:HB3	1:A:74:PRO:HD2	1.83	0.61
1:A:359:LEU:HD11	1:A:651:ARG:NE	2.16	0.60
1:A:88:LEU:CD2	1:A:135:LYS:HB3	2.32	0.60
1:A:504:ARG:HG2	1:A:504:ARG:HH11	1.65	0.60
1:A:22:VAL:HG13	1:A:23:ASN:N	2.16	0.60
1:A:105:ASP:OD2	1:A:108:VAL:HB	2.02	0.60
1:A:96:GLU:HG3	1:A:97:ALA:N	2.17	0.59
1:A:100:THR:HG22	1:A:114:GLU:O	2.02	0.59
1:A:92:ILE:HD13	1:A:132:ILE:HA	1.85	0.59
1:A:80:LEU:HB3	1:A:84:GLU:OE2	2.03	0.59
1:A:538:ALA:HB3	1:A:539:PRO:HD3	1.84	0.58
1:A:143:VAL:HG12	1:A:144:ARG:N	2.18	0.58
1:A:385:ARG:HG3	2:B:5:SSU:C2	2.32	0.58
1:A:485:PHE:CD1	1:A:486:LYS:N	2.72	0.58
1:A:23:ASN:OD1	1:A:32:ILE:HD12	2.03	0.58
1:A:449:ILE:O	1:A:449:ILE:HD12	2.03	0.58
1:A:22:VAL:HG11	1:A:35:ILE:CD1	2.34	0.58
1:A:483:GLN:HE21	1:A:489:TYR:HE2	1.51	0.57
1:A:127:GLU:C	1:A:129:LEU:H	2.06	0.57
1:A:157:ARG:O	1:A:161:GLN:HG2	2.05	0.57
2:C:1:SSU:O2	2:C:1:SSU:H2'	2.05	0.57
1:A:147:PRO:HB2	1:A:493:LEU:HD21	1.86	0.57
1:A:524:MET:HA	1:A:551:GLN:HE22	1.69	0.57
1:A:22:VAL:C	1:A:24:GLN:H	2.06	0.56
1:A:505:GLU:O	1:A:509:ILE:HG13	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:ILE:N	1:A:579:ILE:HD12	2.21	0.56
1:A:73:ARG:CZ	1:A:108:VAL:HG13	2.36	0.56
1:A:100:THR:HG21	1:A:145:THR:HG23	1.88	0.56
1:A:374:ARG:HH12	1:A:445:GLU:HB2	1.71	0.55
1:A:100:THR:HG23	1:A:101:ASN:N	2.22	0.55
1:A:460:GLY:O	1:A:461:MET:HB2	2.06	0.55
1:A:67:LYS:CA	2:B:3:SSU:H1'	2.37	0.55
1:A:144:ARG:NH1	1:A:485:PHE:HB2	2.22	0.55
1:A:265:LEU:HD21	1:A:278:ILE:HD13	1.87	0.55
1:A:96:GLU:HG3	1:A:97:ALA:H	1.71	0.55
1:A:423:GLY:O	1:A:542:LYS:HD3	2.07	0.54
1:A:120:LEU:N	1:A:120:LEU:HD22	2.23	0.54
1:A:104:PHE:HD1	1:A:111:VAL:HG22	1.72	0.54
1:A:75:ASP:O	1:A:78:VAL:HG12	2.07	0.54
1:A:78:VAL:HG22	1:A:78:VAL:O	2.08	0.53
1:A:215:LEU:HD21	1:A:218:PHE:CD1	2.43	0.53
1:A:224:MET:O	1:A:231:ALA:HB2	2.07	0.53
1:A:267:TYR:CZ	1:A:271:TYR:HE2	2.26	0.53
1:A:108:VAL:HG12	1:A:108:VAL:O	2.08	0.53
1:A:110:GLU:HA	1:A:139:ALA:HB3	1.89	0.53
1:A:464:GLU:OE1	1:A:464:GLU:HA	2.07	0.53
1:A:113:ILE:HG21	1:A:121:VAL:HG21	1.91	0.53
1:A:632:HIS:CD2	2:C:1:SSU:O2'	2.63	0.52
1:A:637:ILE:O	1:A:639:THR:HG23	2.10	0.52
1:A:34:GLU:HG2	1:A:35:ILE:N	2.24	0.52
1:A:89:ILE:HA	1:A:92:ILE:HG22	1.92	0.52
2:B:3:SSU:O2'	2:B:4:SSU:H5"	2.09	0.52
1:A:33:THR:HG21	1:A:75:ASP:OD2	2.10	0.52
1:A:31:LYS:NZ	1:A:31:LYS:HB3	2.24	0.52
1:A:18:ILE:O	1:A:21:VAL:HG12	2.11	0.51
1:A:437:GLN:H	1:A:437:GLN:NE2	2.08	0.51
1:A:650:LEU:O	1:A:651:ARG:HB3	2.10	0.51
1:A:198:ARG:HD2	1:A:643:ASN:CG	2.31	0.51
1:A:298:ILE:HD11	5:A:669:HOH:O	2.10	0.51
1:A:10:GLN:O	1:A:14:ILE:HG13	2.10	0.51
1:A:60:LYS:O	1:A:64:LYS:HG3	2.09	0.51
1:A:369:LYS:NZ	1:A:402:GLN:HE22	2.09	0.51
1:A:94:PRO:O	1:A:96:GLU:N	2.42	0.51
1:A:447:ALA:HB2	1:A:452:ILE:HG13	1.93	0.51
1:A:551:GLN:NE2	1:A:557:GLY:HA3	2.25	0.50
1:A:22:VAL:HG11	1:A:35:ILE:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:THR:CG2	1:A:366:GLY:O	2.60	0.50
1:A:569:MET:O	1:A:577:GLU:N	2.31	0.50
1:A:62:LEU:HD22	1:A:70:ILE:CD1	2.38	0.50
1:A:266:PRO:HG2	1:A:308:TYR:CZ	2.47	0.50
1:A:485:PHE:HE1	1:A:486:LYS:HE3	1.76	0.50
1:A:57:GLU:HA	1:A:60:LYS:HE2	1.94	0.50
1:A:80:LEU:HB2	1:A:85:ALA:HB2	1.93	0.50
1:A:197:PHE:CD2	1:A:642:PRO:HG2	2.46	0.50
1:A:406:GLU:O	1:A:410:LYS:HG3	2.12	0.50
1:A:602:ASN:HD21	1:A:606:LYS:HZ3	1.59	0.50
1:A:309:ARG:HB3	1:A:310:PRO:HD2	1.93	0.49
1:A:22:VAL:HG13	1:A:23:ASN:H	1.77	0.49
1:A:620:GLU:HB2	1:A:623:LYS:HD2	1.93	0.49
1:A:216:VAL:HG21	1:A:364:ILE:CD1	2.42	0.49
1:A:216:VAL:HG21	1:A:364:ILE:HD13	1.95	0.49
1:A:604:VAL:O	1:A:607:VAL:HG12	2.13	0.49
1:A:262:CYS:SG	1:A:288:MET:HB2	2.52	0.49
1:A:285:ARG:HH21	1:A:285:ARG:CG	2.16	0.49
1:A:365:THR:HG23	1:A:366:GLY:O	2.13	0.49
1:A:57:GLU:O	1:A:60:LYS:HE2	2.13	0.49
1:A:118:PRO:HA	1:A:121:VAL:HG12	1.95	0.49
1:A:494:SER:OG	1:A:496:ILE:HG12	2.12	0.49
1:A:99:ILE:HA	1:A:115:ALA:HA	1.95	0.49
1:A:128:THR:HG22	1:A:128:THR:O	2.13	0.49
1:A:80:LEU:H	1:A:138:TRP:HE1	1.61	0.49
1:A:422:ARG:NH2	1:A:584:GLU:OE1	2.44	0.49
1:A:483:GLN:NE2	1:A:489:TYR:HE2	2.11	0.49
1:A:207:VAL:HB	1:A:214:VAL:HG22	1.95	0.48
1:A:130:ARG:O	1:A:134:GLN:HG3	2.13	0.48
1:A:89:ILE:HG13	1:A:132:ILE:HD11	1.95	0.48
1:A:21:VAL:CG1	1:A:66:LEU:HD21	2.43	0.48
1:A:424:GLY:O	1:A:515:PRO:HB3	2.14	0.48
1:A:62:LEU:O	1:A:62:LEU:HD23	2.12	0.48
1:A:130:ARG:HG3	1:A:130:ARG:NH1	2.29	0.48
1:A:484:ILE:HG22	1:A:485:PHE:N	2.29	0.47
1:A:138:TRP:O	1:A:140:PRO:HD3	2.14	0.47
1:A:220:VAL:HG22	1:A:221:ASN:N	2.29	0.47
1:A:33:THR:HG21	1:A:47:LYS:HE3	1.97	0.47
1:A:144:ARG:O	1:A:145:THR:C	2.53	0.47
1:A:168:ARG:HD2	1:A:172:ARG:NH2	2.30	0.47
1:A:221:ASN:OD1	1:A:223:ALA:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:HIS:O	1:A:421:LYS:HB2	2.15	0.47
1:A:44:ILE:O	1:A:72:VAL:HG23	2.15	0.47
1:A:369:LYS:HE3	1:A:371:ILE:HG12	1.96	0.47
1:A:446:TYR:CZ	1:A:451:GLY:HA3	2.50	0.47
1:A:565:ARG:HH21	1:A:582:ASN:HA	1.80	0.47
1:A:22:VAL:HG21	1:A:44:ILE:HD13	1.97	0.46
1:A:365:THR:HG21	1:A:392:GLU:H	1.80	0.46
1:A:111:VAL:HG23	1:A:138:TRP:HB3	1.98	0.46
1:A:198:ARG:HH12	1:A:625:LEU:HD23	1.80	0.46
1:A:556:LEU:O	1:A:560:VAL:HG23	2.15	0.46
1:A:570:VAL:HA	1:A:576:THR:HA	1.97	0.46
1:A:643:ASN:O	1:A:646:ASP:HB2	2.15	0.46
1:A:115:ALA:O	1:A:144:ARG:HA	2.15	0.46
1:A:409:GLU:HG3	1:A:442:VAL:HG13	1.98	0.46
1:A:578:VAL:HG23	1:A:578:VAL:O	2.16	0.46
2:B:4:SSU:H6	2:B:4:SSU:O5'	2.15	0.46
1:A:220:VAL:HG12	1:A:263:GLY:HA3	1.98	0.46
1:A:490:ASN:HB3	1:A:493:LEU:HD12	1.98	0.46
1:A:62:LEU:HB3	1:A:70:ILE:CD1	2.47	0.45
1:A:110:GLU:CB	1:A:139:ALA:HB3	2.46	0.45
1:A:553:GLU:HG2	1:A:558:ARG:CZ	2.46	0.45
1:A:524:MET:HB2	1:A:526:VAL:CG2	2.41	0.45
1:A:207:VAL:HB	1:A:214:VAL:CG2	2.47	0.45
1:A:21:VAL:HG22	1:A:25:MET:CE	2.44	0.45
1:A:143:VAL:HG12	1:A:144:ARG:H	1.80	0.45
1:A:359:LEU:CG	1:A:651:ARG:HD3	2.45	0.45
1:A:80:LEU:CD1	1:A:136:VAL:HA	2.47	0.45
1:A:350:ILE:HD11	1:A:379:ALA:HB1	1.99	0.45
1:A:613:ARG:HH11	1:A:613:ARG:CB	2.29	0.44
1:A:485:PHE:HD1	1:A:486:LYS:N	2.13	0.44
1:A:253:ILE:HD13	1:A:337:LEU:HD13	1.99	0.44
1:A:595:ALA:HB1	1:A:599:GLU:HB2	1.99	0.44
1:A:287:LEU:HD22	1:A:433:VAL:HG21	2.00	0.44
1:A:181:LYS:HB2	1:A:182:PRO:HD2	1.98	0.44
1:A:189:ILE:HD12	1:A:651:ARG:HG2	1.99	0.44
1:A:134:GLN:O	1:A:136:VAL:N	2.51	0.44
1:A:526:VAL:O	1:A:526:VAL:HG12	2.17	0.44
1:A:88:LEU:HD22	1:A:136:VAL:HG13	2.00	0.44
1:A:93:VAL:HG11	1:A:99:ILE:HD11	2.00	0.44
1:A:127:GLU:C	1:A:129:LEU:N	2.71	0.44
1:A:346:LEU:HD22	1:A:469:HIS:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:ILE:HD12	1:A:446:TYR:CE2	2.53	0.44
1:A:80:LEU:HD12	1:A:136:VAL:HG12	2.00	0.43
1:A:363:ALA:O	1:A:389:LEU:HD12	2.18	0.43
1:A:567:ILE:HA	1:A:568:PRO:HD3	1.89	0.43
1:A:19:ARG:CA	1:A:22:VAL:HG12	2.44	0.43
1:A:144:ARG:HE	1:A:144:ARG:HB2	1.60	0.43
1:A:385:ARG:HG3	2:B:5:SSU:O2	2.18	0.43
1:A:10:GLN:HG2	1:A:180:ARG:O	2.18	0.43
1:A:104:PHE:CD1	1:A:111:VAL:HG22	2.53	0.43
1:A:374:ARG:HH12	1:A:445:GLU:CB	2.31	0.43
1:A:197:PHE:HB2	1:A:644:ASN:OD1	2.19	0.43
1:A:22:VAL:CG1	1:A:23:ASN:N	2.82	0.43
1:A:57:GLU:CA	1:A:60:LYS:HE2	2.48	0.43
1:A:202:ARG:NH2	3:A:652:SO4:O2	2.52	0.43
1:A:239:GLU:HG2	1:A:240:PHE:N	2.34	0.43
1:A:22:VAL:C	1:A:24:GLN:N	2.73	0.42
1:A:46:VAL:O	1:A:74:PRO:HA	2.20	0.42
1:A:11:VAL:CG1	1:A:12:ASP:N	2.82	0.42
1:A:283:PRO:HG3	1:A:472:TYR:CG	2.55	0.42
1:A:421:LYS:C	1:A:423:GLY:H	2.23	0.42
1:A:116:LYS:O	1:A:117:LYS:HD3	2.20	0.42
1:A:182:PRO:O	1:A:183:GLU:C	2.58	0.42
1:A:447:ALA:HA	1:A:452:ILE:HG12	2.02	0.42
1:A:63:ALA:HB2	1:A:70:ILE:HG12	2.00	0.42
1:A:644:ASN:HB2	3:A:652:SO4:O3	2.20	0.42
1:A:94:PRO:C	1:A:96:GLU:H	2.23	0.42
1:A:132:ILE:HG23	1:A:133:THR:N	2.34	0.42
1:A:93:VAL:O	1:A:95:LYS:N	2.53	0.41
1:A:116:LYS:C	1:A:117:LYS:HD3	2.40	0.41
1:A:598:ARG:HH11	1:A:598:ARG:HG2	1.85	0.41
1:A:102:ILE:C	1:A:102:ILE:HD13	2.41	0.41
1:A:358:GLY:CA	2:B:5:SSU:H1'	2.48	0.41
1:A:30:ALA:HA	1:A:48:ASN:OD1	2.20	0.41
1:A:354:HIS:CE1	2:B:5:SSU:C2	3.03	0.41
1:A:422:ARG:HH22	1:A:584:GLU:CG	2.33	0.41
1:A:632:HIS:CB	2:C:1:SSU:H1'	2.50	0.41
1:A:644:ASN:O	1:A:645:LEU:HB2	2.21	0.41
1:A:454:VAL:HG11	1:A:515:PRO:HB2	2.01	0.41
1:A:493:LEU:O	1:A:494:SER:C	2.58	0.41
1:A:11:VAL:O	1:A:14:ILE:N	2.51	0.41
1:A:422:ARG:HH22	1:A:584:GLU:CD	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:PRO:HA	1:A:582:ASN:ND2	2.34	0.41
1:A:133:THR:O	1:A:137:LYS:N	2.45	0.41
1:A:287:LEU:HD11	1:A:346:LEU:HD23	2.03	0.41
1:A:101:ASN:O	1:A:102:ILE:HB	2.21	0.41
1:A:188:TRP:C	1:A:189:ILE:HG13	2.41	0.41
1:A:110:GLU:CA	1:A:139:ALA:HB3	2.51	0.41
1:A:133:THR:HG23	1:A:134:GLN:N	2.36	0.41
1:A:260:ASP:OD2	1:A:261:HIS:HD2	2.04	0.41
2:C:1:SSU:O2	2:C:1:SSU:C2'	2.68	0.41
1:A:362:ILE:HD11	1:A:650:LEU:HD12	2.03	0.41
1:A:198:ARG:HH22	1:A:625:LEU:HD23	1.87	0.40
1:A:430:ALA:N	1:A:523:GLY:HA2	2.36	0.40
1:A:89:ILE:HG23	1:A:90:PHE:N	2.36	0.40
1:A:432:ALA:HA	1:A:462:ILE:HG12	2.03	0.40
1:A:507:GLN:HE22	1:A:536:GLN:HE22	1.69	0.40
1:A:565:ARG:NH2	1:A:582:ASN:HA	2.36	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	633/651 (97%)	567 (90%)	52 (8%)	14 (2%)	6 12

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	LYS
1	A	102	ILE
1	A	135	LYS
1	A	92	ILE
1	A	97	ALA

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Mol	Chain	Res	Type
1	A	109	GLY
1	A	78	VAL
1	A	98	GLU
1	A	512	SER
1	A	94	PRO
1	A	495	GLU
1	A	124	LYS
1	A	451	GLY
1	A	32	ILE

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	558/570 (98%)	540 (97%)	18 (3%)	39 65

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	ILE
1	A	151	GLN
1	A	245	ARG
1	A	268	LEU
1	A	285	ARG
1	A	332	SER
1	A	365	THR
1	A	385	ARG
1	A	392	GLU
1	A	405	ARG
1	A	437	GLN
1	A	480	LEU
1	A	487	GLU
1	A	597	ARG
1	A	613	ARG
1	A	622	GLN
1	A	625	LEU

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Mol	Chain	Res	Type
1	A	649	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	GLN
1	A	161	GLN
1	A	173	GLN
1	A	292	GLN
1	A	341	ASN
1	A	361	ASN
1	A	380	ASN
1	A	399	ASN
1	A	402	GLN
1	A	437	GLN
1	A	507	GLN
1	A	551	GLN
1	A	561	GLN
1	A	602	ASN
1	A	632	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	0/6	-	-
2	C	0/6	-	-
All	All	0/12	-	-

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

Of 8 non-standard protein/DNA/RNA residues modelled in this entry, 1 is modelled with single atom - leaving 7 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	SSU	B	6	2	0,3,22	-	-	0,3,33	-	-
2	SSU	C	2	2	0,3,22	-	-	0,3,33	-	-
2	SSU	B	3	2	18,21,22	0.36	0	26,30,33	0.68	1 (3%)
2	SSU	B	4	2	18,21,22	0.31	0	26,30,33	0.26	0
2	SSU	C	1	2	18,18,22	0.25	0	26,26,33	0.46	0
2	SSU	B	2	2	18,21,22	0.28	0	26,30,33	0.40	0
2	SSU	B	5	2	18,21,22	0.32	0	26,30,33	0.47	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
2	SSU	B	3	2	-	1/7/25/26	0/2/2/2
2	SSU	B	4	2	-	0/7/25/26	0/2/2/2
2	SSU	C	1	2	-	2/6/22/26	0/2/2/2
2	SSU	B	2	2	-	3/7/25/26	0/2/2/2
2	SSU	B	5	2	-	0/7/25/26	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	3	SSU	C2'-C1'-N1	2.50	120.29	113.22

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	SSU	C2'-C1'-N1-C2
2	C	1	SSU	C2'-C1'-N1-C6
2	B	2	SSU	C3'-C4'-C5'-O5'
2	B	2	SSU	C2'-C1'-N1-C6
2	B	2	SSU	C2'-C1'-N1-C2
2	B	3	SSU	C2'-C1'-N1-C2

There are no ring outliers.

6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	6	SSU	1	0
2	B	3	SSU	4	0
2	B	4	SSU	3	0
2	C	1	SSU	6	0
2	B	2	SSU	1	0
2	B	5	SSU	6	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
3	SO4	A	653	-	4,4,4	0.21	0	6,6,6	0.07	0
3	SO4	A	654	-	4,4,4	0.20	0	6,6,6	0.09	0
3	SO4	A	652	-	4,4,4	0.22	0	6,6,6	0.05	0
3	SO4	A	656	-	4,4,4	0.23	0	6,6,6	0.06	0
3	SO4	A	655	4	4,4,4	0.21	0	6,6,6	0.06	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 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	652	SO4	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	637/651 (97%)	0.60	80 (12%) 3 2	28, 53, 147, 156	0
2	B	0/6	-	-	-	-
2	C	0/6	-	-	-	-
All	All	637/663 (96%)	0.60	80 (12%) 3 2	28, 53, 147, 156	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	125	ASN	8.4
1	A	120	LEU	7.6
1	A	113	ILE	7.4
1	A	135	LYS	7.2
1	A	121	VAL	6.9
1	A	31	LYS	6.9
1	A	83	GLU	6.7
1	A	79	LEU	6.7
1	A	132	ILE	6.6
1	A	130	ARG	6.5
1	A	82	PRO	6.4
1	A	131	LEU	6.3
1	A	103	ALA	6.2
1	A	104	PHE	6.1
1	A	136	VAL	5.9
1	A	124	LYS	5.9
1	A	33	THR	5.4
1	A	138	TRP	5.3
1	A	93	VAL	5.3
1	A	91	GLU	5.1
1	A	112	LEU	5.0
1	A	76	PRO	4.9
1	A	89	ILE	4.8
1	A	127	GLU	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	143	VAL	4.8
1	A	102	ILE	4.8
1	A	133	THR	4.7
1	A	129	LEU	4.6
1	A	80	LEU	4.4
1	A	122	ILE	4.4
1	A	81	PRO	4.3
1	A	29	GLU	4.3
1	A	35	ILE	4.3
1	A	100	THR	4.2
1	A	137	LYS	4.1
1	A	28	LYS	4.1
1	A	84	GLU	3.8
1	A	92	ILE	3.8
1	A	94	PRO	3.8
1	A	30	ALA	3.8
1	A	90	PHE	3.7
1	A	47	LYS	3.7
1	A	96	GLU	3.6
1	A	126	GLY	3.6
1	A	46	VAL	3.6
1	A	99	ILE	3.5
1	A	485	PHE	3.5
1	A	27	PRO	3.4
1	A	118	PRO	3.4
1	A	62	LEU	3.4
1	A	85	ALA	3.3
1	A	95	LYS	3.3
1	A	123	GLY	3.2
1	A	128	THR	3.1
1	A	32	ILE	3.1
1	A	139	ALA	3.0
1	A	70	ILE	3.0
1	A	72	VAL	3.0
1	A	486	LYS	3.0
1	A	117	LYS	2.9
1	A	134	GLN	2.9
1	A	60	LYS	2.8
1	A	111	VAL	2.7
1	A	509	ILE	2.7
1	A	63	ALA	2.6
1	A	86	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	119	GLY	2.5
1	A	489	TYR	2.4
1	A	87	LYS	2.4
1	A	142	VAL	2.3
1	A	98	GLU	2.3
1	A	44	ILE	2.3
1	A	34	GLU	2.2
1	A	281	THR	2.2
1	A	446	TYR	2.2
1	A	534	PHE	2.2
1	A	59	ILE	2.1
1	A	140	PRO	2.1
1	A	141	LYS	2.1
1	A	229	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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
2	SSU	C	1	17/21	0.67	0.42	107,109,112,113	0
2	SSU	B	5	20/21	0.70	0.33	109,115,118,119	0
2	SSU	B	6	4/21	0.77	0.25	119,120,120,121	0
2	SSU	B	3	20/21	0.77	0.26	106,111,115,116	0
2	SSU	B	2	20/21	0.79	0.27	116,118,122,123	0
2	SSU	B	4	20/21	0.82	0.32	111,113,115,116	0
2	SSU	C	2	4/21	0.88	0.15	106,106,107,107	0
2	SSU	B	1	1/21	0.89	0.17	121,121,121,121	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95^{th} 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
3	SO4	A	656	5/5	0.77	0.31	131,131,131,131	0
3	SO4	A	654	5/5	0.83	0.32	95,95,97,97	0
3	SO4	A	655	5/5	0.84	0.31	131,131,131,131	0
4	ZN	A	657	1/1	0.85	0.07	91,91,91,91	0
3	SO4	A	653	5/5	0.86	0.33	122,122,123,123	0
4	ZN	A	658	1/1	0.95	0.12	125,125,125,125	0
3	SO4	A	652	5/5	0.97	0.34	55,59,62,62	0

6.5 Other polymers (i)

There are no such residues in this entry.