Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 01:58 PM EDT

PDB ID	:	6P82
Title	:	Structure of P. aeruginosa ATCC27853 CdnD, Apo form 1
Authors	:	Ye, Q.; Corbett, K.D.
Deposited on	:	2019-06-06
Resolution	:	2.05 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 (i) 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 (1)) were used in the production of this report:

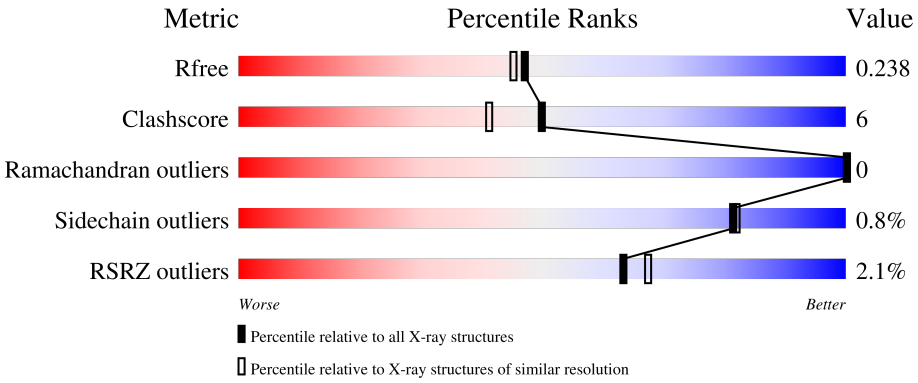
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	302	4% 85% 14%
1	B	302	2% 88% 12%
1	C	302	% 85% 14%
1	D	302	2% 90% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	401	-	-	X	-
2	SO4	B	404	-	-	X	-
2	SO4	C	401	-	-	X	-
2	SO4	D	402	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10437 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.

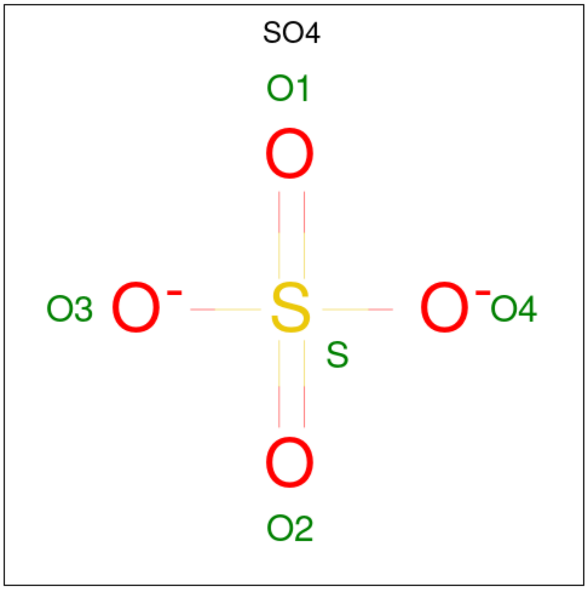
- Molecule 1 is a protein called Nucleotidyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	Se	0	0	0
			2403	1520	431	448	1	3			
1	B	302	Total	C	N	O	S	Se	0	0	0
			2417	1527	434	452	1	3			
1	C	302	Total	C	N	O	S	Se	0	0	0
			2417	1527	434	452	1	3			
1	D	301	Total	C	N	O	S	Se	0	0	0
			2411	1524	433	450	1	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP A0A080VY32
A	0	ASN	-	expression tag	UNP A0A080VY32
A	1	ALA	-	expression tag	UNP A0A080VY32
B	-1	SER	-	expression tag	UNP A0A080VY32
B	0	ASN	-	expression tag	UNP A0A080VY32
B	1	ALA	-	expression tag	UNP A0A080VY32
C	-1	SER	-	expression tag	UNP A0A080VY32
C	0	ASN	-	expression tag	UNP A0A080VY32
C	1	ALA	-	expression tag	UNP A0A080VY32
D	-1	SER	-	expression tag	UNP A0A080VY32
D	0	ASN	-	expression tag	UNP A0A080VY32
D	1	ALA	-	expression tag	UNP A0A080VY32

- 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	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	B	1	Total O S 5 4 1	0	0

Continued on next page...

Continued from previous page...

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

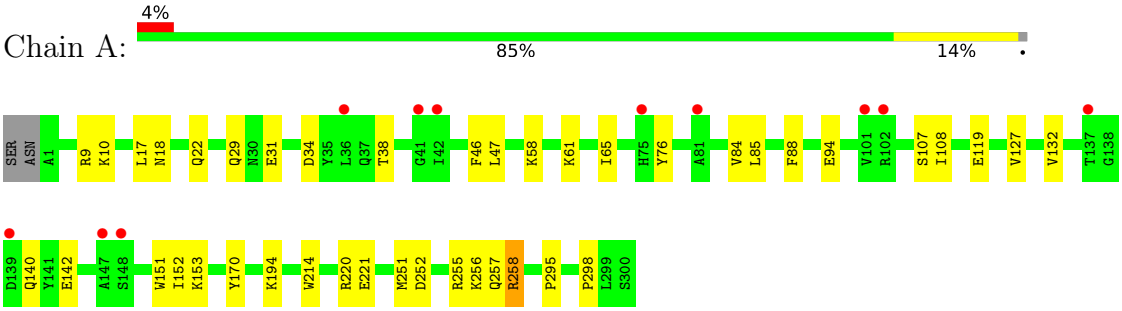
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	151	Total O 151 151	0	0
3	B	144	Total O 144 144	0	0
3	C	137	Total O 137 137	0	0
3	D	187	Total O 187 187	0	0

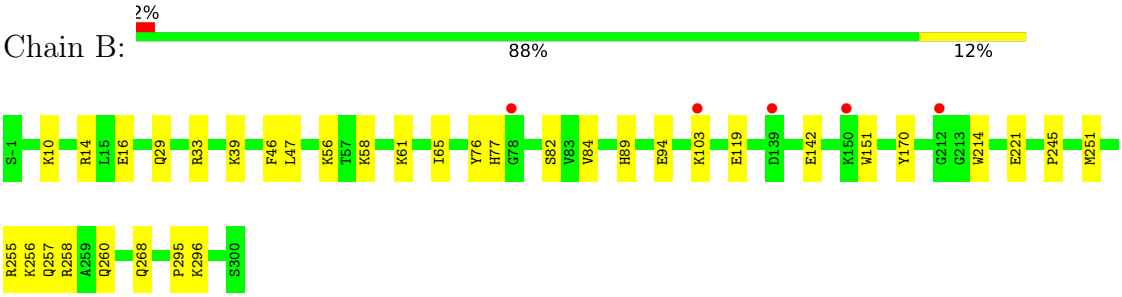
3 Residue-property plots (i)

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.

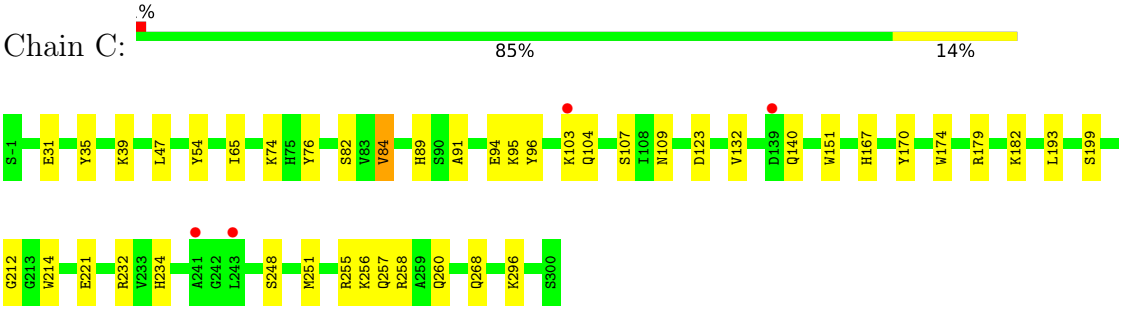
• Molecule 1: Nucleotidyltransferase



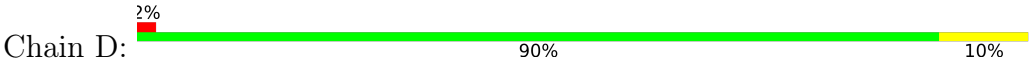
• Molecule 1: Nucleotidyltransferase

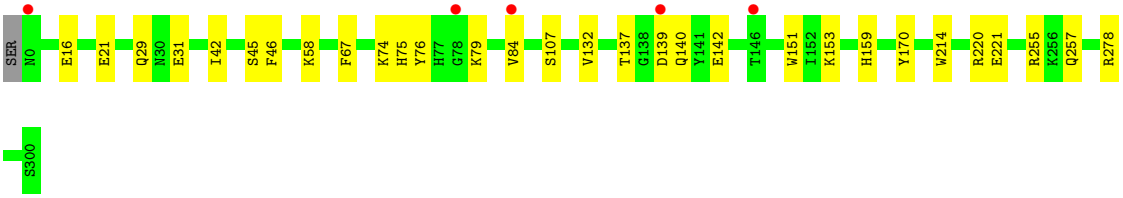


• Molecule 1: Nucleotidyltransferase



• Molecule 1: Nucleotidyltransferase




SER
N0
E16
E21
Q29
N30
E31
I42
S45
F46
K58
F67
K74
H75
Y76
H77
G78
K79
V84
S107
V132
T137
G138
D139
Q140
Y141
E142
T146
W151
I152
K153
H159
Y170
W214
R220
E221
R255
K256
Q257
R278
S300

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.59Å 117.39Å 147.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.92 – 2.05 104.59 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.1 (91.92-2.05) 98.9 (104.59-2.05)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 2.05Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.213 , 0.243 0.208 , 0.238	Depositor DCC
R_{free} test set	5707 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	40.4	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 44.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10437	wwPDB-VP
Average B, all atoms (Å^2)	45.0	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 69.11 % 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 3.9072e-06. 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: 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	0.39	0/2458	0.54	2/3315 (0.1%)
1	B	0.37	0/2472	0.51	0/3334
1	C	0.37	0/2472	0.50	0/3334
1	D	0.40	0/2466	0.55	0/3326
All	All	0.38	0/9868	0.53	2/13309 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	258	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	17	LEU	CA-CB-CG	5.09	127.00	115.30

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	2403	0	2344	30	0
1	B	2417	0	2355	23	0
1	C	2417	0	2355	32	0
1	D	2411	0	2350	22	0
2	A	50	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	40	0	0	4	0
2	C	40	0	0	4	0
2	D	40	0	0	4	0
3	A	151	0	0	7	1
3	B	144	0	0	5	3
3	C	137	0	0	15	1
3	D	187	0	0	8	5
All	All	10437	0	9404	111	5

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 6.

All (111) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:257:GLN:NE2	3:C:502:HOH:O	1.92	0.97
1:C:82:SER:OG	3:C:501:HOH:O	1.90	0.90
1:C:255:ARG:NH2	2:C:401:SO4:O2	2.08	0.86
1:A:220:ARG:NH1	3:A:503:HOH:O	2.09	0.86
1:A:31:GLU:OE1	3:A:501:HOH:O	1.98	0.81
1:C:212:GLY:O	3:C:504:HOH:O	1.96	0.81
1:D:257:GLN:NE2	3:D:503:HOH:O	2.17	0.76
1:A:58:LYS:O	3:A:502:HOH:O	2.04	0.75
1:B:245:PRO:O	3:B:501:HOH:O	2.05	0.72
1:D:84:VAL:HG21	1:D:151:TRP:HZ2	1.54	0.71
1:A:84:VAL:HG21	1:A:151:TRP:HZ2	1.54	0.71
2:C:407:SO4:O4	3:C:505:HOH:O	2.06	0.70
1:B:84:VAL:HG21	1:B:151:TRP:HZ2	1.57	0.70
1:A:84:VAL:HG21	1:A:151:TRP:CZ2	2.27	0.69
1:D:84:VAL:HG21	1:D:151:TRP:CZ2	2.27	0.69
1:D:31:GLU:OE1	3:D:501:HOH:O	2.11	0.69
1:D:220:ARG:HD2	3:D:502:HOH:O	1.95	0.65
2:C:408:SO4:O3	3:C:506:HOH:O	2.12	0.65
1:B:84:VAL:HG21	1:B:151:TRP:CZ2	2.32	0.64
1:B:16:GLU:O	1:B:58:LYS:NZ	2.30	0.64
1:A:94:GLU:OE1	3:A:504:HOH:O	2.14	0.64
2:C:401:SO4:O1	3:C:507:HOH:O	2.14	0.62
1:C:89:HIS:ND1	1:C:103:LYS:HG3	2.15	0.61
1:C:35:TYR:OH	1:C:91:ALA:O	2.11	0.60
1:C:214:TRP:CZ3	1:C:221:GLU:HG3	2.36	0.60
1:A:61:LYS:HE2	1:A:127:VAL:HG11	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:LYS:NZ	1:B:94:GLU:OE2	2.35	0.59
1:C:179:ARG:NH2	3:C:503:HOH:O	1.96	0.58
1:C:84:VAL:HG21	1:C:151:TRP:CZ2	2.38	0.58
1:B:56:LYS:HE3	1:B:61:LYS:O	2.03	0.58
1:A:47:LEU:HD23	1:A:65:ILE:HG12	1.85	0.57
1:B:214:TRP:CZ3	1:B:221:GLU:HG3	2.40	0.57
1:B:255:ARG:NH2	2:B:401:SO4:O4	2.37	0.57
1:C:84:VAL:HG21	1:C:151:TRP:HZ2	1.71	0.56
1:B:47:LEU:HD23	1:B:65:ILE:HG12	1.88	0.56
1:C:182:LYS:HE3	1:C:199:SER:OG	2.06	0.56
1:A:76:TYR:CD1	1:A:84:VAL:HG22	2.40	0.56
1:B:296:LYS:NZ	3:B:512:HOH:O	2.37	0.55
1:A:107:SER:HB3	1:A:132:VAL:HG22	1.88	0.55
1:A:9:ARG:NH2	3:A:510:HOH:O	2.39	0.55
1:D:255:ARG:NH2	2:D:402:SO4:O1	2.33	0.54
2:D:401:SO4:O1	3:D:504:HOH:O	2.18	0.54
1:A:214:TRP:CZ3	1:A:221:GLU:HG3	2.43	0.54
2:D:405:SO4:O3	3:D:505:HOH:O	2.18	0.53
1:C:232:ARG:NH1	3:C:508:HOH:O	2.21	0.53
1:D:29:GLN:NE2	1:D:45:SER:OG	2.40	0.53
1:D:214:TRP:CZ3	1:D:221:GLU:HG3	2.44	0.53
1:C:47:LEU:HD23	1:C:65:ILE:HG12	1.90	0.52
1:C:107:SER:HB3	1:C:132:VAL:HG22	1.90	0.52
1:B:260:GLN:NE2	1:C:268:GLN:HE21	2.08	0.51
1:C:193:LEU:O	1:C:258:ARG:NH2	2.36	0.51
2:A:409:SO4:O4	3:A:505:HOH:O	2.19	0.51
2:B:401:SO4:O3	3:B:502:HOH:O	2.19	0.51
1:C:248:SER:HB2	3:C:546:HOH:O	2.11	0.50
1:C:248:SER:O	1:C:256:LYS:NZ	2.44	0.50
1:A:140:GLN:NE2	1:A:153:LYS:HD3	2.26	0.50
1:D:21:GLU:OE1	1:D:58:LYS:HE3	2.12	0.50
1:D:220:ARG:HH22	1:D:278:ARG:NE	2.10	0.50
1:A:295:PRO:HG3	3:C:628:HOH:O	2.12	0.49
1:A:257:GLN:HE22	1:B:258:ARG:HH11	1.59	0.49
1:B:29:GLN:HE22	1:B:46:PHE:HA	1.78	0.49
1:D:76:TYR:CD1	1:D:84:VAL:HG22	2.48	0.48
1:C:39:LYS:NZ	1:C:94:GLU:OE2	2.46	0.48
1:A:140:GLN:HE22	1:A:153:LYS:HD3	1.79	0.47
1:D:16:GLU:O	1:D:58:LYS:NZ	2.43	0.47
1:B:33:ARG:NH1	3:B:516:HOH:O	2.46	0.46
1:B:119:GLU:HG3	1:B:295:PRO:HB2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:HIS:HA	1:C:174:TRP:HB3	1.97	0.46
1:B:10:LYS:HE2	2:B:404:SO4:O3	2.15	0.46
1:B:76:TYR:CD1	1:B:84:VAL:HG22	2.50	0.46
1:A:29:GLN:HE22	1:A:46:PHE:HA	1.81	0.46
1:A:255:ARG:HD3	3:B:575:HOH:O	2.16	0.46
1:B:268:GLN:HE21	1:C:260:GLN:NE2	2.13	0.45
1:D:75:HIS:HD2	1:D:79:LYS:NZ	2.14	0.45
1:C:182:LYS:NZ	3:C:519:HOH:O	2.50	0.45
1:C:54:TYR:O	1:C:179:ARG:NH1	2.46	0.45
1:C:104:GLN:NE2	1:C:109:ASN:HB2	2.32	0.45
1:C:296:LYS:NZ	3:C:516:HOH:O	2.46	0.45
1:A:10:LYS:HB3	1:A:298:PRO:HG3	1.99	0.45
1:D:139:ASP:O	3:D:507:HOH:O	2.20	0.45
1:D:140:GLN:NE2	1:D:153:LYS:HD3	2.32	0.45
1:D:42:ILE:HD13	1:D:67:PHE:HB3	1.98	0.44
1:C:31:GLU:OE1	3:C:509:HOH:O	2.21	0.44
1:A:194:LYS:O	1:A:258:ARG:NH2	2.50	0.44
1:D:29:GLN:HE22	1:D:46:PHE:HA	1.82	0.44
1:A:61:LYS:HG2	1:A:127:VAL:HB	2.00	0.44
1:B:89:HIS:ND1	1:B:103:LYS:HG3	2.33	0.44
1:D:74:LYS:HD3	1:D:74:LYS:HA	1.64	0.44
1:C:234:HIS:HB2	3:C:523:HOH:O	2.18	0.43
1:C:257:GLN:NE2	3:C:520:HOH:O	2.50	0.43
2:D:402:SO4:O2	3:D:506:HOH:O	2.19	0.43
1:D:220:ARG:HH22	1:D:278:ARG:CZ	2.32	0.43
1:C:251:MSE:O	1:C:256:LYS:HD2	2.18	0.43
1:A:252:ASP:OD2	3:A:506:HOH:O	2.22	0.42
1:D:137:THR:HG21	1:D:142:GLU:HG3	2.00	0.42
1:A:18:ASN:O	1:A:22:GLN:HG3	2.19	0.42
1:A:85:LEU:O	1:A:108:ILE:HD11	2.20	0.42
1:A:258:ARG:HD2	1:B:257:GLN:OE1	2.19	0.42
1:D:107:SER:HB3	1:D:132:VAL:HG22	2.01	0.42
1:B:251:MSE:HE3	1:B:256:LYS:HG2	2.02	0.41
1:D:159:HIS:HD2	3:D:676:HOH:O	2.02	0.41
1:A:34:ASP:O	1:A:38:THR:HG23	2.20	0.41
1:A:88:PHE:HB3	1:A:108:ILE:HD13	2.02	0.41
1:B:14:ARG:NH2	2:B:404:SO4:O3	2.49	0.41
1:A:142:GLU:HA	1:A:152:ILE:O	2.20	0.41
1:A:251:MSE:O	1:A:256:LYS:NZ	2.53	0.41
1:C:74:LYS:O	1:C:74:LYS:HG3	2.21	0.41
1:C:95:LYS:HG2	1:C:96:TYR:CE2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:HIS:NE2	1:B:142:GLU:OE2	2.37	0.41
1:C:76:TYR:HB3	1:C:84:VAL:HG22	2.02	0.40
1:A:119:GLU:HA	1:A:295:PRO:HB2	2.03	0.40

All (5) 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)
3:A:612:HOH:O	3:D:659:HOH:O[3_645]	1.58	0.62
3:C:502:HOH:O	3:D:617:HOH:O[3_645]	1.75	0.45
3:B:634:HOH:O	3:D:672:HOH:O[3_645]	2.01	0.19
3:B:634:HOH:O	3:D:653:HOH:O[3_645]	2.12	0.08
3:B:550:HOH:O	3:D:623:HOH:O[3_645]	2.19	0.01

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	298/302 (99%)	293 (98%)	5 (2%)	0	100	100
1	B	300/302 (99%)	296 (99%)	4 (1%)	0	100	100
1	C	300/302 (99%)	296 (99%)	4 (1%)	0	100	100
1	D	299/302 (99%)	296 (99%)	3 (1%)	0	100	100
All	All	1197/1208 (99%)	1181 (99%)	16 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	248/247 (100%)	247 (100%)	1 (0%)	91	91
1	B	250/247 (101%)	248 (99%)	2 (1%)	81	82
1	C	250/247 (101%)	246 (98%)	4 (2%)	62	59
1	D	249/247 (101%)	248 (100%)	1 (0%)	91	91
All	All	997/988 (101%)	989 (99%)	8 (1%)	81	82

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	TYR
1	B	82	SER
1	B	170	TYR
1	C	84	VAL
1	C	123	ASP
1	C	140	GLN
1	C	170	TYR
1	D	170	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	75	HIS
1	A	190	HIS
1	A	257	GLN
1	A	260	GLN
1	A	265	GLN
1	B	29	GLN
1	B	75	HIS
1	B	104	GLN
1	B	121	ASN
1	B	172	ASN
1	B	190	HIS
1	B	234	HIS
1	B	260	GLN
1	C	121	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	172	ASN
1	C	234	HIS
1	C	260	GLN
1	D	22	GLN
1	D	29	GLN
1	D	75	HIS
1	D	121	ASN
1	D	190	HIS

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)

34 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	C	405	-	4,4,4	0.17	0	6,6,6	0.14	0
2	SO4	C	408	-	4,4,4	0.21	0	6,6,6	0.31	0
2	SO4	A	410	-	4,4,4	0.19	0	6,6,6	0.28	0
2	SO4	D	405	-	4,4,4	0.14	0	6,6,6	0.22	0
2	SO4	A	403	-	4,4,4	0.17	0	6,6,6	0.31	0
2	SO4	A	407	-	4,4,4	0.14	0	6,6,6	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	B	406	-	4,4,4	0.11	0	6,6,6	0.19	0
2	SO4	B	407	-	4,4,4	0.20	0	6,6,6	0.40	0
2	SO4	C	402	-	4,4,4	0.24	0	6,6,6	0.24	0
2	SO4	D	404	-	4,4,4	0.19	0	6,6,6	0.16	0
2	SO4	A	409	-	4,4,4	0.14	0	6,6,6	0.26	0
2	SO4	B	402	-	4,4,4	0.14	0	6,6,6	0.19	0
2	SO4	D	408	-	4,4,4	0.22	0	6,6,6	0.36	0
2	SO4	B	404	-	4,4,4	0.22	0	6,6,6	0.35	0
2	SO4	C	407	-	4,4,4	0.15	0	6,6,6	0.28	0
2	SO4	B	405	-	4,4,4	0.21	0	6,6,6	0.09	0
2	SO4	D	401	-	4,4,4	0.24	0	6,6,6	0.41	0
2	SO4	C	406	-	4,4,4	0.18	0	6,6,6	0.20	0
2	SO4	A	401	-	4,4,4	0.11	0	6,6,6	0.15	0
2	SO4	C	404	-	4,4,4	0.21	0	6,6,6	0.20	0
2	SO4	C	403	-	4,4,4	0.20	0	6,6,6	0.32	0
2	SO4	D	406	-	4,4,4	0.16	0	6,6,6	0.21	0
2	SO4	D	403	-	4,4,4	0.21	0	6,6,6	0.28	0
2	SO4	D	407	-	4,4,4	0.16	0	6,6,6	0.29	0
2	SO4	A	404	-	4,4,4	0.31	0	6,6,6	0.57	0
2	SO4	A	405	-	4,4,4	0.25	0	6,6,6	0.25	0
2	SO4	A	408	-	4,4,4	0.30	0	6,6,6	0.27	0
2	SO4	A	402	-	4,4,4	0.13	0	6,6,6	0.24	0
2	SO4	B	401	-	4,4,4	0.19	0	6,6,6	0.18	0
2	SO4	C	401	-	4,4,4	0.23	0	6,6,6	0.22	0
2	SO4	A	406	-	4,4,4	0.10	0	6,6,6	0.40	0
2	SO4	B	403	-	4,4,4	0.12	0	6,6,6	0.28	0
2	SO4	D	402	-	4,4,4	0.13	0	6,6,6	0.23	0
2	SO4	B	408	-	4,4,4	0.13	0	6,6,6	0.31	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.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	408	SO4	1	0
2	D	405	SO4	1	0
2	A	409	SO4	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	404	SO4	2	0
2	C	407	SO4	1	0
2	D	401	SO4	1	0
2	B	401	SO4	2	0
2	C	401	SO4	2	0
2	D	402	SO4	2	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	297/302 (98%)	0.31	11 (3%) 41 45	28, 41, 59, 71	0
1	B	299/302 (99%)	0.32	5 (1%) 70 73	29, 49, 64, 73	0
1	C	299/302 (99%)	0.19	4 (1%) 77 79	29, 47, 64, 74	0
1	D	298/302 (98%)	0.21	5 (1%) 70 73	29, 40, 54, 77	0
All	All	1193/1208 (98%)	0.26	25 (2%) 63 67	28, 43, 63, 77	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	139	ASP	5.5
1	D	84	VAL	4.6
1	C	139	ASP	4.4
1	D	0	ASN	3.9
1	D	78	GLY	3.8
1	A	102	ARG	2.9
1	A	148	SER	2.9
1	C	103	LYS	2.9
1	D	139	ASP	2.9
1	A	147	ALA	2.7
1	C	241	ALA	2.7
1	B	103	LYS	2.6
1	A	75	HIS	2.5
1	D	146	THR	2.5
1	C	243	LEU	2.5
1	A	41	GLY	2.5
1	A	137	THR	2.4
1	A	81	ALA	2.3
1	B	212	GLY	2.3
1	A	42	ILE	2.1
1	A	36	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	78	GLY	2.1
1	A	101	VAL	2.0
1	A	139	ASP	2.0
1	B	150	LYS	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	405	5/5	0.83	0.28	60,65,71,81	0
2	SO4	A	404	5/5	0.84	0.12	51,52,65,74	0
2	SO4	A	408	5/5	0.88	0.37	50,51,66,82	0
2	SO4	A	407	5/5	0.90	0.31	57,60,68,73	0
2	SO4	B	403	5/5	0.90	0.13	67,69,77,79	0
2	SO4	B	404	5/5	0.92	0.17	62,63,68,75	0
2	SO4	B	405	5/5	0.92	0.39	63,70,75,81	0
2	SO4	C	403	5/5	0.92	0.12	56,61,67,71	0
2	SO4	C	404	5/5	0.92	0.14	60,61,72,73	0
2	SO4	D	401	5/5	0.92	0.16	53,53,66,72	0
2	SO4	D	406	5/5	0.92	0.32	56,61,65,67	0
2	SO4	C	405	5/5	0.93	0.30	61,68,73,79	0
2	SO4	C	406	5/5	0.93	0.24	58,59,71,74	0
2	SO4	A	406	5/5	0.93	0.41	53,63,64,64	0
2	SO4	D	403	5/5	0.93	0.06	52,52,57,67	0
2	SO4	B	406	5/5	0.93	0.26	56,64,68,69	0
2	SO4	C	402	5/5	0.94	0.20	54,61,65,70	0
2	SO4	A	403	5/5	0.94	0.27	53,56,60,65	0
2	SO4	C	407	5/5	0.95	0.12	48,49,59,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	C	401	5/5	0.96	0.16	44,48,60,61	0
2	SO4	D	404	5/5	0.96	0.33	60,63,72,76	0
2	SO4	B	402	5/5	0.96	0.18	60,61,67,70	0
2	SO4	A	401	5/5	0.97	0.14	49,55,57,65	0
2	SO4	B	407	5/5	0.97	0.15	45,51,53,56	0
2	SO4	B	401	5/5	0.97	0.18	51,56,64,68	0
2	SO4	C	408	5/5	0.97	0.12	46,50,58,62	0
2	SO4	A	409	5/5	0.98	0.11	40,43,44,47	0
2	SO4	A	410	5/5	0.98	0.15	39,40,46,47	0
2	SO4	D	405	5/5	0.98	0.13	44,50,56,67	5
2	SO4	D	402	5/5	0.98	0.14	51,52,56,62	0
2	SO4	D	407	5/5	0.98	0.11	37,43,47,50	0
2	SO4	B	408	5/5	0.99	0.11	45,46,47,54	0
2	SO4	A	402	5/5	0.99	0.11	45,49,52,52	0
2	SO4	D	408	5/5	0.99	0.11	36,39,43,44	0

6.5 Other polymers (i)

There are no such residues in this entry.