



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:09 AM UTC

PDB ID : 5XMB / pdb_00005xmb
Title : Mycobacterium tuberculosis Pantothenate kinase mutant F247A
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Deposited on : 2017-05-13
Resolution : 3.20 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

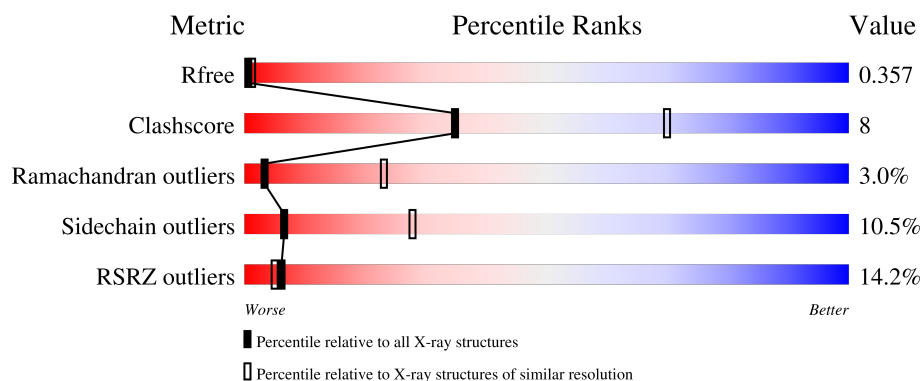
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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 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 $\leq 5\%$. 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	13% 69% 17% • 11%
1	B	312	12% 69% 15% • 14%
1	C	312	13% 62% 19% • 17%
1	D	312	12% 64% 16% • 15%

2 Entry composition

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	C	N	O	S	0	0	0
			2039	1314	358	363	4			
1	B	267	Total	C	N	O	S	0	0	0
			2037	1305	361	367	4			
1	C	260	Total	C	N	O	S	0	0	0
			1966	1259	350	354	3			
1	D	264	Total	C	N	O	S	0	0	0
			1978	1264	357	352	5			

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 (CCD ID: SO4) (formula: O₄S).



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

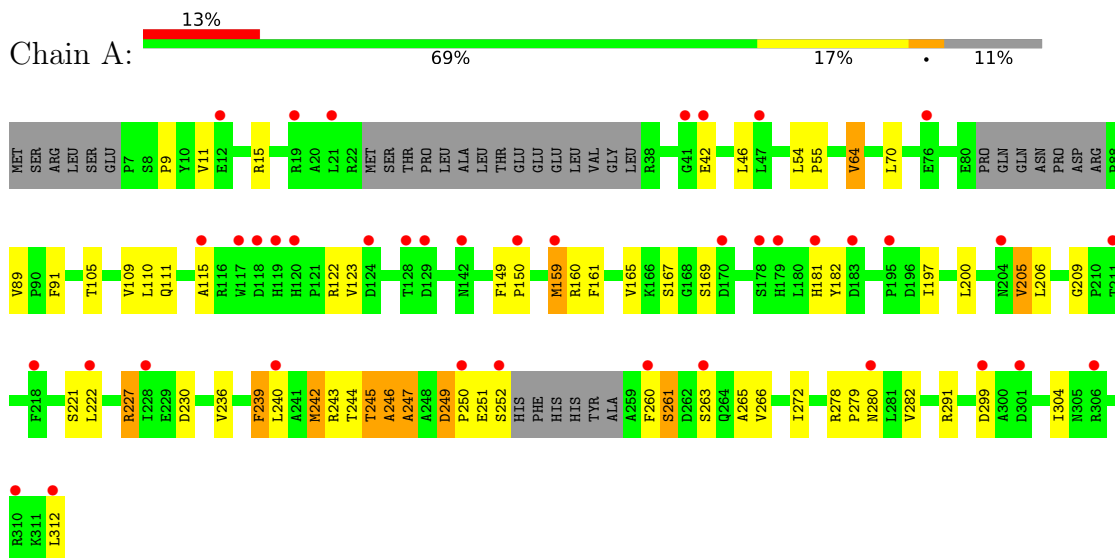
- Molecule 3 is water.

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

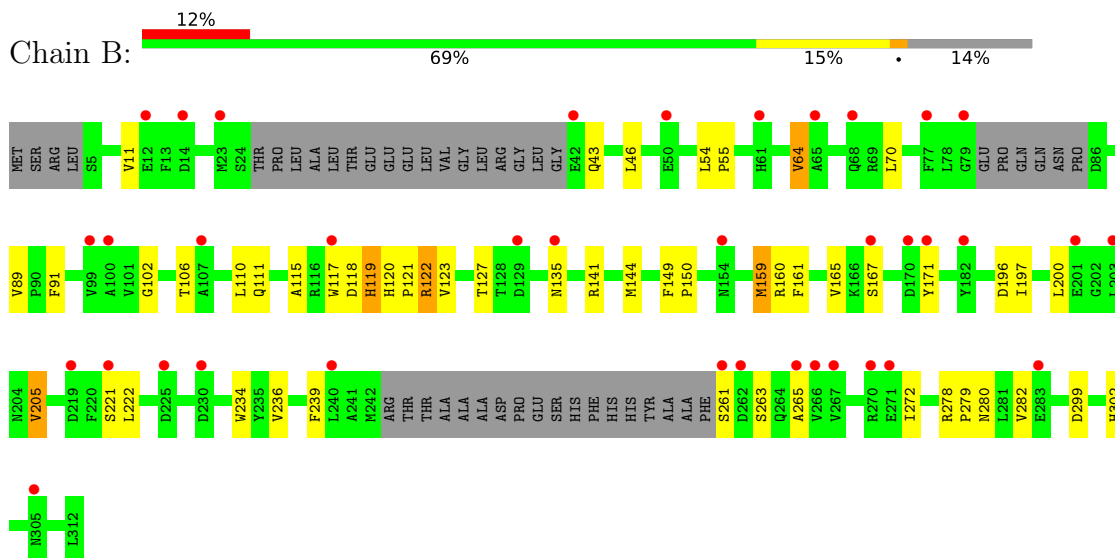
3 Residue-property plots [i](#)

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: Pantothenate kinase

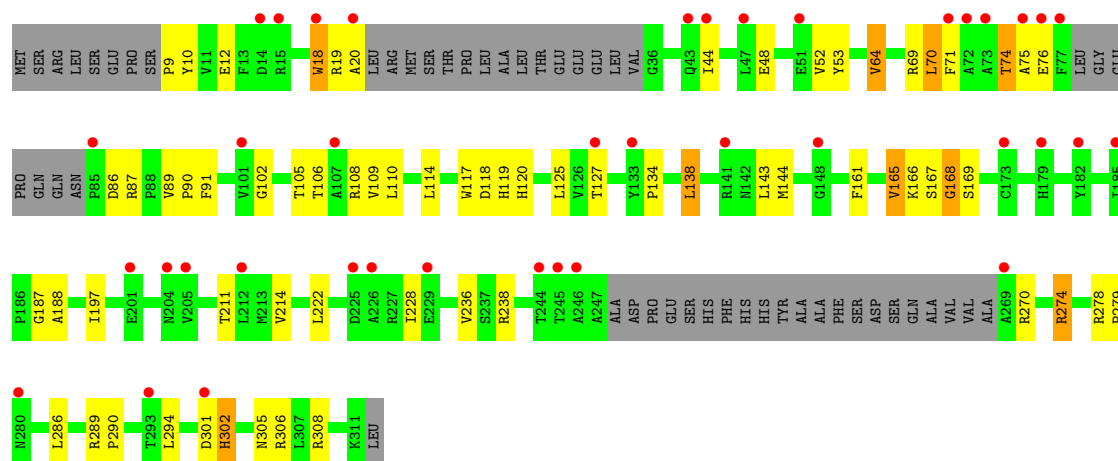


- Molecule 1: Pantothenate kinase

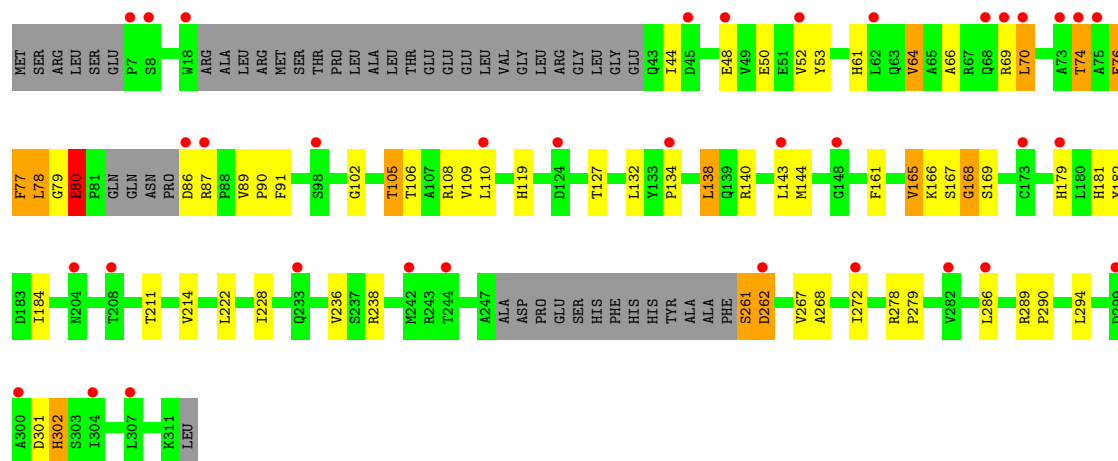


- Molecule 1: Pantothenate kinase





• Molecule 1: Pantothenate kinase



4 Data and refinement statistics

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 84.96 – 3.20	Depositor EDS
% Data completeness (in resolution range)	90.1 (84.96-3.20) 90.1 (84.96-3.20)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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	1051 reflections (4.77%)	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)	0.35 , 58.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.54	0/2078	0.94	3/2838 (0.1%)
1	B	0.53	0/2082	0.89	0/2842
1	C	0.67	4/2006 (0.2%)	0.91	0/2739
1	D	0.64	2/2020 (0.1%)	0.95	2/2760 (0.1%)
All	All	0.60	6/8186 (0.1%)	0.93	5/11179 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	86	ASP	N-CA	-8.10	1.35	1.46
1	C	76	GLU	C-N	7.76	1.44	1.33
1	C	86	ASP	CA-CB	-7.64	1.40	1.53
1	D	78	LEU	CA-C	-6.56	1.44	1.52
1	C	86	ASP	CB-CG	6.03	1.67	1.52
1	D	76	GLU	C-O	5.77	1.31	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	86	ASP	N-CA-CB	-6.81	98.93	110.50
1	D	78	LEU	CB-CA-C	5.77	121.90	110.42
1	A	239	PHE	N-CA-C	-5.73	102.93	110.43
1	A	209	GLY	CA-C-N	5.20	124.83	119.05
1	A	209	GLY	C-N-CA	5.20	124.83	119.05

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	2039	0	1961	32	0
1	B	2037	0	1952	23	0
1	C	1966	0	1877	33	0
1	D	1978	0	1894	34	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	118	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 8.

All (118) 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:O	1:C:120:HIS:CD2	2.36	0.80
1:D:78:LEU:O	1:D:79:GLY:C	2.24	0.78
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:O	1:C:120:HIS:CG	2.58	0.56
1:D:261:SER:O	1:D:262:ASP:C	2.49	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:D:76:GLU:O	1:D:77:PHE:C	2.50	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:119:HIS:O	1:C:120:HIS:HB3	2.08	0.52
1:C:301:ASP:O	1:C:302:HIS:HB2	2.08	0.52
1:C:89:VAL:HG12	1:C:168:GLY:CA	2.40	0.52
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:B:135:ASN:HB3	1:B:144:MET:HE1	1.93	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:B:279:PRO:O	1:B:280:ASN:HB3	2.11	0.49
1:C:9:PRO:CA	1:D:167:SER:HB3	2.43	0.49
1:C:120:HIS:CD2	1:C:197:ILE:HD12	2.46	0.49
1:B:102:GLY:O	1:B:106:THR:OG1	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:278:ARG:CB	1:D:279:PRO:CD	2.92	0.47
1:D:102:GLY:O	1:D:106:THR:OG1	2.29	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:71:PHE:O	1:C:75:ALA:HB3	2.16	0.45
1:C:102:GLY:O	1:C:106:THR:OG1	2.29	0.45
1:D:105:THR:O	1:D:109:VAL:HG23	2.17	0.45
1:A:159:MET:O	1:A:160:ARG:C	2.59	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: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:B:135:ASN:CG	1:B:144:MET:HE1	2.41	0.44
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:B:159:MET:O	1:B:160:ARG:C	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:134:PRO:O	1:D:138:LEU:HB2	2.20	0.42
1:C:187:GLY:O	1:C:188:ALA:C	2.63	0.41
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: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:C:161:PHE:O	1:C:165:VAL:HG23	2.20	0.41
1:A:9:PRO:HA	1:A:312:LEU:HD13	2.03	0.40
1:A:54:LEU:N	1:A:55:PRO:HD2	2.37	0.40
1:A:105:THR:O	1:A:109:VAL:HG23	2.21	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	15
1	B	259/312 (83%)	228 (88%)	27 (10%)	4 (2%)	8	37
1	C	252/312 (81%)	217 (86%)	28 (11%)	7 (3%)	4	25
1	D	256/312 (82%)	222 (87%)	26 (10%)	8 (3%)	3	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1037/1248 (83%)	893 (86%)	113 (11%)	31 (3%)	3 23

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%)	173 (90%)	19 (10%)	7	31
1	B	202/269 (75%)	181 (90%)	21 (10%)	7	28
1	C	191/269 (71%)	171 (90%)	20 (10%)	6	28
1	D	193/269 (72%)	171 (89%)	22 (11%)	5	24
All	All	778/1076 (72%)	696 (90%)	82 (10%)	6	28

All (82) 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	89	VAL
1	A	110	LEU
1	A	159	MET
1	A	167	SER
1	A	169	SER
1	A	200	LEU
1	A	205	VAL
1	A	206	LEU
1	A	221	SER
1	A	222	LEU
1	A	227	ARG
1	A	272	ILE
1	A	282	VAL
1	A	291	ARG
1	A	299	ASP
1	B	11	VAL
1	B	43	GLN
1	B	46	LEU
1	B	64	VAL
1	B	70	LEU
1	B	89	VAL
1	B	110	LEU
1	B	117	TRP
1	B	119	HIS
1	B	127	THR
1	B	141	ARG

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Mol	Chain	Res	Type
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	222	LEU
1	B	272	ILE
1	B	282	VAL
1	B	299	ASP
1	C	12	GLU
1	C	64	VAL
1	C	69	ARG
1	C	74	THR
1	C	108	ARG
1	C	110	LEU
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	286	LEU
1	D	50	GLU
1	D	64	VAL
1	D	69	ARG
1	D	74	THR
1	D	80	GLU
1	D	105	THR
1	D	108	ARG
1	D	110	LEU
1	D	127	THR
1	D	138	LEU
1	D	143	LEU
1	D	144	MET

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Mol	Chain	Res	Type
1	D	165	VAL
1	D	179	HIS
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	267	VAL
1	D	286	LEU

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

Mol	Chain	Res	Type
1	A	190	GLN
1	B	43	GLN
1	B	61	HIS
1	B	190	GLN
1	B	302	HIS
1	C	68	GLN
1	C	120	HIS
1	C	190	GLN
1	D	61	HIS
1	D	63	GLN
1	D	190	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 oligosaccharides 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	0.47	0	6,6,6	0.10	0
2	SO4	C	401	-	4,4,4	0.38	0	6,6,6	0.24	0
2	SO4	D	401	-	4,4,4	0.37	0	6,6,6	0.36	0
2	SO4	A	401	-	4,4,4	0.36	0	6,6,6	0.23	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

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, 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%)	1.10	40 (14%) 6 5	5, 35, 76, 114	0
1	B	267/312 (85%)	1.00	37 (13%) 6 5	4, 36, 83, 115	0
1	C	260/312 (83%)	1.01	39 (15%) 5 4	7, 35, 77, 118	0
1	D	264/312 (84%)	1.06	36 (13%) 7 5	5, 38, 78, 114	0
All	All	1069/1248 (85%)	1.04	152 (14%) 6 5	4, 36, 79, 118	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	244	THR	5.9
1	C	301	ASP	4.9
1	D	74	THR	4.8
1	A	204	ASN	4.7
1	C	20	ALA	4.5
1	C	246	ALA	4.4
1	B	42	GLU	4.3
1	D	68	GLN	4.3
1	B	167	SER	4.2
1	C	72	ALA	4.2
1	A	280	ASN	4.1
1	B	225	ASP	4.0
1	B	170	ASP	3.9
1	B	271	GLU	3.7
1	A	118	ASP	3.7
1	C	76	GLU	3.7
1	B	182	TYR	3.6
1	A	195	PRO	3.5
1	A	260	PHE	3.5
1	B	283	GLU	3.4
1	B	266	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	179	HIS	3.4
1	D	86	ASP	3.4
1	A	181	HIS	3.4
1	A	170	ASP	3.4
1	D	18	TRP	3.3
1	D	48	GLU	3.3
1	C	44	ILE	3.3
1	A	119	HIS	3.3
1	C	280	ASN	3.3
1	A	250	PRO	3.3
1	A	117	TRP	3.3
1	A	211	THR	3.2
1	D	7	PRO	3.2
1	D	173	CYS	3.1
1	B	240	LEU	3.1
1	C	148	GLY	3.1
1	A	41	GLY	3.1
1	B	154	ASN	3.0
1	D	124	ASP	3.0
1	C	201	GLU	2.9
1	A	312	LEU	2.9
1	C	204	ASN	2.9
1	B	261	SER	2.9
1	C	15	ARG	2.9
1	A	263	SER	2.9
1	D	272	ILE	2.9
1	D	148	GLY	2.9
1	A	150	PRO	2.8
1	D	233	GLN	2.8
1	C	101	VAL	2.8
1	A	142	ASN	2.8
1	B	265	ALA	2.8
1	D	300	ALA	2.8
1	B	262	ASP	2.7
1	B	99	VAL	2.7
1	C	127	THR	2.7
1	A	178	SER	2.7
1	C	141	ARG	2.6
1	D	244	THR	2.6
1	D	52	VAL	2.6
1	D	208	THR	2.6
1	C	226	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	228	ILE	2.6
1	A	19	ARG	2.6
1	D	242	MET	2.6
1	B	61	HIS	2.6
1	A	159	MET	2.5
1	D	98	SER	2.5
1	D	70	LEU	2.5
1	D	87	ARG	2.5
1	C	75	ALA	2.5
1	C	225	ASP	2.5
1	B	203	LEU	2.5
1	B	201	GLU	2.5
1	C	229	GLU	2.5
1	B	117	TRP	2.5
1	C	77	PHE	2.5
1	C	18	TRP	2.5
1	D	143	LEU	2.5
1	C	269	ALA	2.4
1	A	183	ASP	2.4
1	B	77	PHE	2.4
1	A	129	ASP	2.4
1	C	173	CYS	2.4
1	A	42	GLU	2.4
1	A	299	ASP	2.4
1	D	282	VAL	2.4
1	C	205	VAL	2.3
1	D	304	ILE	2.3
1	B	219	ASP	2.3
1	D	299	ASP	2.3
1	B	267	VAL	2.3
1	D	8	SER	2.3
1	C	182	TYR	2.3
1	A	21	LEU	2.3
1	A	47	LEU	2.3
1	A	76	GLU	2.3
1	B	12	GLU	2.3
1	C	185	ILE	2.3
1	A	115	ALA	2.3
1	B	230	ASP	2.3
1	C	43	GLN	2.3
1	B	65	ALA	2.3
1	A	222	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	135	ASN	2.3
1	B	129	ASP	2.3
1	C	51	GLU	2.2
1	C	212	LEU	2.2
1	D	307	LEU	2.2
1	C	14	ASP	2.2
1	D	262	ASP	2.2
1	B	107	ALA	2.2
1	A	310	ARG	2.2
1	A	124	ASP	2.2
1	D	134	PRO	2.2
1	C	293	THR	2.2
1	B	171	TYR	2.2
1	D	204	ASN	2.2
1	A	120	HIS	2.2
1	A	240	LEU	2.2
1	C	47	LEU	2.2
1	D	62	LEU	2.2
1	B	50	GLU	2.2
1	B	305	ASN	2.2
1	C	107	ALA	2.2
1	B	14	ASP	2.2
1	C	245	THR	2.1
1	B	23	MET	2.1
1	D	75	ALA	2.1
1	A	306	ARG	2.1
1	C	73	ALA	2.1
1	A	218	PHE	2.1
1	A	179	HIS	2.1
1	A	128	THR	2.1
1	D	110	LEU	2.1
1	D	286	LEU	2.1
1	D	73	ALA	2.1
1	A	301	ASP	2.1
1	C	179	HIS	2.1
1	D	45	ASP	2.1
1	C	133	TYR	2.1
1	B	100	ALA	2.1
1	B	68	GLN	2.1
1	A	252	SER	2.1
1	B	79	GLY	2.1
1	C	85	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	270	ARG	2.0
1	B	221	SER	2.0
1	C	71	PHE	2.0
1	A	12	GLU	2.0
1	D	69	ARG	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 oligosaccharides 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	0.09	30,30,30,30	0
2	SO4	D	401	5/5	0.96	0.10	30,30,30,30	0
2	SO4	B	401	5/5	0.97	0.11	30,30,30,30	0
2	SO4	A	401	5/5	0.98	0.06	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.