Full wwPDB X-ray Structure Validation Report (i)

Aug 21, 2020 – 04:21 PM BST

PDB ID	:	5XMB
Title	:	Mycobacterium tuberculosis Pantothenate kinase mutant F247A
Authors	:	Paul, A.; Kumar, P.; Surolia, A.; Vijayan, M.
Deposited on	:	2017-05-13
Resolution	:	3.20 Å(reported)

The following versions of software and data (see references (i)) 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 3.20 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	Percentile Ranks	Value
Rfree		0.357
Clashscore		7
Ramachandran outliers		3.0%
Sidechain outliers		8.9%
RSRZ outliers		2.2%

Worse .... *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
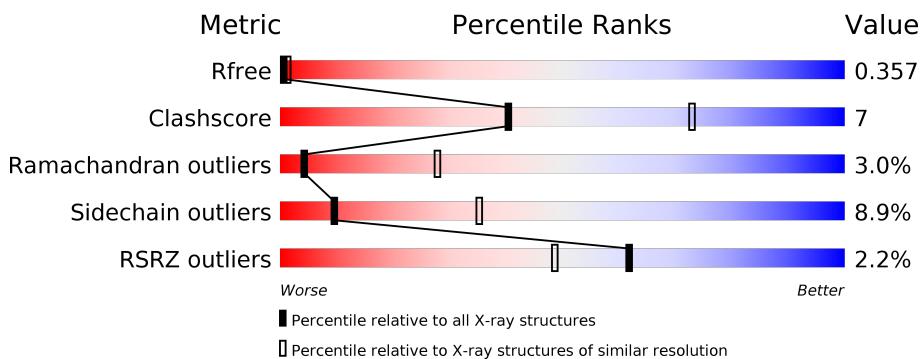
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	312	2% 70% 16% • 11%
1	B	312	3% 71% 13% • 14%
1	C	312	2% 63% 17% • 17%
1	D	312	% 66% 14% • 15%
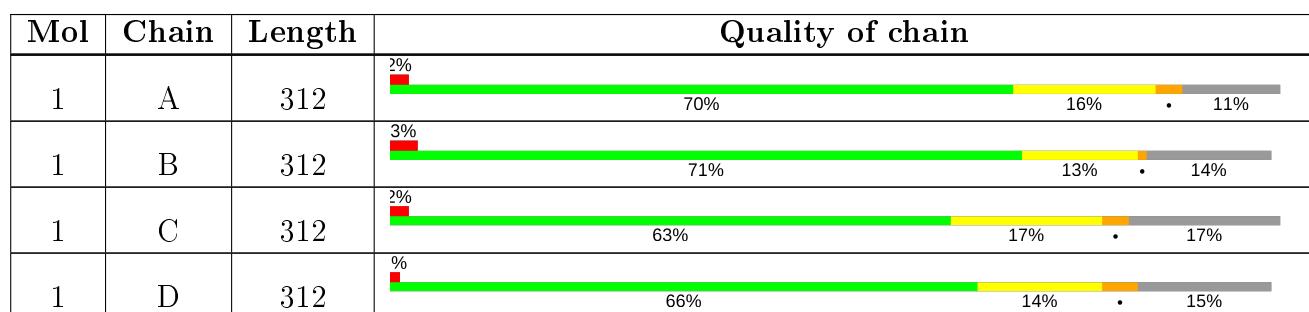
2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8073 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 Pantothenate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total 2039	C 1314	N 358	O 363	S 4	0	0	0
1	B	267	Total 2037	C 1305	N 361	O 367	S 4	0	0	0
1	C	260	Total 1966	C 1259	N 350	O 354	S 3	0	0	0
1	D	264	Total 1978	C 1264	N 357	O 352	S 5	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	247	ALA	PHE	engineered mutation	UNP P9WPA7
B	247	ALA	PHE	engineered mutation	UNP P9WPA7
C	247	ALA	PHE	engineered mutation	UNP P9WPA7
D	247	ALA	PHE	engineered mutation	UNP P9WPA7

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
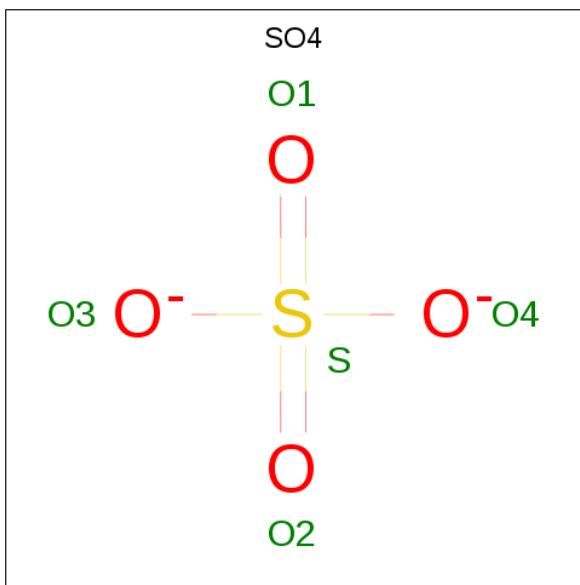
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	C	1	Total 5	O 4	S 1	0	0
2	D	1	Total 5	O 4	S 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total 10	O 10	0	0
3	B	14	Total 14	O 14	0	0
3	C	3	Total 3	O 3	0	0
3	D	6	Total 6	O 6	0	0

3 Residue-property plots ⓘ

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: Pantothenate kinase

Chain A:

- Molecule 1: Pantothenate kinase

Chain B:

- Molecule 1: Pantothenate kinase

Chain C:

HIS PHE HIS HIS TYR ALA ALA PHE SER ASP SER GLN ALA VAL VAL ALA A269 R270 R274 R278 P279 R289 P290 L294 D301 H302 N305 R306 L307 R308 K311 LEU

• Molecule 1: Pantothenate kinase

Chain D:

%

66% 14% 15%

MET SER ARG LEU SER GLU P7 W18 ARG ALA LEU ARG MET SER THR PRO LEU ALA LEU THR GLU GLU GLU LEU VAL GLY LEU GLU ARG GLY LEU GLY GLU Q43 I44 E48 V49 E50 E51 V52 Y53 H61 V64 A65 A66 R69 L70 T74 A75 E76 F77 L78 G79 E80 P81

GLN GLN ASN PRO D86 R87 P88 V89 P90 F91 T105 R108 V109 H119 T127 L132 Y133 P134 L138 Q139 R140 L143 M144 F161 V165 K166 S167 G168 S169 H179 L180 H181 Y182 D183 I184 T211 V214 L222 I228 V236 S237 R238 A247 ALA

ASP PRO GLU SER HIS PHE HIS TYR ALA ALA PHE S261 D262 A268 I272 R278 P279 R289 P290 R291 L294 D301 H302 K311 LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.83Å 104.72Å 145.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	84.96 – 3.20 73.26 – 3.20	Depositor EDS
% Data completeness (in resolution range)	90.1 (84.96-3.20) 90.1 (73.26-3.20)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.73 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.291 , 0.359 0.291 , 0.357	Depositor DCC
R_{free} test set	1034 reflections (5.21%)	wwPDB-VP
Wilson B-factor (Å^2)	41.3	Xtriage
Anisotropy	1.516	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 58.2	EDS
L-test for twinning[2]	$<|L|> = 0.42, <L^2> = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	8073	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.36% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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	0.36	0/2078	0.65	0/2838
1	B	0.36	0/2082	0.61	0/2842
1	C	0.48	3/2006 (0.1%)	0.67	2/2739 (0.1%)
1	D	0.44	1/2020 (0.0%)	0.69	3/2760 (0.1%)
All	All	0.41	4/8186 (0.0%)	0.66	5/11179 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	86	ASP	CB-CG	7.32	1.67	1.51
1	C	86	ASP	CA-CB	-6.09	1.40	1.53
1	C	86	ASP	N-CA	-5.31	1.35	1.46
1	D	79	GLY	N-CA	-5.13	1.38	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	77	PHE	CB-CG-CD2	-6.57	116.20	120.80
1	D	86	ASP	N-CA-CB	-6.49	98.93	110.60
1	C	77	PHE	CB-CG-CD1	6.25	125.17	120.80
1	D	78	LEU	CB-CA-C	6.16	121.90	110.20
1	D	78	LEU	CA-C-N	-5.12	105.97	116.20

There are no chirality outliers.

There are no planarity outliers.

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	2039	0	1961	32	0
1	B	2037	0	1952	20	0
1	C	1966	0	1877	32	0
1	D	1978	0	1894	33	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	10	0	0	0	0
3	B	14	0	0	0	0
3	C	3	0	0	0	0
3	D	6	0	0	0	0
All	All	8073	0	7684	113	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 7.

All (113) 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:242:MET:O	1:A:247:ALA:HB2	1.65	0.95
1:C:120:HIS:CD2	1:C:120:HIS:O	2.36	0.80
1:D:78:LEU:O	1:D:79:GLY:C	2.24	0.73
1:D:61:HIS:CE1	1:D:119:HIS:CE1	2.80	0.69
1:B:120:HIS:O	1:B:120:HIS:ND1	2.26	0.68
1:C:70:LEU:HG	1:C:71:PHE:N	2.10	0.67
1:D:167:SER:O	1:D:169:SER:N	2.30	0.64
1:C:167:SER:O	1:C:169:SER:N	2.32	0.63
1:A:15:ARG:HG2	1:A:304:ILE:O	1.99	0.63
1:A:123:VAL:HG12	1:A:197:ILE:HB	1.81	0.62
1:D:61:HIS:CE1	1:D:119:HIS:NE2	2.68	0.62
1:B:123:VAL:HG12	1:B:197:ILE:HB	1.82	0.61
1:D:61:HIS:HE1	1:D:119:HIS:NE2	1.98	0.60
1:C:120:HIS:CD2	1:C:197:ILE:CD1	2.83	0.60
1:B:121:PRO:O	1:B:122:ARG:CB	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:HIS:CD2	1:C:197:ILE:HD11	2.36	0.60
1:C:222:LEU:HD12	1:C:294:LEU:HD23	1.85	0.58
1:D:61:HIS:HE1	1:D:119:HIS:CE1	2.20	0.58
1:D:222:LEU:HD12	1:D:294:LEU:HD23	1.85	0.58
1:C:70:LEU:O	1:C:74:THR:HG22	2.04	0.58
1:C:120:HIS:CG	1:C:120:HIS:O	2.58	0.56
1:D:278:ARG:HB3	1:D:279:PRO:CD	2.35	0.56
1:A:240:LEU:HD23	1:A:240:LEU:O	2.05	0.56
1:A:261:SER:HB3	1:A:265:ALA:HB2	1.88	0.56
1:C:70:LEU:HD13	1:D:66:ALA:HB2	1.87	0.55
1:D:70:LEU:O	1:D:74:THR:HG22	2.06	0.55
1:D:181:HIS:O	1:D:182:TYR:HB3	2.05	0.55
1:C:18:TRP:O	1:C:20:ALA:N	2.40	0.54
1:D:301:ASP:O	1:D:302:HIS:HB2	2.08	0.54
1:B:261:SER:HB3	1:B:265:ALA:HB2	1.90	0.54
1:C:89:VAL:HG11	1:C:166:LYS:O	2.08	0.53
1:C:301:ASP:O	1:C:302:HIS:HB2	2.08	0.53
1:C:119:HIS:O	1:C:120:HIS:HB3	2.08	0.52
1:C:89:VAL:HG12	1:C:168:GLY:CA	2.40	0.52
1:D:261:SER:O	1:D:262:ASP:C	2.49	0.51
1:D:268:ALA:O	1:D:272:ILE:HG12	2.10	0.51
1:A:279:PRO:O	1:A:280:ASN:HB3	2.11	0.51
1:C:278:ARG:CB	1:C:279:PRO:CD	2.89	0.51
1:B:278:ARG:HB3	1:B:279:PRO:HD3	1.94	0.50
1:D:132:LEU:O	1:D:184:ILE:HD11	2.12	0.50
1:D:89:VAL:HG11	1:D:166:LYS:O	2.10	0.50
1:A:278:ARG:HB3	1:A:279:PRO:HD3	1.94	0.50
1:B:236:VAL:O	1:B:239:PHE:O	2.29	0.50
1:D:76:GLU:O	1:D:77:PHE:C	2.50	0.49
1:B:279:PRO:O	1:B:280:ASN:HB3	2.11	0.49
1:C:120:HIS:CD2	1:C:197:ILE:HD12	2.46	0.49
1:C:9:PRO:CA	1:D:167:SER:HB3	2.43	0.49
1:B:111:GLN:O	1:B:123:VAL:HG21	2.13	0.49
1:A:111:GLN:O	1:A:123:VAL:HG21	2.13	0.49
1:D:89:VAL:HG12	1:D:168:GLY:CA	2.43	0.49
1:A:239:PHE:O	1:A:240:LEU:HB3	2.13	0.48
1:A:249:ASP:CB	1:A:250:PRO:HD3	2.42	0.48
1:D:76:GLU:O	1:D:78:LEU:N	2.47	0.48
1:C:9:PRO:HA	1:D:167:SER:HB3	1.94	0.48
1:A:161:PHE:O	1:A:165:VAL:HG23	2.14	0.48
1:A:242:MET:O	1:A:247:ALA:CB	2.50	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:278:ARG:CB	1:D:279:PRO:CD	2.92	0.47
1:C:105:THR:O	1:C:109:VAL:HG23	2.15	0.47
1:B:149:PHE:HB3	1:B:150:PRO:HD2	1.96	0.47
1:D:278:ARG:HB3	1:D:279:PRO:HD3	1.96	0.47
1:D:48:GLU:O	1:D:52:VAL:HB	2.15	0.46
1:B:115:ALA:HB2	1:B:123:VAL:HG22	1.97	0.46
1:C:48:GLU:O	1:C:52:VAL:HB	2.15	0.46
1:D:52:VAL:HG12	1:D:53:TYR:N	2.31	0.46
1:A:149:PHE:HB3	1:A:150:PRO:HD2	1.96	0.46
1:C:52:VAL:HG12	1:C:53:TYR:N	2.31	0.46
1:C:102:GLY:O	1:C:106:THR:OG1	2.29	0.45
1:C:71:PHE:O	1:C:75:ALA:HB3	2.16	0.45
1:D:105:THR:O	1:D:109:VAL:HG23	2.17	0.45
1:A:260:PHE:O	1:A:261:SER:HB2	2.16	0.45
1:B:279:PRO:O	1:B:280:ASN:CB	2.65	0.45
1:A:115:ALA:HB2	1:A:123:VAL:HG22	1.98	0.45
1:A:279:PRO:O	1:A:280:ASN:CB	2.65	0.45
1:B:135:ASN:HB3	1:B:144:MET:HE1	1.98	0.45
1:C:64:VAL:HG23	1:C:91:PHE:CG	2.51	0.45
1:D:64:VAL:HG23	1:D:91:PHE:CG	2.52	0.45
1:A:15:ARG:CG	1:A:304:ILE:O	2.64	0.44
1:A:227:ARG:HB3	1:A:230:ASP:HB2	1.98	0.44
1:B:278:ARG:HB3	1:B:279:PRO:CD	2.47	0.44
1:D:90:PRO:HG2	1:D:165:VAL:HG12	1.99	0.44
1:A:240:LEU:CD1	1:A:266:VAL:CG1	2.96	0.43
1:C:289:ARG:N	1:C:290:PRO:CD	2.82	0.43
1:A:278:ARG:HB3	1:A:279:PRO:CD	2.48	0.43
1:B:118:ASP:O	1:B:121:PRO:HD3	2.18	0.43
1:C:90:PRO:HG2	1:C:165:VAL:HG12	1.99	0.43
1:A:181:HIS:O	1:A:182:TYR:CB	2.67	0.43
1:A:243:ARG:HA	1:A:247:ALA:CB	2.49	0.43
1:A:245:THR:O	1:A:246:ALA:HB3	2.19	0.43
1:C:114:LEU:O	1:C:117:TRP:HB2	2.19	0.43
1:D:289:ARG:N	1:D:290:PRO:CD	2.82	0.42
1:B:234:TRP:CD2	1:B:302:HIS:CE1	3.06	0.42
1:A:250:PRO:O	1:A:252:SER:N	2.52	0.42
1:C:10:TYR:CB	1:C:308:ARG:HG2	2.48	0.42
1:B:161:PHE:O	1:B:165:VAL:HG23	2.19	0.42
1:C:305:ASN:OD1	1:C:306:ARG:N	2.53	0.42
1:B:234:TRP:CE3	1:B:302:HIS:CE1	3.07	0.42
1:C:270:ARG:O	1:C:274:ARG:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:PRO:O	1:D:138:LEU:HB2	2.20	0.42
1:C:134:PRO:O	1:C:138:LEU:HB2	2.21	0.41
1:D:80:GLU:O	1:D:80:GLU:HG2	2.19	0.41
1:A:236:VAL:O	1:A:239:PHE:O	2.38	0.41
1:D:161:PHE:O	1:D:165:VAL:HG23	2.20	0.41
1:B:54:LEU:N	1:B:55:PRO:HD2	2.35	0.41
1:B:64:VAL:HG23	1:B:91:PHE:CG	2.55	0.41
1:A:64:VAL:HG23	1:A:91:PHE:CG	2.55	0.41
1:C:161:PHE:O	1:C:165:VAL:HG23	2.20	0.41
1:A:239:PHE:CD1	1:A:240:LEU:N	2.89	0.41
1:A:239:PHE:HD1	1:A:240:LEU:N	2.19	0.41
1:B:171:TYR:OH	1:D:140:ARG:NE	2.54	0.41
1:A:159:MET:O	1:A:160:ARG:C	2.59	0.40
1:A:9:PRO:HA	1:A:312:LEU:HD13	2.03	0.40
1:A:105:THR:O	1:A:109:VAL:HG23	2.21	0.40
1:A:54:LEU:N	1:A:55:PRO:HD2	2.37	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	270/312 (86%)	226 (84%)	32 (12%)	12 (4%)	2	19
1	B	259/312 (83%)	228 (88%)	27 (10%)	4 (2%)	10	44
1	C	252/312 (81%)	217 (86%)	28 (11%)	7 (3%)	5	29
1	D	256/312 (82%)	222 (87%)	26 (10%)	8 (3%)	4	26
All	All	1037/1248 (83%)	893 (86%)	113 (11%)	31 (3%)	4	28

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	THR
1	A	251	GLU
1	C	18	TRP
1	C	19	ARG
1	C	44	ILE
1	C	168	GLY
1	D	44	ILE
1	D	77	PHE
1	D	168	GLY
1	D	262	ASP
1	A	42	GLU
1	A	205	VAL
1	A	242	MET
1	A	247	ALA
1	A	261	SER
1	A	263	SER
1	B	122	ARG
1	B	205	VAL
1	B	263	SER
1	A	122	ARG
1	A	245	THR
1	B	119	HIS
1	C	70	LEU
1	C	302	HIS
1	D	70	LEU
1	A	246	ALA
1	A	249	ASP
1	D	302	HIS
1	D	80	GLU
1	D	87	ARG
1	C	87	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	192/269 (71%)	177 (92%)	15 (8%)	12	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	202/269 (75%)	184 (91%)	18 (9%)	9	35
1	C	191/269 (71%)	173 (91%)	18 (9%)	8	33
1	D	193/269 (72%)	175 (91%)	18 (9%)	9	33
All	All	778/1076 (72%)	709 (91%)	69 (9%)	9	35

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	VAL
1	A	46	LEU
1	A	64	VAL
1	A	70	LEU
1	A	110	LEU
1	A	139	GLN
1	A	159	MET
1	A	167	SER
1	A	169	SER
1	A	200	LEU
1	A	205	VAL
1	A	221	SER
1	A	227	ARG
1	A	282	VAL
1	A	291	ARG
1	B	11	VAL
1	B	43	GLN
1	B	46	LEU
1	B	64	VAL
1	B	70	LEU
1	B	110	LEU
1	B	117	TRP
1	B	119	HIS
1	B	127	THR
1	B	141	ARG
1	B	146	ARG
1	B	159	MET
1	B	167	SER
1	B	196	ASP
1	B	200	LEU
1	B	205	VAL
1	B	221	SER
1	B	282	VAL

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Mol	Chain	Res	Type
1	C	64	VAL
1	C	69	ARG
1	C	74	THR
1	C	108	ARG
1	C	118	ASP
1	C	125	LEU
1	C	127	THR
1	C	138	LEU
1	C	143	LEU
1	C	144	MET
1	C	165	VAL
1	C	211	THR
1	C	214	VAL
1	C	228	ILE
1	C	236	VAL
1	C	238	ARG
1	C	274	ARG
1	C	301	ASP
1	D	50	GLU
1	D	64	VAL
1	D	69	ARG
1	D	74	THR
1	D	108	ARG
1	D	127	THR
1	D	138	LEU
1	D	143	LEU
1	D	144	MET
1	D	165	VAL
1	D	211	THR
1	D	214	VAL
1	D	228	ILE
1	D	236	VAL
1	D	238	ARG
1	D	261	SER
1	D	291	ARG
1	D	301	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	61	HIS
1	B	302	HIS

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Mol	Chain	Res	Type
1	C	120	HIS
1	C	142	ASN
1	D	61	HIS
1	D	142	ASN

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)

4 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	B	401	-	4,4,4	0.37	0	6,6,6	0.08	0
2	SO4	A	401	-	4,4,4	0.25	0	6,6,6	0.22	0
2	SO4	D	401	-	4,4,4	0.26	0	6,6,6	0.34	0
2	SO4	C	401	-	4,4,4	0.27	0	6,6,6	0.25	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.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	278/312 (89%)	0.22	5 (1%)	68	55	5, 35, 76, 114	0
1	B	267/312 (85%)	0.30	9 (3%)	45	29	4, 36, 83, 115	0
1	C	260/312 (83%)	0.25	6 (2%)	60	47	7, 35, 77, 118	0
1	D	264/312 (84%)	0.33	4 (1%)	73	61	5, 39, 78, 114	0
All	All	1069/1248 (85%)	0.27	24 (2%)	62	48	4, 36, 79, 118	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	42	GLU	5.2
1	D	74	THR	4.9
1	B	261	SER	4.2
1	C	301	ASP	4.1
1	D	7	PRO	3.2
1	B	170	ASP	3.1
1	D	86	ASP	2.9
1	C	44	ILE	2.9
1	B	229	GLU	2.7
1	C	201	GLU	2.7
1	A	204	ASN	2.7
1	B	14	ASP	2.6
1	A	22	ARG	2.5
1	B	271	GLU	2.5
1	D	179	HIS	2.5
1	A	118	ASP	2.4
1	C	85	PRO	2.3
1	B	79	GLY	2.2
1	A	142	ASN	2.2
1	C	229	GLU	2.1
1	C	20	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	283	GLU	2.1
1	A	21	LEU	2.0
1	B	167	SER	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, 95th 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	C	401	5/5	0.95	0.15	30,30,30,30	0
2	SO4	D	401	5/5	0.96	0.17	30,30,30,30	0
2	SO4	B	401	5/5	0.97	0.17	30,30,30,30	0
2	SO4	A	401	5/5	0.97	0.16	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.