Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:56 PM GMT

PDB ID	:	4DWR
Title	:	RNA ligase RtcB/Mn2+ complex
Authors	:	Xia, S.; Englert, M.; Soll, D.; Wang, J.
Deposited on	:	2012-02-26
Resolution	:	1.48 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

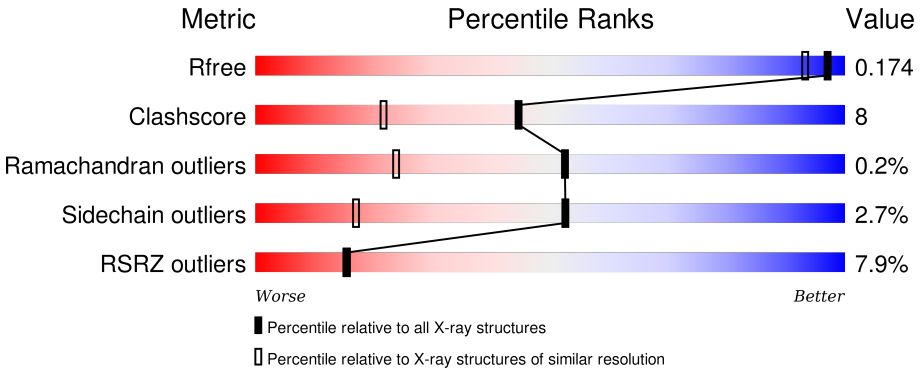
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.48 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	3129 (1.50-1.46)
Clashscore	102246	3380 (1.50-1.46)
Ramachandran outliers	100387	3310 (1.50-1.46)
Sidechain outliers	100360	3308 (1.50-1.46)
RSRZ outliers	91569	3133 (1.50-1.46)

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 <=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	487	9%, 90%, 9%
1	B	487	9%, 84%, 15%
1	C	487	5%, 86%, 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	SUC	C	601	-	-	-	X
4	SO4	A	605	-	-	-	X
4	SO4	A	606	-	-	-	X
4	SO4	B	608	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13603 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.

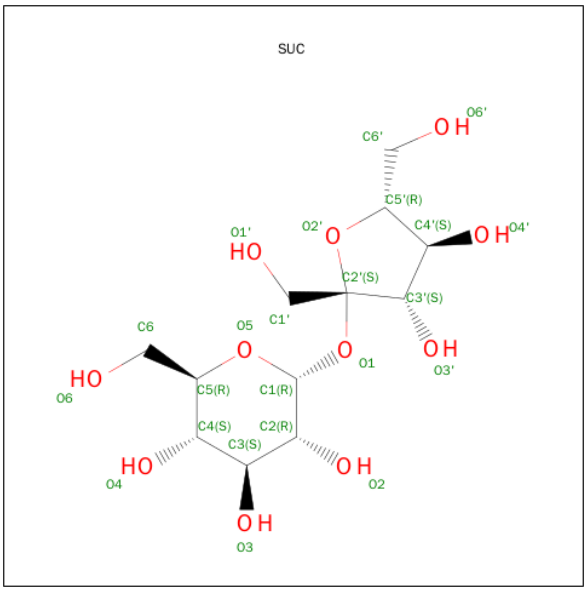
- Molecule 1 is a protein called tRNA-splicing ligase RtcB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	486	Total	C	N	O	S	0	25	0
			3944	2503	724	701	16			
1	A	483	Total	C	N	O	S	0	16	0
			3874	2449	712	697	16			
1	C	481	Total	C	N	O	S	0	32	0
			3951	2517	718	700	16			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	482	ALA	-	EXPRESSION TAG	UNP O59245
B	483	ALA	-	EXPRESSION TAG	UNP O59245
B	484	ALA	-	EXPRESSION TAG	UNP O59245
B	485	LEU	-	EXPRESSION TAG	UNP O59245
B	486	GLU	-	EXPRESSION TAG	UNP O59245
B	487	HIS	-	EXPRESSION TAG	UNP O59245
A	482	ALA	-	EXPRESSION TAG	UNP O59245
A	483	ALA	-	EXPRESSION TAG	UNP O59245
A	484	ALA	-	EXPRESSION TAG	UNP O59245
A	485	LEU	-	EXPRESSION TAG	UNP O59245
A	486	GLU	-	EXPRESSION TAG	UNP O59245
A	487	HIS	-	EXPRESSION TAG	UNP O59245
C	482	ALA	-	EXPRESSION TAG	UNP O59245
C	483	ALA	-	EXPRESSION TAG	UNP O59245
C	484	ALA	-	EXPRESSION TAG	UNP O59245
C	485	LEU	-	EXPRESSION TAG	UNP O59245
C	486	GLU	-	EXPRESSION TAG	UNP O59245
C	487	HIS	-	EXPRESSION TAG	UNP O59245

- Molecule 2 is SUGAR (SUCROSE) (three-letter code: SUC) (formula: $C_{12}H_{22}O_{11}$).

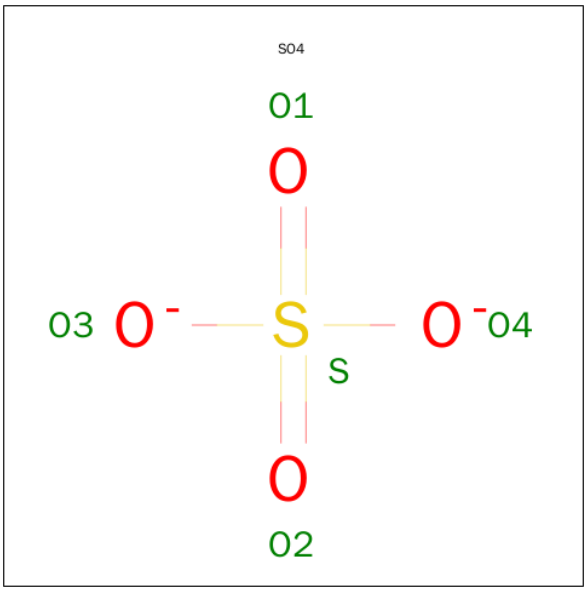


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 23 12 11	0	0
2	A	1	Total C O 23 12 11	0	0
2	C	1	Total C O 23 12 11	0	0

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

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

- Molecule 5 is water.

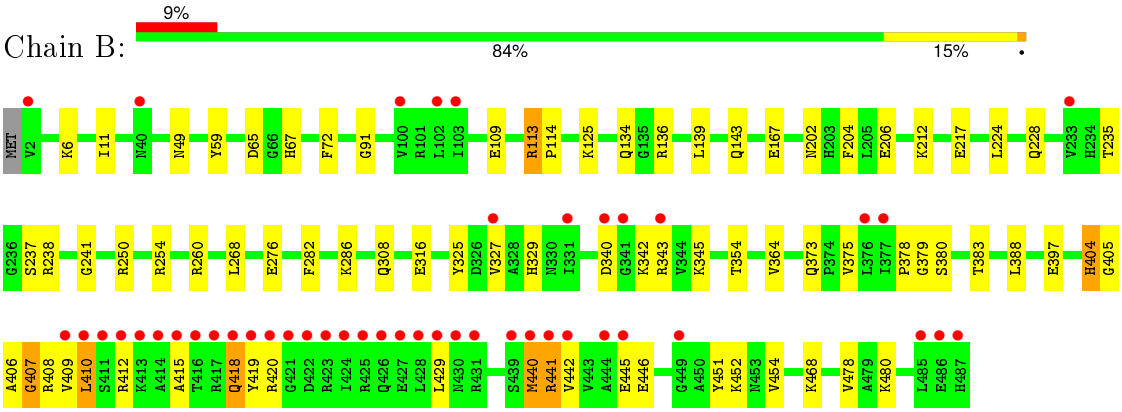
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	574	Total O 574 574	0	0
5	A	550	Total O 550 550	0	0
5	C	530	Total O 530 530	0	0

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 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.

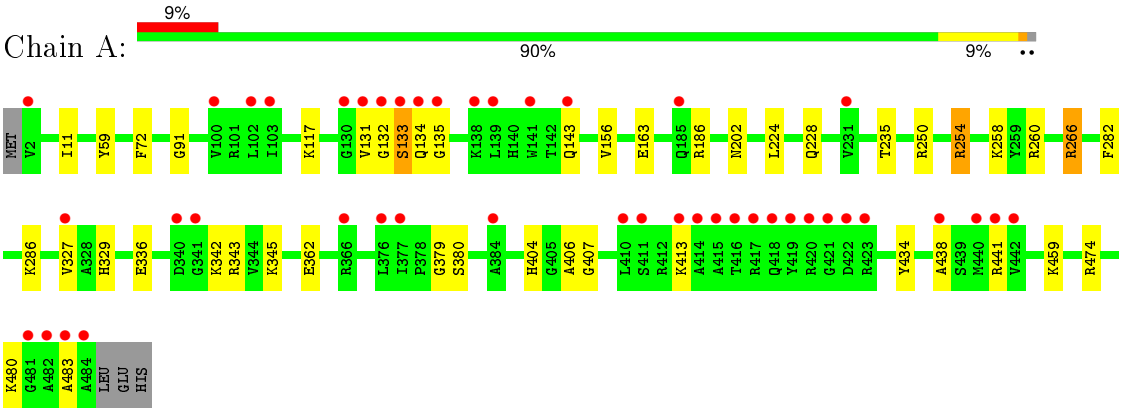
- Molecule 1: tRNA-splicing ligase RtcB

Chain B:



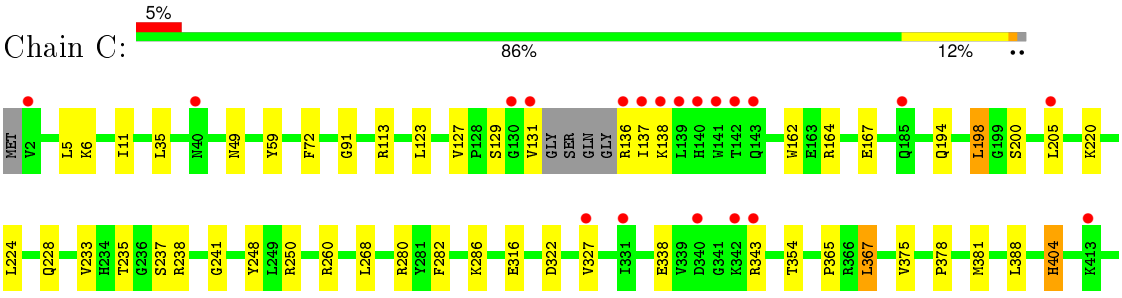
- Molecule 1: tRNA-splicing ligase RtcB

Chain A:



- Molecule 1: tRNA-splicing ligase RtcB

Chain C:




R417
Q418
R423
L429
A437
A438
K459
V478
A479
K480
G481
A484
L485
E486
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	114.08Å 84.90Å 124.20Å 90.00° 115.65° 90.00°	Depositor
Resolution (Å)	46.74 – 1.48 43.22 – 1.48	Depositor EDS
% Data completeness (in resolution range)	87.7 (46.74-1.48) 87.7 (43.22-1.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 1.48Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.142 , 0.178 0.139 , 0.174	Depositor DCC
R_{free} test set	17819 reflections (6.06%)	DCC
Wilson B-factor (Å^2)	22.8	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 51.1	EDS
Estimated twinning fraction	0.010 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 309709 reflections	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	13603	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 3.17% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.52	0/4002	0.62	0/5394
1	B	0.52	0/4095	0.63	0/5517
1	C	0.51	0/4123	0.64	0/5553
All	All	0.51	0/12220	0.63	0/16464

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	3874	0	3946	36	0
1	B	3944	0	4060	83	1
1	C	3951	0	4104	69	0
2	A	23	0	22	1	0
2	B	23	0	22	2	0
2	C	23	0	22	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
4	A	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	40	0	0	1	0
4	C	35	0	0	0	0
5	A	550	0	0	16	0
5	B	574	0	0	45	0
5	C	530	0	0	19	1
All	All	13603	0	12176	190	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 8.

All (190) 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:454:VAL:HG11	5:B:1173:HOH:O	1.37	1.19
1:B:316[A]:GLU:OE1	5:B:1255:HOH:O	1.59	1.18
1:C:113[B]:ARG:HH11	1:C:113[B]:ARG:CG	1.63	1.11
1:B:408[B]:ARG:HD3	1:B:410:LEU:O	1.51	1.10
1:A:254[A]:ARG:HH11	1:A:254[A]:ARG:CG	1.72	1.03
1:C:194[A]:GLN:NE2	1:C:238:ARG:O	1.92	1.02
1:C:113[B]:ARG:HG2	1:C:113[B]:ARG:HH11	0.87	1.02
1:B:412:ARG:NH2	1:B:446:GLU:OE2	1.91	1.01
1:B:406[B]:ALA:O	5:B:949:HOH:O	1.79	1.00
1:A:254[A]:ARG:HH11	1:A:254[A]:ARG:HG2	1.25	0.99
1:A:254[B]:ARG:NH1	5:A:1243:HOH:O	1.91	0.96
1:C:113[B]:ARG:HG2	1:C:113[B]:ARG:NH1	1.64	0.95
1:C:327[B]:VAL:HG11	1:C:354:THR:HG23	1.51	0.93
1:B:342[B]:LYS:HD2	5:B:957:HOH:O	1.68	0.93
1:C:429[A]:LEU:CD2	5:C:1151:HOH:O	2.18	0.92
1:B:418:GLN:HG2	1:B:419:TYR:N	1.84	0.92
1:C:220:LYS:NZ	5:C:1163:HOH:O	2.02	0.91
1:C:162:TRP:CZ2	1:C:316[A]:GLU:HG2	2.06	0.91
1:B:442:VAL:HG21	5:B:1224:HOH:O	1.72	0.89
1:C:429[A]:LEU:HD23	5:C:1151:HOH:O	1.73	0.88
1:C:131:VAL:HG13	1:C:136:ARG:N	1.88	0.88
1:C:438:ALA:H	1:C:480[B]:LYS:HD2	1.38	0.87
1:B:408[B]:ARG:CD	1:B:410:LEU:O	2.28	0.81
1:A:266:ARG:NH1	5:A:1188:HOH:O	2.08	0.81
5:B:1180:HOH:O	1:C:6[A]:LYS:HG2	1.80	0.81
1:B:415:ALA:HB3	5:B:1178:HOH:O	1.79	0.80
1:C:327[B]:VAL:HG11	1:C:354:THR:CG2	2.11	0.80
1:C:437:ALA:HA	1:C:480[B]:LYS:CG	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338[B]:GLU:OE2	1:C:343:ARG:HG2	1.82	0.79
1:B:480:LYS:HE2	5:B:740:HOH:O	1.82	0.78
1:C:327[B]:VAL:CG1	5:C:765:HOH:O	2.31	0.78
1:B:441:ARG:H	1:B:441:ARG:HE	1.31	0.76
1:C:167:GLU:HB2	5:C:1222:HOH:O	1.85	0.76
1:C:131:VAL:CG1	1:C:136:ARG:N	2.49	0.75
1:C:437:ALA:HA	1:C:480[B]:LYS:HG2	1.66	0.75
1:C:343:ARG:HH11	1:C:343:ARG:HG3	1.51	0.75
1:C:480[B]:LYS:HD3	1:C:481:GLY:O	1.88	0.74
1:B:167:GLU:OE2	5:B:1263:HOH:O	2.06	0.73
1:B:418:GLN:HG2	1:B:419:TYR:H	1.52	0.72
1:B:238:ARG:O	5:B:1023:HOH:O	2.07	0.71
1:C:123:LEU:HD22	1:C:205[B]:LEU:HD21	1.74	0.70
1:B:445:GLU:O	5:B:1178:HOH:O	2.10	0.69
1:C:322:ASP:HB2	5:C:1167:HOH:O	1.92	0.69
1:C:429[B]:LEU:HG	5:C:860:HOH:O	1.93	0.68
1:A:132:GLY:HA3	1:A:133:SER:HB3	1.74	0.68
1:B:134:GLN:HE22	1:B:136:ARG:HH11	1.42	0.66
1:B:454:VAL:CG1	5:B:1173:HOH:O	2.12	0.66
1:B:329:HIS:CE1	1:B:404[B]:HIS:CE1	2.84	0.66
1:C:429[A]:LEU:HD21	5:C:1151:HOH:O	1.87	0.65
1:B:397:GLU:OE1	5:B:1146:HOH:O	2.14	0.65
1:C:437:ALA:HA	1:C:480[B]:LYS:HG3	1.79	0.63
1:B:415:ALA:CB	5:B:1178:HOH:O	2.41	0.63
1:B:139:LEU:HD13	5:B:1041:HOH:O	1.97	0.63
1:B:404[B]:HIS:NE2	5:B:970:HOH:O	2.19	0.63
1:A:254[A]:ARG:NH1	1:A:254[A]:ARG:HG2	2.05	0.62
1:C:438:ALA:H	1:C:480[B]:LYS:CD	2.10	0.62
1:B:418:GLN:CG	1:B:419:TYR:N	2.62	0.62
1:A:254[A]:ARG:HG3	1:A:254[A]:ARG:HH11	1.64	0.61
1:C:327[B]:VAL:CG1	1:C:354:THR:HG23	2.29	0.61
1:A:329:HIS:HD2	5:A:1133:HOH:O	1.84	0.61
1:A:474:ARG:HG3	5:A:1163:HOH:O	2.01	0.60
1:A:407:GLY:N	5:A:1155:HOH:O	2.33	0.60
1:A:254[A]:ARG:NH1	1:A:254[A]:ARG:CG	2.43	0.60
1:C:418:GLN:NE2	5:C:1224:HOH:O	2.34	0.59
1:B:406[A]:ALA:CB	5:B:1038:HOH:O	2.49	0.59
1:C:327[B]:VAL:HG13	5:C:765:HOH:O	1.98	0.59
1:C:343:ARG:HG3	1:C:343:ARG:NH1	2.18	0.58
1:B:418:GLN:CG	1:B:419:TYR:H	2.15	0.58
1:B:325:TYR:CD2	1:B:327[B]:VAL:HG22	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113[B]:ARG:NH1	1:C:113[B]:ARG:CG	2.36	0.57
1:B:134:GLN:NE2	1:B:136:ARG:HH11	2.02	0.57
1:B:408[B]:ARG:CG	1:B:410:LEU:O	2.52	0.56
1:C:164:ARG:NH2	1:C:316[B]:GLU:OE2	2.38	0.56
1:C:248:TYR:OH	1:C:280:ARG:HG2	2.05	0.56
1:A:132:GLY:HA3	1:A:133:SER:CB	2.33	0.56
1:B:212[B]:LYS:HD3	5:B:1271:HOH:O	2.06	0.56
1:C:423:ARG:HD2	5:C:928:HOH:O	2.04	0.56
1:C:164:ARG:O	1:C:167:GLU:HG2	2.06	0.55
1:B:125[B]:LYS:HG3	5:B:844:HOH:O	2.07	0.55
4:B:606:SO4:O4	5:B:1252:HOH:O	2.18	0.55
1:C:137:ILE:HG22	5:C:1216:HOH:O	2.06	0.55
1:C:164:ARG:HH22	1:C:316[B]:GLU:CD	2.11	0.54
1:A:132:GLY:CA	1:A:133:SER:CB	2.85	0.54
1:A:254[A]:ARG:HG3	5:A:1227:HOH:O	2.08	0.54
1:A:329:HIS:CD2	5:A:1133:HOH:O	2.57	0.54
1:B:202:ASN:ND2	5:B:1037:HOH:O	2.41	0.53
1:B:109:GLU:OE2	1:B:113[A]:ARG:NH1	2.41	0.53
1:B:345:LYS:HE2	5:B:1220:HOH:O	2.07	0.53
1:B:308[B]:GLN:OE1	5:B:992:HOH:O	2.19	0.53
2:B:601:SUC:H4	5:B:1218:HOH:O	2.08	0.53
1:A:250[B]:ARG:HE	1:A:254[B]:ARG:HH12	1.55	0.52
1:C:198:LEU:HD21	1:C:205[A]:LEU:HG	1.90	0.52
1:C:123:LEU:HB3	1:C:205[B]:LEU:HD23	1.91	0.52
1:C:438:ALA:CB	1:C:480[B]:LYS:HD2	2.40	0.51
1:B:325:TYR:CD2	1:B:327[A]:VAL:HG13	2.44	0.51
1:A:379:GLY:N	5:A:1138:HOH:O	2.39	0.51
1:C:485:LEU:HD23	1:C:485:LEU:H	1.76	0.51
1:B:345:LYS:CE	5:B:1220:HOH:O	2.59	0.51
1:B:125[A]:LYS:HE3	2:A:601:SUC:H62	1.92	0.51
1:C:49:ASN:HB3	1:C:268:LEU:HD22	1.93	0.51
1:C:282:PHE:CE1	1:C:286:LYS:HE3	2.47	0.50
1:A:362:GLU:OE2	5:A:1050:HOH:O	2.18	0.50
1:C:429[B]:LEU:HD12	5:C:1104:HOH:O	2.11	0.49
1:B:378:PRO:HG3	1:B:404[B]:HIS:HE1	1.77	0.49
1:B:383:THR:HB	5:B:1173:HOH:O	2.12	0.49
1:C:200[B]:SER:HB3	5:C:1114:HOH:O	2.11	0.49
1:C:327[B]:VAL:HG12	5:C:765:HOH:O	2.06	0.49
1:A:117[A]:LYS:HG3	1:A:434:TYR:CZ	2.47	0.49
1:C:235:THR:HG23	5:C:713:HOH:O	2.12	0.49
1:B:237:SER:OG	1:B:241:GLY:HA3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:PHE:HE2	5:B:1037:HOH:O	1.96	0.48
1:C:381:MET:HG3	1:C:478:VAL:HG11	1.95	0.48
1:A:327:VAL:HG23	5:A:1133:HOH:O	2.13	0.48
1:B:406[B]:ALA:HA	5:B:1161:HOH:O	2.14	0.48
1:B:379:GLY:N	5:B:1011:HOH:O	2.40	0.48
1:C:129[B]:SER:CB	1:C:480[B]:LYS:HE2	2.43	0.48
1:B:134:GLN:HE21	1:B:136:ARG:HD2	1.79	0.47
1:C:437:ALA:CA	1:C:480[B]:LYS:HG2	2.40	0.47
1:B:383:THR:HG21	5:B:1231:HOH:O	2.13	0.47
1:B:412:ARG:NE	5:B:1269:HOH:O	2.26	0.47
1:C:113[B]:ARG:HH11	1:C:113[B]:ARG:CB	2.25	0.47
1:B:440:MET:H	1:B:441:ARG:HH21	1.61	0.47
1:A:202:ASN:HD21	1:A:380:SER:HA	1.80	0.47
1:C:480[B]:LYS:HB2	1:C:480[B]:LYS:HE3	1.66	0.47
1:A:254[A]:ARG:HG3	1:A:254[A]:ARG:NH1	2.23	0.46
1:C:316[A]:GLU:HG3	5:C:1116:HOH:O	2.16	0.46
1:C:129[B]:SER:HB2	1:C:480[B]:LYS:HE2	1.97	0.46
1:C:220:LYS:NZ	5:C:849:HOH:O	2.48	0.46
1:A:156:VAL:HG11	1:A:163:GLU:HA	1.97	0.46
1:B:224:LEU:HA	1:B:228:GLN:OE1	2.16	0.46
1:C:378:PRO:HD2	1:C:404:HIS:O	2.14	0.46
1:B:206:GLU:HG2	1:B:478:VAL:HG22	1.97	0.46
1:B:327[B]:VAL:HG11	1:B:354:THR:CG2	2.46	0.46
1:C:5:LEU:HD13	1:C:35:LEU:HD21	1.96	0.46
1:B:340:ASP:OD1	2:B:601:SUC:O4'	2.31	0.46
1:C:365:PRO:HB2	1:C:367[A]:LEU:HD23	1.98	0.46
1:C:127:VAL:HG21	1:C:205[A]:LEU:HD11	1.98	0.45
1:C:438:ALA:N	1:C:480[B]:LYS:HD2	2.18	0.45
1:A:235:THR:HG23	5:A:736:HOH:O	2.16	0.45
1:B:250:ARG:HE	1:B:254:ARG:HH11	1.64	0.45
1:A:474:ARG:HD3	5:A:1085:HOH:O	2.16	0.45
1:B:378:PRO:HG3	1:B:404[B]:HIS:CE1	2.52	0.45
1:C:459[A]:LYS:HB3	1:C:459[A]:LYS:HE3	1.76	0.45
1:B:383:THR:CB	5:B:1173:HOH:O	2.65	0.45
1:B:325:TYR:CE2	1:B:327[B]:VAL:HG22	2.51	0.45
1:B:143:GLN:NE2	5:B:1188:HOH:O	2.49	0.45
1:A:258:LYS:NZ	5:A:1141:HOH:O	2.50	0.45
1:B:235:THR:HG23	5:B:783:HOH:O	2.16	0.45
1:B:325:TYR:HD2	1:B:327[A]:VAL:HG13	1.81	0.44
1:B:308[B]:GLN:NE2	1:A:342:LYS:HB2	2.33	0.44
1:B:451:TYR:HB2	5:B:1231:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:SER:OG	1:C:241:GLY:HA3	2.18	0.44
1:C:375:VAL:HB	1:C:388[A]:LEU:HB2	1.99	0.44
1:B:202:ASN:HD21	1:B:380:SER:HA	1.83	0.43
1:A:438:ALA:HB1	1:A:483:ALA:HB2	2.00	0.43
1:B:49:ASN:HB3	1:B:268:LEU:HD22	2.00	0.43
1:B:441:ARG:H	1:B:441:ARG:NE	2.08	0.43
1:B:217[B]:GLU:OE1	5:B:1153:HOH:O	2.21	0.43
1:A:282:PHE:CE1	1:A:286:LYS:HE3	2.54	0.43
1:C:224:LEU:HA	1:C:228:GLN:OE1	2.19	0.43
1:B:364:VAL:HG22	1:B:373:GLN:HB2	2.01	0.43
1:A:72:PHE:CG	1:A:91:GLY:HA2	2.54	0.42
1:C:113[B]:ARG:HA	1:C:113[B]:ARG:HD3	1.80	0.42
1:C:205[A]:LEU:CD2	1:C:233:VAL:HG22	2.48	0.42
1:B:412:ARG:HG3	5:B:1196:HOH:O	2.19	0.42
1:B:480:LYS:NZ	5:B:1264:HOH:O	2.50	0.42
1:A:406:ALA:HB2	5:A:1138:HOH:O	2.18	0.42
1:A:336[A]:GLU:OE1	1:A:343:ARG:HB3	2.20	0.42
1:C:72:PHE:CG	1:C:91:GLY:HA2	2.53	0.42
1:A:131:VAL:HG13	1:A:135:GLY:HA3	2.00	0.42
1:B:67:HIS:NE2	1:B:407:GLY:HA2	2.35	0.42
1:B:67:HIS:HE1	5:B:1132:HOH:O	2.02	0.42
1:A:224:LEU:HA	1:A:228:GLN:OE1	2.19	0.42
1:A:345[A]:LYS:NZ	5:A:1210:HOH:O	2.36	0.42
1:B:276:GLU:HG2	5:B:1192:HOH:O	2.19	0.42
1:B:468[B]:LYS:NZ	5:B:882:HOH:O	2.51	0.42
1:B:342[B]:LYS:HE2	5:B:1151:HOH:O	2.19	0.42
1:B:406[A]:ALA:HB2	5:B:1011:HOH:O	2.20	0.41
1:B:113[B]:ARG:HB3	1:B:114:PRO:HD3	2.02	0.41
1:B:418:GLN:HE21	1:B:418:GLN:HB3	1.63	0.41
1:B:375:VAL:HB	1:B:388[A]:LEU:HB2	2.02	0.41
1:B:72:PHE:CG	1:B:91:GLY:HA2	2.55	0.41
1:B:113[A]:ARG:HD2	1:B:113[A]:ARG:HA	1.89	0.41
1:B:282:PHE:CE1	1:B:286:LYS:HE3	2.56	0.41
1:B:452:LYS:CE	5:B:1182:HOH:O	2.69	0.41
1:B:379:GLY:HA2	5:B:1161:HOH:O	2.20	0.41
1:B:65:ASP:OD2	1:B:405:GLY:N	2.49	0.40
1:A:459:LYS:HD3	5:A:1205:HOH:O	2.19	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:B:6[B]:LYS:NZ	5:C:1167:HOH:O[2_747]	1.67	0.53

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	498/487 (102%)	487 (98%)	10 (2%)	1 (0%)	52 24
1	B	509/487 (104%)	491 (96%)	16 (3%)	2 (0%)	39 14
1	C	509/487 (104%)	497 (98%)	12 (2%)	0	100 100
All	All	1516/1461 (104%)	1475 (97%)	38 (2%)	3 (0%)	52 24

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	407	GLY
1	A	133	SER
1	B	420	ARG

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	406/393 (103%)	391 (96%)	15 (4%)	41 9
1	B	416/393 (106%)	401 (96%)	15 (4%)	42 10
1	C	421/393 (107%)	411 (98%)	10 (2%)	57 21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1243/1179 (105%)	1203 (97%)	40 (3%)	52 12

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	11	ILE
1	B	59	TYR
1	B	113[A]	ARG
1	B	113[B]	ARG
1	B	260	ARG
1	B	343[A]	ARG
1	B	343[B]	ARG
1	B	404[A]	HIS
1	B	404[B]	HIS
1	B	409	VAL
1	B	410	LEU
1	B	418	GLN
1	B	429	LEU
1	B	440	MET
1	B	441	ARG
1	A	11	ILE
1	A	59	TYR
1	A	134	GLN
1	A	143[A]	GLN
1	A	143[B]	GLN
1	A	186	ARG
1	A	254[A]	ARG
1	A	254[B]	ARG
1	A	260	ARG
1	A	266	ARG
1	A	404	HIS
1	A	413	LYS
1	A	441[A]	ARG
1	A	441[B]	ARG
1	A	480	LYS
1	C	11	ILE
1	C	59	TYR
1	C	138	LYS
1	C	198	LEU
1	C	250[A]	ARG
1	C	250[B]	ARG
1	C	367[A]	LEU

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Mol	Chain	Res	Type
1	C	367[B]	LEU
1	C	404	HIS
1	C	485	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	134	GLN
1	B	202	ASN
1	B	418	GLN
1	A	40	ASN
1	A	134	GLN
1	A	202	ASN
1	A	274	GLN
1	A	329	HIS
1	A	418	GLN
1	C	40	ASN
1	C	185	GLN
1	C	418	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 30 ligands modelled in this entry, 6 are monoatomic - leaving 24 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	SUC	A	601	-	24,24,24	0.46	0	36,36,36	0.93	3 (8%)
4	SO4	A	604	-	4,4,4	0.32	0	6,6,6	0.37	0
4	SO4	A	605	-	4,4,4	0.08	0	6,6,6	0.30	0
4	SO4	A	606	-	4,4,4	0.41	0	6,6,6	0.59	0
4	SO4	A	607	-	4,4,4	0.18	0	6,6,6	0.15	0
4	SO4	A	608	3	4,4,4	0.13	0	6,6,6	0.16	0
4	SO4	A	609	-	4,4,4	0.12	0	6,6,6	0.13	0
2	SUC	B	601	-	24,24,24	0.43	0	36,36,36	0.61	0
4	SO4	B	604	-	4,4,4	0.41	0	6,6,6	0.23	0
4	SO4	B	605	-	4,4,4	0.22	0	6,6,6	0.22	0
4	SO4	B	606	-	4,4,4	0.55	0	6,6,6	0.53	0
4	SO4	B	607	3	4,4,4	0.28	0	6,6,6	0.28	0
4	SO4	B	608	-	4,4,4	0.16	0	6,6,6	0.15	0
4	SO4	B	609	-	4,4,4	0.20	0	6,6,6	0.18	0
4	SO4	B	610	-	4,4,4	0.08	0	6,6,6	0.07	0
4	SO4	B	611	-	4,4,4	0.13	0	6,6,6	0.15	0
2	SUC	C	601	-	24,24,24	0.43	0	36,36,36	0.65	0
4	SO4	C	604	-	4,4,4	0.45	0	6,6,6	0.48	0
4	SO4	C	605	-	4,4,4	0.35	0	6,6,6	0.19	0
4	SO4	C	606	-	4,4,4	0.21	0	6,6,6	0.25	0
4	SO4	C	607	-	4,4,4	0.17	0	6,6,6	0.07	0
4	SO4	C	608	3	4,4,4	0.10	0	6,6,6	0.14	0
4	SO4	C	609	-	4,4,4	0.12	0	6,6,6	0.17	0
4	SO4	C	610	-	4,4,4	0.15	0	6,6,6	0.13	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	SUC	A	601	-	-	0/12/51/51	0/2/2/2
4	SO4	A	604	-	-	0/0/0/0	0/0/0/0
4	SO4	A	605	-	-	0/0/0/0	0/0/0/0
4	SO4	A	606	-	-	0/0/0/0	0/0/0/0
4	SO4	A	607	-	-	0/0/0/0	0/0/0/0
4	SO4	A	608	3	-	0/0/0/0	0/0/0/0
4	SO4	A	609	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SUC	B	601	-	-	0/12/51/51	0/2/2/2
4	SO4	B	604	-	-	0/0/0/0	0/0/0/0
4	SO4	B	605	-	-	0/0/0/0	0/0/0/0
4	SO4	B	606	-	-	0/0/0/0	0/0/0/0
4	SO4	B	607	3	-	0/0/0/0	0/0/0/0
4	SO4	B	608	-	-	0/0/0/0	0/0/0/0
4	SO4	B	609	-	-	0/0/0/0	0/0/0/0
4	SO4	B	610	-	-	0/0/0/0	0/0/0/0
4	SO4	B	611	-	-	0/0/0/0	0/0/0/0
2	SUC	C	601	-	-	0/12/51/51	0/2/2/2
4	SO4	C	604	-	-	0/0/0/0	0/0/0/0
4	SO4	C	605	-	-	0/0/0/0	0/0/0/0
4	SO4	C	606	-	-	0/0/0/0	0/0/0/0
4	SO4	C	607	-	-	0/0/0/0	0/0/0/0
4	SO4	C	608	3	-	0/0/0/0	0/0/0/0
4	SO4	C	609	-	-	0/0/0/0	0/0/0/0
4	SO4	C	610	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	SUC	C1-O5-C5	2.01	117.65	113.75
2	A	601	SUC	O5-C5-C4	2.03	113.50	109.68
2	A	601	SUC	C3-C4-C5	2.49	114.54	110.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	SUC	1	0
2	B	601	SUC	2	0
4	B	606	SO4	1	0

5.7 Other polymers (i)

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	483/487 (99%)	0.25	44 (9%)	11 11	16, 24, 48, 68	0
1	B	486/487 (99%)	0.27	46 (9%)	10 10	16, 22, 54, 82	0
1	C	481/487 (98%)	-0.04	25 (5%)	31 32	16, 24, 41, 66	0
All	All	1450/1461 (99%)	0.16	115 (7%)	15 15	16, 23, 47, 82	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	133	SER	10.6
1	A	484	ALA	10.4
1	A	132	GLY	9.7
1	B	419	TYR	9.5
1	A	134	GLN	9.3
1	B	416	THR	9.2
1	A	483	ALA	8.7
1	B	423	ARG	8.3
1	A	131	VAL	8.3
1	B	487	HIS	8.1
1	C	141	TRP	8.0
1	C	131	VAL	7.7
1	B	424	ILE	7.6
1	B	421	GLY	7.5
1	A	135	GLY	7.5
1	C	137	ILE	7.3
1	B	415	ALA	7.1
1	B	417	ARG	7.0
1	B	420	ARG	6.8
1	B	422	ASP	6.5
1	B	409	VAL	6.4
1	A	420	ARG	6.3
1	A	417	ARG	6.3

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Mol	Chain	Res	Type	RSRZ
1	C	139	LEU	5.8
1	B	410	LEU	5.8
1	C	138	LYS	5.7
1	B	486	GLU	5.7
1	B	430	ASN	5.6
1	B	414	ALA	5.6
1	B	2	VAL	5.6
1	B	429	LEU	5.5
1	C	143[A]	GLN	5.2
1	B	442	VAL	4.9
1	C	485	LEU	4.8
1	A	481	GLY	4.6
1	B	426	GLN	4.6
1	C	136	ARG	4.5
1	A	419	TYR	4.5
1	B	428	LEU	4.5
1	B	413	LYS	4.5
1	B	440	MET	4.4
1	B	441	ARG	4.4
1	B	418	GLN	4.4
1	A	442	VAL	4.2
1	A	482	ALA	4.1
1	A	422[A]	ASP	4.1
1	B	444	ALA	4.1
1	A	416	THR	3.9
1	C	480[A]	LYS	3.9
1	A	438	ALA	3.9
1	A	141	TRP	3.8
1	B	427	GLU	3.8
1	A	421	GLY	3.8
1	C	140	HIS	3.7
1	B	411	SER	3.6
1	B	327[A]	VAL	3.6
1	C	142	THR	3.6
1	B	425	ARG	3.6
1	C	2	VAL	3.5
1	A	130	GLY	3.5
1	A	410	LEU	3.5
1	C	205[A]	LEU	3.4
1	A	423[A]	ARG	3.4
1	A	441[A]	ARG	3.4
1	B	412	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	440	MET	3.3
1	A	340[A]	ASP	3.3
1	B	376	LEU	3.1
1	A	413	LYS	3.1
1	A	414	ALA	3.1
1	B	449	GLY	3.1
1	A	102	LEU	3.1
1	A	2	VAL	3.0
1	B	431	ARG	3.0
1	A	376	LEU	3.0
1	A	418	GLN	3.0
1	B	343[A]	ARG	2.9
1	C	343	ARG	2.9
1	A	377	ILE	2.9
1	A	100	VAL	2.8
1	A	231	VAL	2.7
1	C	484	ALA	2.7
1	B	40[A]	ASN	2.7
1	B	341	GLY	2.7
1	B	102	LEU	2.7
1	C	185	GLN	2.7
1	C	130	GLY	2.6
1	B	485	LEU	2.6
1	B	100	VAL	2.5
1	C	331	ILE	2.5
1	A	366	ARG	2.5
1	A	138	LYS	2.4
1	B	377	ILE	2.4
1	A	341	GLY	2.4
1	B	103	ILE	2.4
1	C	40	ASN	2.3
1	A	327	VAL	2.2
1	B	445	GLU	2.2
1	C	327[A]	VAL	2.2
1	A	139	LEU	2.2
1	C	429[A]	LEU	2.2
1	A	185	GLN	2.2
1	B	340	ASP	2.2
1	C	342	LYS	2.2
1	B	233	VAL	2.2
1	B	331	ILE	2.2
1	A	103	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	439	SER	2.1
1	C	413	LYS	2.1
1	C	417	ARG	2.1
1	C	340	ASP	2.1
1	A	411	SER	2.1
1	A	415	ALA	2.0
1	A	143[A]	GLN	2.0
1	A	384	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, 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	LLDF	B-factors(Å^2)	Q<0.9
4	SO4	A	605	5/5	0.96	0.17	5.26	44,44,47,48	0
4	SO4	B	608	5/5	0.96	0.29	4.50	61,62,64,67	0
4	SO4	A	606	5/5	0.90	0.16	2.66	17,28,36,38	5
2	SUC	C	601	23/23	0.91	0.20	2.52	28,34,44,52	0
2	SUC	B	601	23/23	0.91	0.17	1.96	27,33,39,54	0
4	SO4	B	605	5/5	0.97	0.11	1.93	30,37,41,44	5
2	SUC	A	601	23/23	0.83	0.25	1.35	27,40,49,57	0
4	SO4	B	606	5/5	0.93	0.12	1.09	16,27,32,35	5
4	SO4	C	608	5/5	0.95	0.11	0.48	34,41,46,46	5
4	SO4	C	607	5/5	0.96	0.19	0.28	74,74,76,77	0
4	SO4	C	606	5/5	0.94	0.11	0.21	34,41,45,46	5
4	SO4	B	607	5/5	0.95	0.10	-0.49	45,48,49,51	5
4	SO4	C	604	5/5	0.99	0.05	-1.00	24,26,32,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	SO4	B	604	5/5	1.00	0.04	-1.32	22,23,24,24	0
4	SO4	A	604	5/5	0.99	0.04	-1.43	26,27,31,31	0
4	SO4	C	605	5/5	0.98	0.07	-1.66	29,31,33,34	5
3	MN	A	603	1/1	1.00	0.04	-2.06	28,28,28,28	0
3	MN	B	603	1/1	1.00	0.05	-2.07	30,30,30,30	0
3	MN	C	602	1/1	1.00	0.05	-2.41	26,26,26,26	0
3	MN	B	602	1/1	1.00	0.02	-3.77	28,28,28,28	0
4	SO4	B	611	5/5	0.91	0.34	-	61,61,65,66	0
4	SO4	A	609	5/5	0.96	0.36	-	52,54,57,57	0
4	SO4	B	610	5/5	0.87	0.31	-	65,65,67,70	0
3	MN	C	603	1/1	1.00	0.03	-	28,28,28,28	0
4	SO4	C	609	5/5	0.98	0.34	-	74,75,79,80	0
4	SO4	A	608	5/5	0.92	0.14	-	33,40,43,45	5
4	SO4	A	607	5/5	0.97	0.20	-	66,70,72,73	0
4	SO4	C	610	5/5	0.97	0.21	-	67,67,70,71	0
4	SO4	B	609	5/5	0.97	0.18	-	57,61,61,63	0
3	MN	A	602	1/1	1.00	0.03	-	28,28,28,28	0

6.5 Other polymers

There are no such residues in this entry.