Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 12:32 pm BST

PDB ID	:	4M5D
Title	:	Crystal structure of the Utp22 and Rrp7 complex from Saccharomyces cerevisiae
Authors	:	Lin, J.; Ye, K.
Deposited on	:	2013-08-08
Resolution	:	1.97 Å(reported)

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

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

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

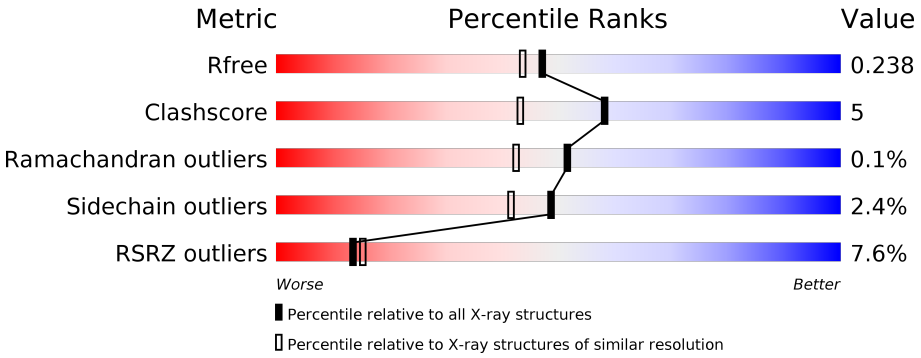
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance

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

The reported resolution of this entry is 1.97 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1237	6% 78% 9% • 11%
2	B	297	8% 52% 5% 43%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11079 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.

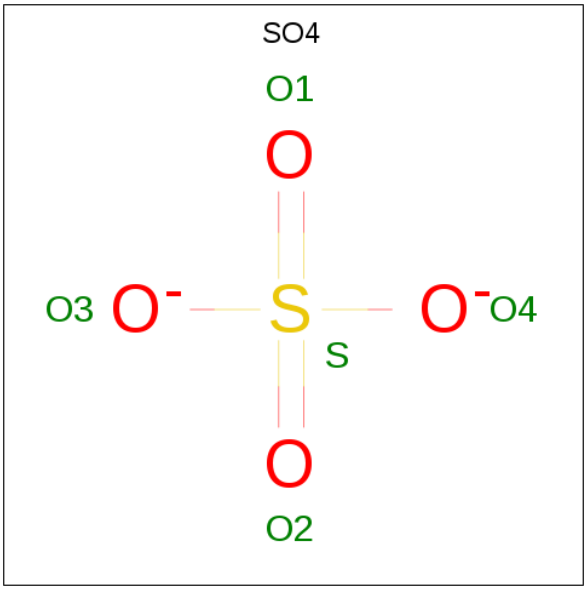
- Molecule 1 is a protein called U3 small nucleolar RNA-associated protein 22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1098	Total	C	N	O	S	0	0	0
			8870	5763	1462	1621	24			

- Molecule 2 is a protein called Ribosomal RNA-processing protein 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	169	Total	C	N	O	S	0	0	0
			1368	884	225	252	7			

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



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

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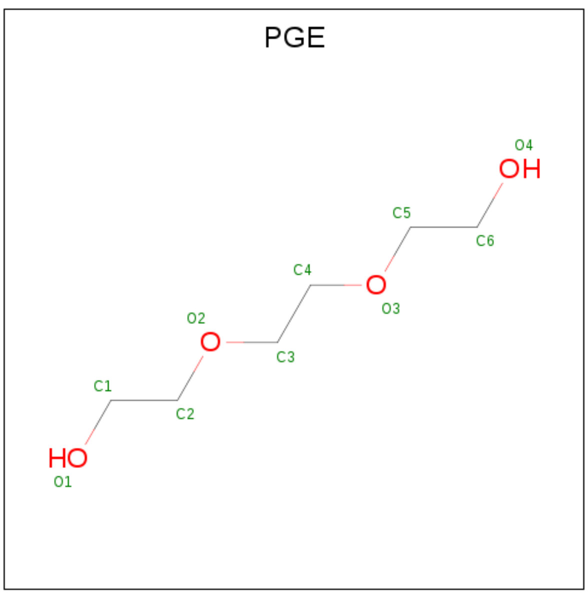
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 10 6 4	0	0
4	A	1	Total C O 7 4 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	4	2		

- Molecule 5 is water.

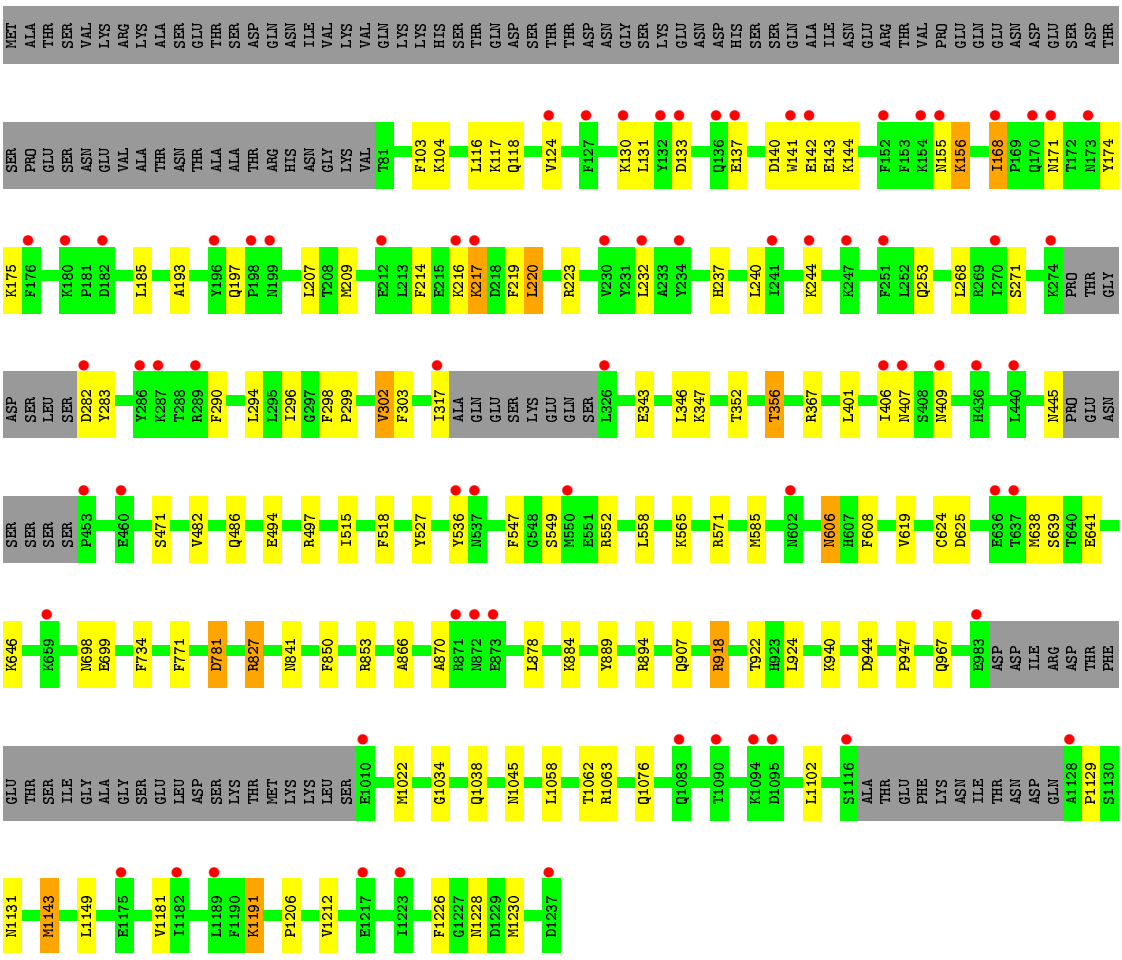
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	690	Total	O	0	0
			690	690		
5	B	73	Total	O	0	0
			73	73		

3 Residue-property plots (i)

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

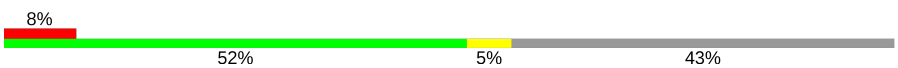
- Molecule 1: U3 small nucleolar RNA-associated protein 22

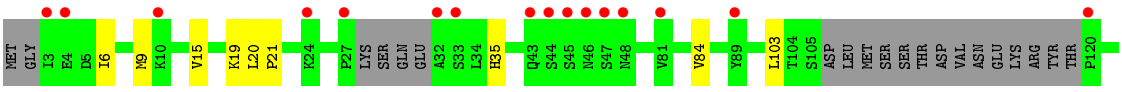
Chain A:

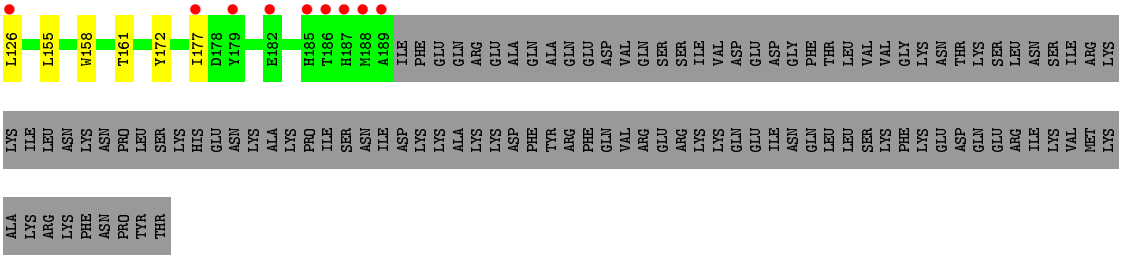


- Molecule 2: Ribosomal RNA-processing protein 7

Chain B:






L126
L155
W158
T161
Y172
I177
D178
Y179
E182
H185
T186
H187
M188
A189
ILE PHE GLU GLN ARG GLU ALA GLN ALA GLN GLU ASP VAL GLN SER SER ILE VAL ASP GLU ASP GLY PHE THR LEU VAL VAL GLY LYS ASN THR LYS SER LEU ASN SER ILE ARG LYS
LYS ILE LEU ASN LYS ASN PRO LEU SER LYS HIS GLU ASN LYS ALA LYS PRO ILE SER ASN ILE ASP LYS LYS ALA LYS LYS ASP PHE TYR ARG PHE GLN VAL ARG GLU ARG LYS LYS GLN GLU ILE ASN GLN LEU LEU SER LYS PHE LYS GLU ASP GLN GLU GLU ARG ILE LYS VAL MET LYS
ALA LYS ARG LYS PHE ASN PRO TYR THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	126.26Å 129.56Å 214.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 1.97 19.94 – 1.97	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.94-1.97) 100.0 (19.94-1.97)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.208 , 0.238 0.207 , 0.238	Depositor DCC
R_{free} test set	6183 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	25.7	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 56.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.009 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11079	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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: PGE, 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	0.49	0/9081	0.55	0/12283
2	B	0.45	0/1405	0.52	0/1903
All	All	0.48	0/10486	0.55	0/14186

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8870	0	8975	88	0
2	B	1368	0	1330	15	0
3	A	55	0	0	0	0
4	A	17	0	23	2	0
4	B	6	0	7	0	0
5	A	690	0	0	13	0
5	B	73	0	0	0	0
All	All	11079	0	10335	100	0

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

All (100) 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:168:ILE:HD13	1:A:171:ASN:HB2	1.46	0.97
1:A:168:ILE:HD12	1:A:168:ILE:H	1.31	0.92
1:A:606:ASN:HD22	1:A:608:PHE:H	1.21	0.89
1:A:878:LEU:HD21	2:B:103:LEU:HD13	1.55	0.88
1:A:168:ILE:CD1	1:A:171:ASN:HB2	2.09	0.83
1:A:117:LYS:HB3	4:A:1313:PGE:H4	1.63	0.79
1:A:142:GLU:O	1:A:144:LYS:HG2	1.87	0.75
1:A:356:THR:HG21	1:A:401:LEU:HD13	1.68	0.74
2:B:6:ILE:CG2	2:B:9:MET:HE1	2.20	0.71
1:A:352:THR:O	1:A:356:THR:HG23	1.91	0.69
1:A:209:MET:HE3	1:A:298:PHE:CD1	2.29	0.67
1:A:1063:ARG:HD3	5:A:1898:HOH:O	1.97	0.64
1:A:317:ILE:HG12	1:A:549:SER:HB3	1.80	0.62
1:A:232:LEU:HD13	1:A:296:ILE:HD11	1.81	0.62
1:A:209:MET:HE3	1:A:298:PHE:CE1	2.35	0.62
1:A:870:ALA:HB2	1:A:878:LEU:HD22	1.82	0.61
1:A:168:ILE:HD13	1:A:171:ASN:CB	2.27	0.61
1:A:518:PHE:CZ	1:A:1076:GLN:HG2	2.36	0.61
1:A:1143:MET:HB3	2:B:172:TYR:CE2	2.36	0.60
1:A:1149:LEU:HD12	1:A:1226:PHE:CD2	2.37	0.60
1:A:606:ASN:ND2	1:A:608:PHE:H	1.95	0.59
2:B:9:MET:HE2	2:B:15:VAL:CG2	2.31	0.59
2:B:6:ILE:HG22	2:B:9:MET:HE1	1.84	0.59
1:A:209:MET:CE	1:A:298:PHE:CE1	2.87	0.58
1:A:781:ASP:OD2	5:A:2089:HOH:O	2.17	0.58
1:A:918:ARG:O	1:A:922:THR:HG23	2.04	0.57
1:A:219:PHE:CE2	1:A:220:LEU:HD13	2.40	0.57
1:A:536:TYR:OH	1:A:552:ARG:HD3	2.06	0.56
1:A:406:ILE:H	1:A:406:ILE:HD12	1.71	0.56
2:B:9:MET:HE2	2:B:15:VAL:HG21	1.89	0.54
1:A:299:PRO:HB2	1:A:302:VAL:HG13	1.89	0.54
2:B:6:ILE:HG21	2:B:9:MET:HE1	1.90	0.53
1:A:827:ARG:NH2	5:A:1789:HOH:O	2.41	0.53
1:A:209:MET:CE	1:A:298:PHE:CD1	2.92	0.52
2:B:9:MET:CE	2:B:15:VAL:HG21	2.38	0.52
1:A:268:LEU:HD23	1:A:294:LEU:HD12	1.92	0.51
1:A:1191:LYS:HE2	5:A:1991:HOH:O	2.10	0.51
1:A:156:LYS:HG2	1:A:237:HIS:CE1	2.45	0.51
1:A:299:PRO:O	1:A:302:VAL:HG22	2.11	0.51
1:A:547:PHE:CZ	1:A:552:ARG:HG2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:LEU:HG	1:A:558:LEU:O	2.08	0.51
1:A:494:GLU:CD	1:A:497:ARG:HH12	2.14	0.50
1:A:143:GLU:HG2	1:A:175:LYS:HG3	1.92	0.50
1:A:639:SER:OG	1:A:641:GLU:HG3	2.12	0.49
1:A:240:LEU:O	1:A:244:LYS:HG2	2.13	0.49
1:A:1063:ARG:CD	5:A:1898:HOH:O	2.59	0.49
1:A:209:MET:HE3	1:A:298:PHE:HD1	1.77	0.49
1:A:133:ASP:O	1:A:137:GLU:HG3	2.12	0.49
1:A:185:LEU:O	1:A:346:LEU:HD22	2.13	0.49
2:B:6:ILE:HG22	2:B:9:MET:CE	2.43	0.49
2:B:6:ILE:CG2	2:B:9:MET:CE	2.91	0.48
1:A:894:ARG:HD2	1:A:1045:ASN:OD1	2.14	0.48
1:A:853:ARG:HD3	1:A:889:TYR:CZ	2.49	0.47
1:A:884:LYS:HE3	5:A:1913:HOH:O	2.15	0.47
1:A:209:MET:CE	1:A:298:PHE:HE1	2.27	0.47
1:A:445:ASN:C	5:A:2006:HOH:O	2.52	0.47
1:A:116:LEU:HD11	1:A:290:PHE:HZ	1.80	0.46
1:A:565:LYS:HE2	5:A:1632:HOH:O	2.16	0.46
1:A:168:ILE:N	1:A:168:ILE:HD12	2.12	0.46
1:A:515:ILE:CG2	1:A:947:PRO:HG2	2.46	0.46
1:A:352:THR:O	1:A:356:THR:CG2	2.63	0.46
2:B:20:LEU:HD21	2:B:35:HIS:HB2	1.98	0.46
1:A:1034:GLY:O	1:A:1038:GLN:HG3	2.16	0.45
1:A:193:ALA:O	1:A:367:ARG:NH2	2.50	0.45
1:A:924:LEU:HD21	1:A:1181:VAL:HG13	1.99	0.45
1:A:1143:MET:HB3	2:B:172:TYR:CD2	2.53	0.44
1:A:619:VAL:HG13	1:A:624:CYS:HB3	2.00	0.44
2:B:21:PRO:HD3	2:B:158:TRP:O	2.18	0.44
1:A:1058:LEU:O	1:A:1062:THR:HG23	2.17	0.44
1:A:232:LEU:HD13	1:A:296:ILE:CD1	2.47	0.44
1:A:1131:ASN:HB2	5:A:2061:HOH:O	2.17	0.43
1:A:343:GLU:HG2	1:A:347:LYS:HE3	1.99	0.43
2:B:19:LYS:HE2	2:B:155:LEU:O	2.17	0.43
1:A:527:TYR:CD2	1:A:698:ASN:HB2	2.54	0.43
1:A:124:VAL:HG11	1:A:290:PHE:CD2	2.54	0.43
1:A:445:ASN:HD22	1:A:471:SER:HB3	1.83	0.43
1:A:253:GLN:HB2	1:A:271:SER:OG	2.19	0.43
1:A:207:LEU:HD11	1:A:294:LEU:HD22	2.01	0.42
1:A:606:ASN:ND2	5:A:1769:HOH:O	2.53	0.42
1:A:104:LYS:HB2	5:A:2055:HOH:O	2.19	0.42
1:A:118:GLN:H	4:A:1313:PGE:H2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:PHE:HB3	1:A:303:PHE:CG	2.54	0.42
1:A:209:MET:HE3	1:A:214:PHE:HZ	1.84	0.42
1:A:130:LYS:HD2	1:A:283:TYR:CZ	2.55	0.42
1:A:140:ASP:OD1	1:A:140:ASP:N	2.52	0.42
1:A:940:LYS:HD2	1:A:944:ASP:HB3	2.01	0.42
1:A:482:VAL:O	1:A:486:GLN:HG2	2.18	0.42
1:A:1206:PRO:HA	1:A:1212:VAL:HG12	2.01	0.42
1:A:116:LEU:HD11	1:A:290:PHE:CZ	2.55	0.42
1:A:217:LYS:HA	1:A:217:LYS:HD3	1.79	0.41
1:A:638:MET:CE	1:A:646:LYS:HD2	2.50	0.41
2:B:84:VAL:HG11	2:B:126:LEU:HD11	2.02	0.41
1:A:866:ALA:C	1:A:878:LEU:HD23	2.41	0.41
1:A:1102:LEU:HA	1:A:1230:MET:O	2.21	0.41
1:A:907:GLN:HG2	5:A:1885:HOH:O	2.20	0.41
1:A:699:GLU:N	5:A:1992:HOH:O	2.52	0.41
1:A:771:PHE:HB2	1:A:1129:PRO:HB2	2.02	0.41
1:A:734:PHE:HB2	1:A:850:PHE:CZ	2.56	0.40
1:A:841:ASN:HD22	1:A:841:ASN:N	2.19	0.40
1:A:174:TYR:CE1	1:A:223:ARG:HG2	2.57	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	1086/1237 (88%)	1070 (98%)	15 (1%)	1 (0%)	51 42
2	B	163/297 (55%)	158 (97%)	5 (3%)	0	100 100
All	All	1249/1534 (81%)	1228 (98%)	20 (2%)	1 (0%)	51 42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1228	ASN

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	1000/1125 (89%)	974 (97%)	26 (3%)	46	37
2	B	154/274 (56%)	152 (99%)	2 (1%)	69	64
All	All	1154/1399 (82%)	1126 (98%)	28 (2%)	49	41

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	PHE
1	A	131	LEU
1	A	141	TRP
1	A	155	ASN
1	A	156	LYS
1	A	168	ILE
1	A	197	GLN
1	A	216	LYS
1	A	217	LYS
1	A	220	LEU
1	A	282	ASP
1	A	302	VAL
1	A	356	THR
1	A	407	ASN
1	A	409	ASN
1	A	571	ARG
1	A	585	MET
1	A	606	ASN
1	A	625	ASP
1	A	781	ASP
1	A	827	ARG
1	A	918	ARG
1	A	967	GLN

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Mol	Chain	Res	Type
1	A	1022	MET
1	A	1143	MET
1	A	1191	LYS
2	B	161	THR
2	B	177	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	ASN
1	A	344	ASN
1	A	407	ASN
1	A	409	ASN
1	A	436	HIS
1	A	445	ASN
1	A	606	ASN
1	A	683	ASN
1	A	841	ASN
1	A	967	GLN
1	A	1083	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

14 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	$\#\|Z\| > 2$
3	SO4	A	1301	-	4,4,4	0.16	0	6,6,6	0.09	0
4	PGE	A	1312	-	9,9,9	0.43	0	8,8,8	0.51	0
3	SO4	A	1305	-	4,4,4	0.15	0	6,6,6	0.19	0
3	SO4	A	1304	-	4,4,4	0.17	0	6,6,6	0.18	0
3	SO4	A	1309	-	4,4,4	0.16	0	6,6,6	0.14	0
4	PGE	B	301	-	5,5,9	0.51	0	4,4,8	0.23	0
3	SO4	A	1303	-	4,4,4	0.16	0	6,6,6	0.19	0
4	PGE	A	1313	-	6,6,9	0.42	0	5,5,8	0.35	0
3	SO4	A	1307	-	4,4,4	0.15	0	6,6,6	0.16	0
3	SO4	A	1310	-	4,4,4	0.17	0	6,6,6	0.17	0
3	SO4	A	1311	-	4,4,4	0.20	0	6,6,6	0.11	0
3	SO4	A	1302	-	4,4,4	0.15	0	6,6,6	0.24	0
3	SO4	A	1308	-	4,4,4	0.18	0	6,6,6	0.10	0
3	SO4	A	1306	-	4,4,4	0.14	0	6,6,6	0.06	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PGE	A	1313	-	-	2/4/4/7	-
4	PGE	A	1312	-	-	2/7/7/7	-
4	PGE	B	301	-	-	1/3/3/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1313	PGE	O2-C3-C4-O3
4	A	1312	PGE	O2-C3-C4-O3
4	B	301	PGE	O1-C1-C2-O2
4	A	1313	PGE	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
4	A	1312	PGE	O3-C5-C6-O4

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1313	PGE	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	1098/1237 (88%)	0.45	71 (6%) 18 20	13, 26, 51, 63	0
2	B	169/297 (56%)	0.94	25 (14%) 2 2	24, 35, 54, 60	0
All	All	1267/1534 (82%)	0.51	96 (7%) 13 15	13, 28, 51, 63	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	171	ASN	6.5
2	B	47	SER	5.9
1	A	286	TYR	5.9
1	A	155	ASN	5.8
1	A	168	ILE	5.8
2	B	32	ALA	5.7
1	A	326	LEU	5.7
2	B	179	TYR	5.4
1	A	317	ILE	5.4
1	A	274	LYS	5.3
2	B	45	SER	5.2
1	A	133	ASP	5.2
2	B	3	ILE	5.2
2	B	43	GLN	5.0
1	A	198	PRO	4.8
1	A	1116	SER	4.8
1	A	170	GLN	4.8
1	A	196	TYR	4.8
1	A	453	PRO	4.7
1	A	199	ASN	4.5
1	A	637	THR	4.5
1	A	1237	ASP	4.4
2	B	187	HIS	4.3
1	A	407	ASN	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	136	GLN	4.1
2	B	27	PRO	4.1
2	B	24	LYS	4.0
1	A	154	LYS	4.0
2	B	188	MET	3.9
2	B	189	ALA	3.9
1	A	141	TRP	3.9
2	B	48	ASN	3.9
2	B	126	LEU	3.8
1	A	247	LYS	3.8
1	A	217	LYS	3.8
2	B	46	ASN	3.7
2	B	44	SER	3.6
1	A	1189	LEU	3.6
1	A	132	TYR	3.6
1	A	1128	ALA	3.3
1	A	289	ARG	3.1
1	A	142	GLU	3.1
1	A	406	ILE	3.1
1	A	1094	LYS	3.1
2	B	33	SER	3.0
1	A	241	ILE	3.0
2	B	185	HIS	3.0
1	A	1175	GLU	2.9
2	B	186	THR	2.9
1	A	232	LEU	2.8
2	B	182	GLU	2.8
1	A	287	LYS	2.8
1	A	659	LYS	2.7
1	A	212	GLU	2.7
1	A	182	ASP	2.7
1	A	871	ARG	2.7
1	A	1010	GLU	2.7
1	A	244	LYS	2.6
1	A	536	TYR	2.6
1	A	460	GLU	2.6
1	A	983	GLU	2.6
1	A	180	LYS	2.6
1	A	1083	GLN	2.6
1	A	282	ASP	2.6
1	A	1223	ILE	2.6
2	B	89	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	636	GLU	2.6
2	B	4	GLU	2.5
1	A	873	GLU	2.5
1	A	1095	ASP	2.5
2	B	81	VAL	2.5
1	A	440	LEU	2.5
1	A	124	VAL	2.5
1	A	436	HIS	2.5
1	A	173	ASN	2.4
1	A	152	PHE	2.4
1	A	251	PHE	2.4
1	A	550	MET	2.4
1	A	872	ASN	2.4
1	A	216	LYS	2.3
1	A	230	VAL	2.3
1	A	602	ASN	2.3
1	A	176	PHE	2.3
1	A	130	LYS	2.3
1	A	1090	THR	2.2
2	B	177	ILE	2.2
1	A	1182	ILE	2.2
1	A	1217	GLU	2.1
1	A	537	ASN	2.1
1	A	234	TYR	2.1
2	B	120	PRO	2.1
2	B	10	LYS	2.1
1	A	270	ILE	2.1
1	A	127	PHE	2.1
1	A	409	ASN	2.1
1	A	137	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
4	PGE	A	1312	10/10	0.81	0.19	38,41,44,46	0
4	PGE	A	1313	7/10	0.82	0.15	47,49,50,51	0
3	SO4	A	1304	5/5	0.86	0.21	55,55,57,57	0
3	SO4	A	1306	5/5	0.86	0.30	88,88,88,88	0
4	PGE	B	301	6/10	0.90	0.13	37,38,39,41	0
3	SO4	A	1308	5/5	0.91	0.22	82,82,82,82	0
3	SO4	A	1311	5/5	0.92	0.36	54,55,56,56	0
3	SO4	A	1305	5/5	0.93	0.21	66,67,67,68	0
3	SO4	A	1303	5/5	0.93	0.28	64,64,65,65	0
3	SO4	A	1301	5/5	0.93	0.27	80,80,80,80	0
3	SO4	A	1309	5/5	0.94	0.10	54,54,55,55	0
3	SO4	A	1307	5/5	0.97	0.12	44,44,45,45	0
3	SO4	A	1302	5/5	0.97	0.20	46,48,48,48	0
3	SO4	A	1310	5/5	0.98	0.14	44,45,46,46	0

6.5 Other polymers (i)

There are no such residues in this entry.