Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 05:56 PM BST

PDB ID	:	6QH8
Title	:	Structure of knotted YibK from P. aeruginosa
Authors	:	Mikula, K.M.; Tascon, I.; Iwai, H.
Deposited on	:	2019-01-16
Resolution	:	2.20 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:

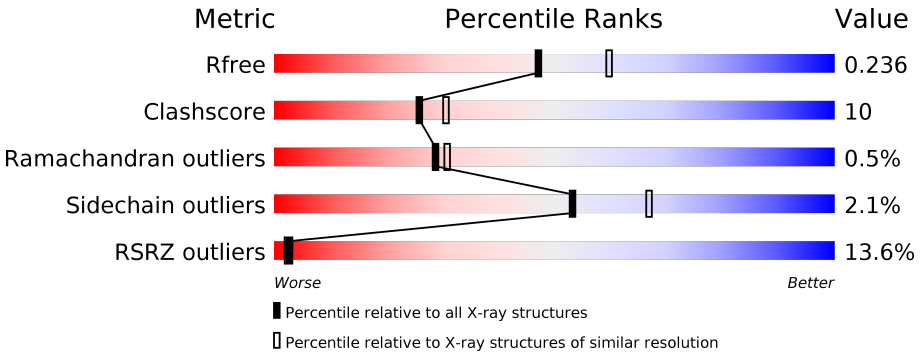
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	162	9% 83% 15%
1	B	162	12% 82% 10% 6%
1	C	162	14% 80% 15%
1	D	162	19% 77% 17%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	202	-	-	X	-
2	SO4	C	201	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10108 atoms, of which 4907 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 (cytidine(34)-2'-O)-methyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	162	Total	C	H	N	O	S	0	0	0
			2537	808	1259	235	228	7			
1	B	153	Total	C	H	N	O	S	0	0	0
			2382	760	1181	218	216	7			
1	C	157	Total	C	H	N	O	S	0	0	0
			2467	787	1225	227	221	7			
1	D	155	Total	C	H	N	O	S	0	0	0
			2427	767	1212	226	215	7			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP A0A071LCY6
A	2	GLY	-	expression tag	UNP A0A071LCY6
A	3	GLY	-	expression tag	UNP A0A071LCY6
A	4	GLY	-	expression tag	UNP A0A071LCY6
A	5	SER	-	expression tag	UNP A0A071LCY6
A	67	TYR	ASP	engineered mutation	UNP A0A071LCY6
A	158	GLY	-	expression tag	UNP A0A071LCY6
A	159	LEU	-	expression tag	UNP A0A071LCY6
A	160	PRO	-	expression tag	UNP A0A071LCY6
A	161	GLU	-	expression tag	UNP A0A071LCY6
A	162	THR	-	expression tag	UNP A0A071LCY6
B	1	GLY	-	expression tag	UNP A0A071LCY6
B	2	GLY	-	expression tag	UNP A0A071LCY6
B	3	GLY	-	expression tag	UNP A0A071LCY6
B	4	GLY	-	expression tag	UNP A0A071LCY6
B	5	SER	-	expression tag	UNP A0A071LCY6
B	67	TYR	ASP	engineered mutation	UNP A0A071LCY6
B	158	GLY	-	expression tag	UNP A0A071LCY6
B	159	LEU	-	expression tag	UNP A0A071LCY6
B	160	PRO	-	expression tag	UNP A0A071LCY6
B	161	GLU	-	expression tag	UNP A0A071LCY6

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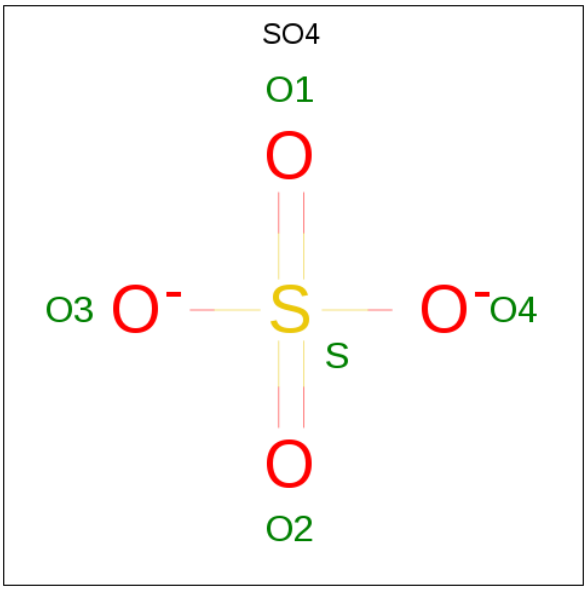
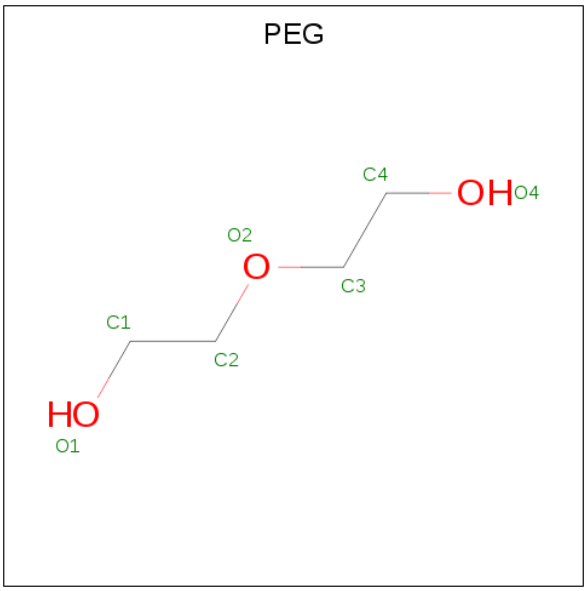
Chain	Residue	Modelled	Actual	Comment	Reference
B	162	THR	-	expression tag	UNP A0A071LCY6
C	1	GLY	-	expression tag	UNP A0A071LCY6
C	2	GLY	-	expression tag	UNP A0A071LCY6
C	3	GLY	-	expression tag	UNP A0A071LCY6
C	4	GLY	-	expression tag	UNP A0A071LCY6
C	5	SER	-	expression tag	UNP A0A071LCY6
C	67	TYR	ASP	engineered mutation	UNP A0A071LCY6
C	158	GLY	-	expression tag	UNP A0A071LCY6
C	159	LEU	-	expression tag	UNP A0A071LCY6
C	160	PRO	-	expression tag	UNP A0A071LCY6
C	161	GLU	-	expression tag	UNP A0A071LCY6
C	162	THR	-	expression tag	UNP A0A071LCY6
D	1	GLY	-	expression tag	UNP A0A071LCY6
D	2	GLY	-	expression tag	UNP A0A071LCY6
D	3	GLY	-	expression tag	UNP A0A071LCY6
D	4	GLY	-	expression tag	UNP A0A071LCY6
D	5	SER	-	expression tag	UNP A0A071LCY6
D	67	TYR	ASP	engineered mutation	UNP A0A071LCY6
D	158	GLY	-	expression tag	UNP A0A071LCY6
D	159	LEU	-	expression tag	UNP A0A071LCY6
D	160	PRO	-	expression tag	UNP A0A071LCY6
D	161	GLU	-	expression tag	UNP A0A071LCY6
D	162	THR	-	expression tag	UNP A0A071LCY6

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C H O 17 4 10 3	0	0
3	B	1	Total C H O 17 4 10 3	0	0
3	D	1	Total C H O 17 4 10 3	0	0

- Molecule 4 is water.

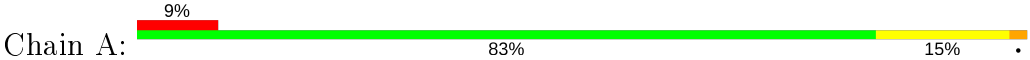
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	44	Total O 44 44	0	0
4	B	43	Total O 43 43	0	0
4	C	46	Total O 46 46	0	0
4	D	31	Total O 31 31	0	0

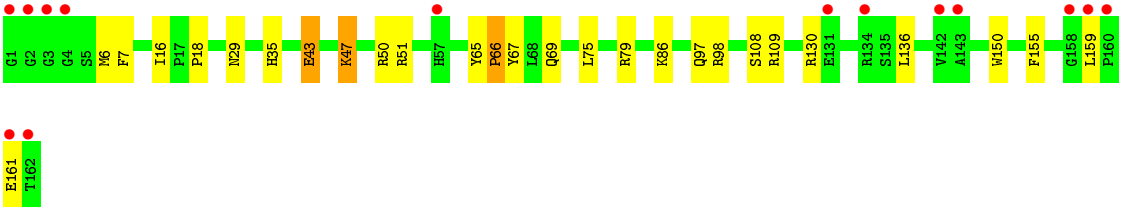
3 Residue-property plots (i)

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: tRNA (cytidine(34)-2'-O)-methyltransferase

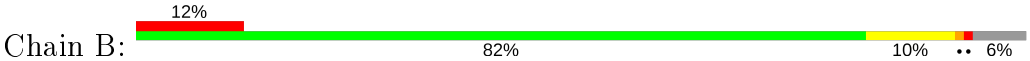
Chain A:

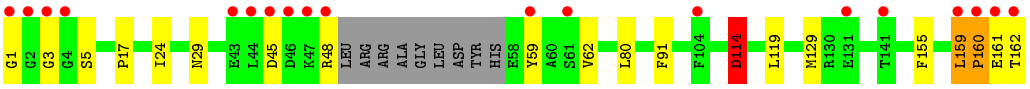




- Molecule 1: tRNA (cytidine(34)-2'-O)-methyltransferase

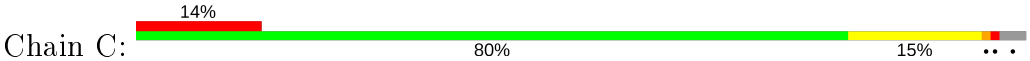
Chain B:

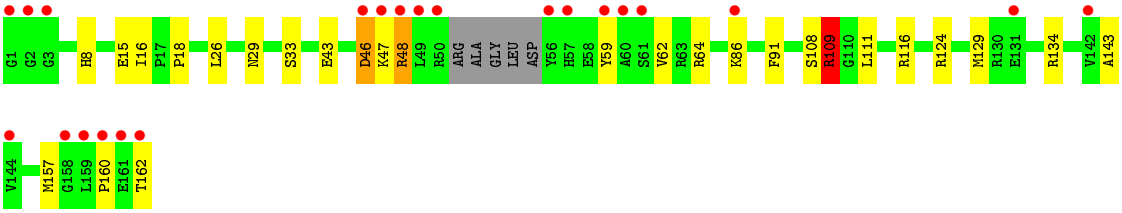




- Molecule 1: tRNA (cytidine(34)-2'-O)-methyltransferase

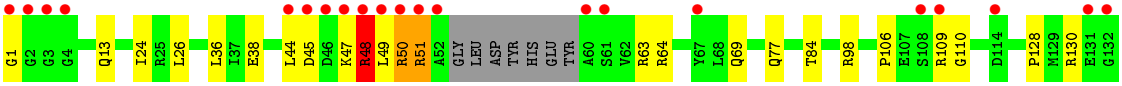
Chain C:

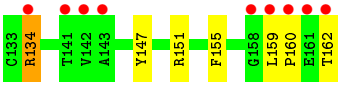




- Molecule 1: tRNA (cytidine(34)-2'-O)-methyltransferase

Chain D:




C133
R134
T141
V142
A143
Y147
R151
F155
G158
L159
P160
E161
T162

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	48.93Å 85.73Å 167.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.17 – 2.20 29.80 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (28.17-2.20) 99.6 (29.80-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.185 , 0.236 0.185 , 0.236	Depositor DCC
R_{free} test set	1858 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	38.4	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 44.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10108	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.44 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3589e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: PEG, 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	0.87	3/1309 (0.2%)	0.85	4/1771 (0.2%)
1	B	0.77	2/1229 (0.2%)	1.01	6/1662 (0.4%)
1	C	0.66	1/1272 (0.1%)	0.90	4/1720 (0.2%)
1	D	0.71	2/1242 (0.2%)	1.08	2/1678 (0.1%)
All	All	0.76	8/5052 (0.2%)	0.96	16/6831 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	C	0	1
All	All	0	3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	PRO	CB-CG	-19.43	0.52	1.50
1	B	114	ASP	CB-CG	-8.70	1.33	1.51
1	D	63	ARG	CZ-NH1	7.42	1.42	1.33
1	D	63	ARG	CD-NE	-7.13	1.34	1.46
1	A	66	PRO	N-CD	-6.37	1.39	1.47
1	A	43	GLU	CB-CG	-5.90	1.41	1.52
1	B	159	LEU	CG-CD2	5.40	1.71	1.51
1	C	109	ARG	CG-CD	5.20	1.65	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	63	ARG	NE-CZ-NH2	-22.79	108.91	120.30
1	D	63	ARG	NE-CZ-NH1	20.97	130.78	120.30
1	B	114	ASP	CB-CG-OD1	-16.65	103.31	118.30
1	A	47	LYS	CD-CE-NZ	-13.08	81.61	111.70
1	C	109	ARG	NE-CZ-NH1	10.29	125.45	120.30
1	C	109	ARG	NE-CZ-NH2	-10.01	115.30	120.30
1	A	66	PRO	CA-N-CD	-9.71	97.91	111.50
1	A	66	PRO	CB-CG-CD	7.90	137.31	106.50
1	B	159	LEU	CB-CG-CD1	6.84	122.63	111.00
1	A	66	PRO	N-CD-CG	-6.19	93.92	103.20
1	B	45	ASP	CB-CG-OD2	-5.97	112.93	118.30
1	B	159	LEU	CB-CG-CD2	5.69	120.67	111.00
1	C	111	LEU	CB-CG-CD2	-5.52	101.61	111.00
1	C	111	LEU	CA-CB-CG	5.31	127.52	115.30
1	B	62	VAL	CG1-CB-CG2	5.29	119.36	110.90
1	B	159	LEU	CB-CA-C	5.11	119.91	110.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	114	ASP	Sidechain,Mainchain
1	C	46	ASP	Peptide

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	1278	1259	1263	29	4
1	B	1201	1181	1186	16	2
1	C	1242	1225	1226	29	0
1	D	1215	1212	1213	35	2
2	A	35	0	0	2	0
2	B	15	0	0	0	0
2	C	15	0	0	2	0
2	D	15	0	0	1	0
3	B	14	20	20	0	0
3	D	7	10	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	44	0	0	3	0
4	B	43	0	0	2	0
4	C	46	0	0	4	0
4	D	31	0	0	3	0
All	All	5201	4907	4918	104	4

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 10.

All (104) 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:51:ARG:NH1	2:A:202:SO4:O1	1.95	0.99
1:D:159:LEU:HD23	1:D:159:LEU:O	1.63	0.97
1:B:1:GLY:N	1:B:162:THR:OG1	2.02	0.90
1:D:84:THR:OG1	2:D:202:SO4:O4	1.93	0.85
1:D:130:ARG:NH1	4:D:301:HOH:O	2.10	0.79
1:A:69:GLN:NE2	4:A:301:HOH:O	2.14	0.79
1:C:109:ARG:NH1	4:C:301:HOH:O	2.17	0.78
1:D:48:ARG:HB3	1:D:51:ARG:HB3	1.67	0.77
1:A:35:HIS:CE1	1:A:65:TYR:HH	2.03	0.76
1:C:129:MET:HE3	1:C:134:ARG:O	1.87	0.75
1:D:48:ARG:HB3	1:D:51:ARG:CB	2.17	0.74
1:A:86:LYS:NZ	4:A:302:HOH:O	2.15	0.73
1:A:35:HIS:CD2	4:A:303:HOH:O	2.43	0.72
1:B:80:LEU:HD23	1:B:119:LEU:HD21	1.73	0.71
1:D:47:LYS:O	1:D:49:LEU:N	2.25	0.69
1:B:159:LEU:HD23	1:B:160:PRO:HD3	1.76	0.66
1:A:136:LEU:HD11	1:C:26:LEU:HD12	1.76	0.66
1:D:38:GLU:O	4:D:302:HOH:O	2.13	0.66
1:C:26:LEU:HD21	1:C:143:ALA:HA	1.78	0.65
1:A:35:HIS:ND1	1:A:65:TYR:OH	2.31	0.63
1:D:38:GLU:OE2	1:D:64:ARG:NE	2.26	0.63
1:A:130:ARG:HA	1:C:157:MET:CE	2.30	0.61
2:C:201:SO4:S	4:C:302:HOH:O	2.56	0.61
1:C:108:SER:O	1:C:109:ARG:HG3	2.01	0.61
1:A:35:HIS:NE2	1:A:75:LEU:HD21	2.16	0.60
1:B:159:LEU:CD2	1:B:160:PRO:HD3	2.30	0.60
1:A:130:ARG:HA	1:C:157:MET:HE2	1.85	0.59
1:D:128:PRO:HG3	4:D:306:HOH:O	2.03	0.59
1:D:44:LEU:HD23	1:D:47:LYS:HD2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:PRO:HB2	1:C:162:THR:HG23	1.86	0.57
1:D:48:ARG:CB	1:D:51:ARG:HB3	2.35	0.56
1:B:29:ASN:HB3	4:B:307:HOH:O	2.05	0.56
1:C:108:SER:C	1:C:109:ARG:HG3	2.25	0.55
1:D:48:ARG:HB3	1:D:51:ARG:HB2	1.88	0.55
1:B:159:LEU:CG	1:B:160:PRO:HD3	2.36	0.55
1:B:1:GLY:H1	1:B:162:THR:CB	2.16	0.55
1:D:36:LEU:HD12	1:D:36:LEU:N	2.22	0.55
1:D:24:ILE:HD11	1:D:45:ASP:OD2	2.07	0.54
1:C:48:ARG:O	1:C:48:ARG:HG2	2.07	0.54
1:D:151:ARG:HB2	1:D:155:PHE:CZ	2.43	0.54
1:B:129:MET:HE1	4:B:337:HOH:O	2.08	0.53
1:C:116:ARG:HG2	1:C:124:ARG:HD3	1.91	0.52
1:C:16:ILE:HG22	1:C:18:PRO:HD2	1.92	0.52
1:B:155:PHE:CD1	1:D:128:PRO:HG2	2.45	0.51
1:B:159:LEU:HG	1:B:160:PRO:HD3	1.92	0.51
1:A:35:HIS:HB3	1:A:65:TYR:CE2	2.44	0.51
1:A:98:ARG:NH1	1:A:161:GLU:OE2	2.43	0.51
1:D:159:LEU:HD23	1:D:159:LEU:C	2.30	0.49
1:A:79:ARG:NH2	1:A:97:GLN:HG2	2.28	0.49
1:A:66:PRO:HG2	1:A:67:TYR:CD2	2.48	0.49
1:C:47:LYS:O	1:C:48:ARG:C	2.50	0.49
1:D:50:ARG:O	1:D:50:ARG:CG	2.61	0.49
1:B:3:GLY:O	1:B:161:GLU:HA	2.12	0.48
1:C:108:SER:HB3	4:C:304:HOH:O	2.13	0.48
1:D:1:GLY:O	1:D:162:THR:C	2.52	0.48
1:D:47:LYS:C	1:D:49:LEU:N	2.67	0.48
1:C:46:ASP:O	1:C:48:ARG:N	2.47	0.48
1:D:159:LEU:N	1:D:160:PRO:HD2	2.28	0.48
1:B:159:LEU:N	1:B:160:PRO:CD	2.77	0.48
1:D:47:LYS:C	1:D:49:LEU:H	2.17	0.47
1:A:159:LEU:HB2	1:A:161:GLU:OE1	2.14	0.47
1:A:35:HIS:CE1	1:A:65:TYR:OH	2.66	0.47
1:B:1:GLY:CA	1:B:162:THR:OG1	2.62	0.47
1:B:24:ILE:HG21	1:B:59:TYR:CE1	2.50	0.47
1:C:86:LYS:HD3	1:C:116:ARG:CZ	2.45	0.47
1:C:108:SER:OG	1:C:109:ARG:HD2	2.15	0.47
1:C:59:TYR:O	1:C:62:VAL:HG23	2.15	0.47
1:D:130:ARG:HB2	1:D:130:ARG:HH21	1.80	0.46
1:A:66:PRO:HB2	1:A:67:TYR:CD2	2.49	0.46
2:C:201:SO4:O2	4:C:302:HOH:O	2.21	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ARG:HG2	1:C:29:ASN:O	2.16	0.46
1:B:17:PRO:HB2	1:B:48:ARG:HB3	1.97	0.45
1:A:47:LYS:HD2	1:A:50:ARG:HH21	1.80	0.45
1:C:15:GLU:OE2	1:C:109:ARG:CD	2.65	0.45
1:A:51:ARG:NH1	2:A:202:SO4:S	2.89	0.45
1:D:106:PRO:HD2	1:D:110:GLY:O	2.17	0.44
1:C:8:HIS:ND1	1:C:33:SER:OG	2.45	0.44
1:C:108:SER:OG	1:C:109:ARG:CD	2.65	0.44
1:D:106:PRO:HD2	1:D:110:GLY:C	2.38	0.44
1:C:43:GLU:OE1	1:C:64:ARG:NH1	2.46	0.44
1:A:130:ARG:HA	1:C:157:MET:HE1	1.99	0.44
1:D:130:ARG:HB2	1:D:130:ARG:NH2	2.33	0.44
1:A:35:HIS:HB3	1:A:65:TYR:HE2	1.82	0.43
1:B:24:ILE:HG21	1:B:59:TYR:CD1	2.54	0.43
1:A:130:ARG:NH1	1:C:157:MET:O	2.51	0.43
1:A:6:MET:HG2	1:A:7:PHE:CE2	2.54	0.43
1:D:26:LEU:HD11	1:D:147:TYR:CE1	2.54	0.43
1:A:108:SER:OG	1:A:109:ARG:HG2	2.19	0.42
1:C:16:ILE:CG2	1:C:18:PRO:HD2	2.49	0.42
1:D:49:LEU:O	1:D:50:ARG:HB3	2.18	0.42
1:A:16:ILE:HG22	1:A:18:PRO:HD2	2.01	0.42
1:C:86:LYS:HD3	1:C:116:ARG:NH2	2.35	0.42
1:D:134:ARG:HD3	1:D:134:ARG:HA	1.94	0.42
1:A:150:TRP:CD1	1:A:155:PHE:HA	2.55	0.42
1:D:13:GLN:O	1:D:106:PRO:HB3	2.20	0.41
1:D:69:GLN:HE21	1:D:77:GLN:HE22	1.68	0.41
1:D:24:ILE:CD1	1:D:45:ASP:OD2	2.69	0.41
1:D:51:ARG:HB3	1:D:51:ARG:HE	1.71	0.41
1:A:98:ARG:HD2	1:A:161:GLU:OE2	2.21	0.41
1:C:108:SER:C	1:C:109:ARG:CG	2.89	0.41
1:D:49:LEU:H	1:D:49:LEU:HD23	1.85	0.41
1:C:8:HIS:HD1	1:C:33:SER:HG	1.59	0.40
1:A:6:MET:HG2	1:A:7:PHE:CD2	2.56	0.40
1:D:69:GLN:NE2	1:D:77:GLN:HE22	2.19	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:GLU:OE2	1:D:48:ARG:H[1_655]	1.43	0.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:GLU:OE2	1:D:48:ARG:N[1_655]	2.11	0.09
1:A:47:LYS:HZ1	1:B:114:ASP:CG[3_654]	1.58	0.02
1:A:47:LYS:NZ	1:B:114:ASP:CG[3_654]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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	160/162 (99%)	156 (98%)	4 (2%)	0	100 100
1	B	149/162 (92%)	142 (95%)	6 (4%)	1 (1%)	22 22
1	C	153/162 (94%)	141 (92%)	12 (8%)	0	100 100
1	D	151/162 (93%)	140 (93%)	9 (6%)	2 (1%)	12 9
All	All	613/648 (95%)	579 (94%)	31 (5%)	3 (0%)	29 31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	48	ARG
1	D	50	ARG
1	B	160	PRO

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	133/133 (100%)	132 (99%)	1 (1%)	81 90
1	B	126/133 (95%)	124 (98%)	2 (2%)	62 76
1	C	130/133 (98%)	127 (98%)	3 (2%)	50 63
1	D	127/133 (96%)	122 (96%)	5 (4%)	32 41
All	All	516/532 (97%)	505 (98%)	11 (2%)	53 67

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	B	5	SER
1	B	91	PHE
1	C	48	ARG
1	C	91	PHE
1	C	109	ARG
1	D	48	ARG
1	D	51	ARG
1	D	98	ARG
1	D	109	ARG
1	D	134	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	8	HIS
1	D	69	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 monosaccharides 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	$\#\|Z\| > 2$
3	PEG	B	205	-	6,6,6	0.48	0	5,5,5	0.20	0
2	SO4	D	201	-	4,4,4	0.26	0	6,6,6	0.52	0
2	SO4	B	202	-	4,4,4	0.26	0	6,6,6	0.47	0
3	PEG	D	204	-	6,6,6	0.51	0	5,5,5	0.45	0
2	SO4	A	207	-	4,4,4	0.14	0	6,6,6	0.20	0
2	SO4	B	203	-	4,4,4	0.20	0	6,6,6	0.46	0
2	SO4	D	203	-	4,4,4	0.30	0	6,6,6	0.37	0
2	SO4	A	203	-	4,4,4	0.19	0	6,6,6	0.42	0
2	SO4	A	204	-	4,4,4	0.18	0	6,6,6	0.25	0
2	SO4	C	203	-	4,4,4	0.26	0	6,6,6	0.84	0
2	SO4	C	202	-	4,4,4	0.27	0	6,6,6	0.34	0
2	SO4	A	206	-	4,4,4	0.16	0	6,6,6	0.30	0
3	PEG	B	204	-	6,6,6	0.55	0	5,5,5	0.49	0
2	SO4	A	202	-	4,4,4	0.22	0	6,6,6	0.18	0
2	SO4	A	205	-	4,4,4	0.29	0	6,6,6	0.68	0
2	SO4	C	201	-	4,4,4	0.23	0	6,6,6	1.42	1 (16%)
2	SO4	A	201	-	4,4,4	0.27	0	6,6,6	0.50	0
2	SO4	B	201	-	4,4,4	0.25	0	6,6,6	0.97	0
2	SO4	D	202	-	4,4,4	0.19	0	6,6,6	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
3	PEG	B	205	-	-	3/4/4/4	-
3	PEG	B	204	-	-	1/4/4/4	-
3	PEG	D	204	-	-	1/4/4/4	-

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	C	201	SO4	O4-S-O3	2.46	119.55	109.06

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	204	PEG	O2-C3-C4-O4
3	B	204	PEG	O2-C3-C4-O4
3	B	205	PEG	O2-C3-C4-O4
3	B	205	PEG	O1-C1-C2-O2
3	B	205	PEG	C4-C3-O2-C2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	202	SO4	2	0
2	C	201	SO4	2	0
2	D	202	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, 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	162/162 (100%)	0.52	14 (8%)	10	9	27, 44, 95, 139	0
1	B	153/162 (94%)	0.60	19 (12%)	4	3	24, 37, 108, 147	0
1	C	157/162 (96%)	0.69	22 (14%)	2	2	26, 38, 113, 140	0
1	D	155/162 (95%)	1.03	30 (19%)	1	1	26, 48, 126, 144	0
All	All	627/648 (96%)	0.71	85 (13%)	3	2	24, 41, 119, 147	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	162	THR	15.0
1	D	2	GLY	13.4
1	D	45	ASP	13.0
1	B	3	GLY	12.4
1	D	3	GLY	12.0
1	B	2	GLY	11.9
1	C	162	THR	11.4
1	C	2	GLY	11.1
1	A	1	GLY	11.0
1	C	56	TYR	10.8
1	D	159	LEU	10.4
1	A	3	GLY	10.1
1	C	159	LEU	9.3
1	D	44	LEU	9.2
1	B	1	GLY	9.0
1	B	160	PRO	9.0
1	B	159	LEU	8.7
1	A	2	GLY	8.4
1	D	162	THR	8.3
1	C	3	GLY	8.3
1	C	49	LEU	7.9

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Mol	Chain	Res	Type	RSRZ
1	C	48	ARG	7.8
1	D	160	PRO	7.3
1	D	1	GLY	7.3
1	A	160	PRO	7.3
1	C	1	GLY	7.0
1	C	60	ALA	6.9
1	B	48	ARG	6.6
1	B	59	TYR	6.6
1	A	4	GLY	6.6
1	B	161	GLU	6.4
1	A	159	LEU	6.3
1	A	161	GLU	6.1
1	A	162	THR	6.0
1	D	46	ASP	6.0
1	D	49	LEU	5.5
1	C	57	HIS	5.3
1	B	46	ASP	5.3
1	C	50	ARG	5.1
1	C	160	PRO	5.0
1	B	45	ASP	4.8
1	D	60	ALA	4.6
1	C	59	TYR	4.6
1	D	131	GLU	4.5
1	D	47	LYS	4.4
1	C	158	GLY	4.2
1	D	134	ARG	4.1
1	D	67	TYR	4.1
1	D	132	GLY	4.1
1	B	44	LEU	3.8
1	C	47	LYS	3.7
1	D	50	ARG	3.7
1	A	57	HIS	3.7
1	D	161	GLU	3.7
1	A	158	GLY	3.7
1	D	48	ARG	3.6
1	D	51	ARG	3.6
1	C	161	GLU	3.3
1	D	109	ARG	3.2
1	B	47	LYS	3.2
1	D	61	SER	3.1
1	A	131	GLU	3.0
1	C	61	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	158	GLY	2.8
1	B	131	GLU	2.8
1	B	61	SER	2.8
1	D	108	SER	2.8
1	D	4	GLY	2.7
1	C	46	ASP	2.5
1	C	86	LYS	2.5
1	B	4	GLY	2.4
1	A	142	VAL	2.4
1	D	141	THR	2.4
1	D	142	VAL	2.4
1	C	131	GLU	2.3
1	D	114	ASP	2.3
1	D	143	ALA	2.3
1	A	134	ARG	2.2
1	A	143	ALA	2.2
1	D	52	ALA	2.2
1	B	43	GLU	2.2
1	C	142	VAL	2.1
1	B	104	PHE	2.1
1	B	141	THR	2.1
1	C	144	VAL	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 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
2	SO4	A	207	5/5	0.79	0.31	137,140,143,143	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	A	206	5/5	0.80	0.31	84,86,101,108	0
2	SO4	D	203	5/5	0.82	0.17	68,72,80,90	0
3	PEG	B	204	7/7	0.85	0.37	56,69,80,86	0
3	PEG	B	205	7/7	0.89	0.26	59,71,87,87	0
3	PEG	D	204	7/7	0.91	0.23	45,59,70,85	0
2	SO4	A	205	5/5	0.92	0.12	47,51,64,72	0
2	SO4	A	201	5/5	0.92	0.14	73,77,78,101	0
2	SO4	C	202	5/5	0.93	0.12	74,77,85,93	0
2	SO4	D	202	5/5	0.93	0.13	69,73,79,82	0
2	SO4	A	204	5/5	0.95	0.09	77,79,86,86	0
2	SO4	B	203	5/5	0.96	0.09	56,60,67,80	0
2	SO4	C	201	5/5	0.96	0.12	39,41,42,50	0
2	SO4	D	201	5/5	0.98	0.12	47,47,50,65	0
2	SO4	B	201	5/5	0.98	0.10	39,45,52,65	0
2	SO4	A	202	5/5	0.98	0.10	62,67,67,70	0
2	SO4	A	203	5/5	0.99	0.07	47,49,51,63	0
2	SO4	B	202	5/5	0.99	0.10	39,39,46,49	0
2	SO4	C	203	5/5	0.99	0.10	46,46,49,59	0

6.5 Other polymers (i)

There are no such residues in this entry.