



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:03 PM UTC

PDB ID : 5XLV / pdb_00005xlv
Title : Mycobacterium tuberculosis Pantothenate kinase mutant F254A
Authors : Paul, A.; Kumar, P.; Surolia, A.; Vijayan, M.
Deposited on : 2017-05-11
Resolution : 1.80 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

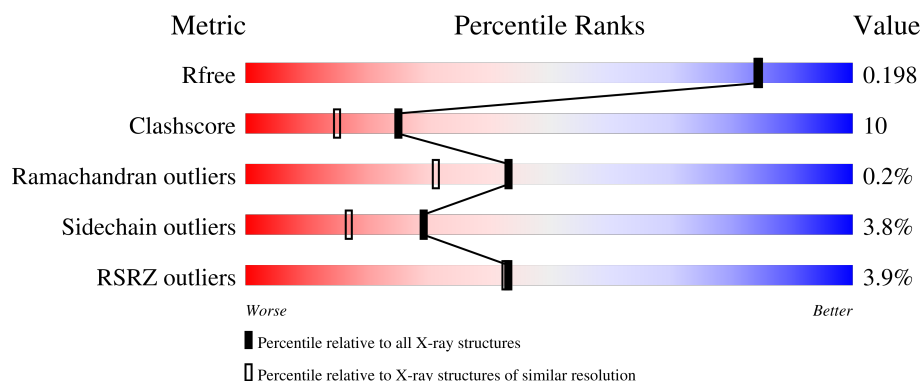
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	4% 80% 16% ..
1	B	312	4% 78% 13% 8%

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
4	EDO	B	406	-	-	X	-
4	EDO	B	413	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5648 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	306	Total	C	N	O	S	0	6	0
			2479	1578	451	443	7			
1	B	288	Total	C	N	O	S	0	4	0
			2326	1482	423	414	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	254	ALA	PHE	engineered mutation	UNP P9WPA7
B	254	ALA	PHE	engineered mutation	UNP P9WPA7

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



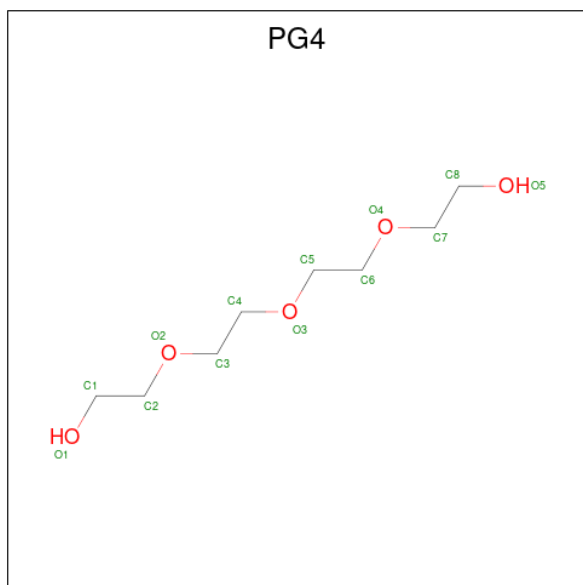
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

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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	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	8	5		
3	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

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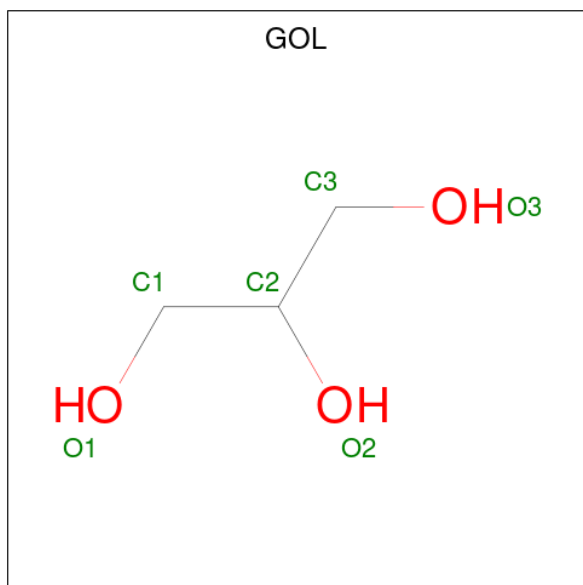
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	331	Total	O	0	0
			331	331		
6	B	296	Total	O	0	0
			296	296		

i

- Molecule 1: Pantothenate kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	120.82Å 120.82Å 125.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.58 – 1.80 24.58 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (24.58-1.80) 99.8 (24.58-1.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.178 , 0.213 (Not available) , 0.198	Depositor DCC
R_{free} test set	4891 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5648	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, PG4, EDO, GOL

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	1.22	0/2556	1.15	4/3476 (0.1%)
1	B	1.24	2/2383 (0.1%)	1.17	2/3240 (0.1%)
All	All	1.23	2/4939 (0.0%)	1.16	6/6716 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	194	HIS	C-O	7.71	1.27	1.23
1	B	194	HIS	CA-CB	5.21	1.56	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	HIS	CA-C-N	-6.61	116.23	122.37
1	A	119	HIS	C-N-CA	-6.61	116.23	122.37
1	A	136	ALA	N-CA-C	-5.93	104.89	111.36
1	B	67	ARG	CB-CG-CD	-5.78	98.01	111.30
1	A	194	HIS	CB-CA-C	-5.14	106.53	111.00
1	B	30	THR	N-CA-C	-5.13	101.62	109.41

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	2479	0	2488	39	0
1	B	2326	0	2348	37	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
3	A	13	0	18	1	0
3	B	13	0	18	6	0
4	A	76	0	114	14	0
4	B	76	0	114	27	0
5	A	12	0	16	3	0
5	B	6	0	8	0	0
6	A	331	0	0	10	0
6	B	296	0	0	17	0
All	All	5648	0	5124	98	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 10.

All (98) 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)
4:A:421:EDO:H11	6:A:756:HOH:O	1.54	1.06
1:B:141:ARG:HH12	4:B:404:EDO:H21	1.40	0.86
4:B:415:EDO:H12	6:B:672:HOH:O	1.76	0.84
1:B:299:ASP:OD1	1:B:301:ASP:OD1	1.96	0.84
1:B:160:ARG:HH22	4:B:406:EDO:H21	1.43	0.82
4:B:417:EDO:O1	6:B:501:HOH:O	1.95	0.80
5:A:423:GOL:O2	6:A:501:HOH:O	2.04	0.76
1:B:28:ALA:O	1:B:33:GLU:HG3	1.88	0.73
1:A:308:ARG:HH12	4:A:405:EDO:H21	1.56	0.70
4:B:412:EDO:C1	6:B:593:HOH:O	2.38	0.70
4:B:412:EDO:H12	6:B:593:HOH:O	1.92	0.70
3:B:403:PG4:H82	6:B:741:HOH:O	1.92	0.68
1:B:173[B]:CYS:SG	1:B:189:GLU:HB2	2.34	0.67
1:A:16:ARG:HH11	1:A:16:ARG:HG2	1.59	0.67
1:B:274:ARG:NH2	6:B:502:HOH:O	2.28	0.67
1:A:144:MET:HB2	4:A:407:EDO:H21	1.76	0.67
1:A:8:SER:HA	6:A:504:HOH:O	1.94	0.66
1:A:171:TYR:CZ	1:A:173[A]:CYS:SG	2.90	0.65
1:B:278:ARG:HH12	4:B:415:EDO:H11	1.61	0.65
1:A:173[B]:CYS:SG	1:A:189:GLU:HB2	2.37	0.65
4:A:416:EDO:H12	6:A:578:HOH:O	1.99	0.62
1:B:41:GLY:C	1:B:43:GLN:H	2.05	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:GLU:O	5:A:424:GOL:H31	2.00	0.61
1:A:267:VAL:HG12	4:A:420:EDO:H22	1.82	0.60
1:A:18:TRP:CZ2	1:A:23:MET:HE1	2.37	0.59
1:B:156:ARG:HH12	4:B:406:EDO:H11	1.67	0.59
1:A:16:ARG:HG2	1:A:16:ARG:NH1	2.16	0.59
4:B:412:EDO:H11	6:B:593:HOH:O	2.02	0.58
1:A:238:ARG:O	1:A:242:MET:HG2	2.04	0.58
1:A:306:ARG:HH22	4:A:405:EDO:H11	1.69	0.56
1:B:117:TRP:CE2	4:B:405:EDO:H12	2.40	0.56
1:A:177:TYR:CE2	3:A:403:PG4:H81	2.41	0.56
3:B:403:PG4:H81	6:B:747:HOH:O	2.06	0.56
4:B:413:EDO:H12	6:B:762:HOH:O	2.07	0.55
1:A:81:PRO:HB2	1:A:83:GLN:OE1	2.07	0.55
1:B:14:ASP:OD1	1:B:17:GLN:HG3	2.08	0.54
1:B:160:ARG:HH22	4:B:406:EDO:C2	2.18	0.53
1:A:211:THR:OG1	1:A:212:LEU:N	2.41	0.53
4:B:418:EDO:C2	6:B:552:HOH:O	2.58	0.52
1:A:293:THR:HA	1:A:310[A]:ARG:HG3	1.92	0.52
3:B:403:PG4:H21	6:B:620:HOH:O	2.10	0.52
1:B:170:ASP:H	4:B:422:EDO:H21	1.75	0.52
1:A:229:GLU:H	1:A:229:GLU:CD	2.17	0.51
4:B:413:EDO:H21	6:B:762:HOH:O	2.10	0.51
1:B:125:LEU:HG	4:B:417:EDO:H21	1.91	0.51
3:B:403:PG4:H32	6:B:620:HOH:O	2.09	0.50
4:A:411:EDO:H21	6:A:533:HOH:O	2.11	0.50
1:A:53:TYR:OH	6:A:502:HOH:O	2.11	0.49
1:B:41:GLY:C	1:B:43:GLN:N	2.61	0.49
1:B:278:ARG:HH12	4:B:415:EDO:C1	2.25	0.49
1:B:160:ARG:NH2	4:B:406:EDO:H21	2.22	0.49
4:B:413:EDO:C2	6:B:762:HOH:O	2.61	0.49
4:A:414:EDO:H21	6:A:510:HOH:O	2.11	0.49
1:A:267:VAL:HG12	4:A:420:EDO:C2	2.44	0.48
1:A:171:TYR:OH	1:A:173[A]:CYS:SG	2.58	0.48
1:B:173[B]:CYS:SG	1:B:189:GLU:OE1	2.71	0.48
1:A:16:ARG:NH2	4:A:422:EDO:O1	2.46	0.47
1:A:179:HIS:CG	5:A:423:GOL:H2	2.50	0.47
1:B:50:GLU:HA	1:B:54:LEU:HD22	1.97	0.47
1:A:299:ASP:OD1	1:A:301:ASP:OD1	2.32	0.46
1:B:162:VAL:HG12	1:B:217:LEU:HD23	1.97	0.46
4:B:413:EDO:C1	6:B:762:HOH:O	2.62	0.46
1:B:122:ARG:NH2	1:B:193:ARG:O	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:ARG:NH1	4:A:405:EDO:H21	2.27	0.45
1:B:240:LEU:HD22	4:B:411:EDO:H22	1.98	0.45
1:A:208:THR:HA	1:A:213:MET:SD	2.57	0.45
1:A:159:MET:HE1	1:A:214:VAL:N	2.31	0.45
3:B:403:PG4:H52	6:B:620:HOH:O	2.18	0.44
1:B:30:THR:OG1	1:B:33:GLU:HG2	2.18	0.44
1:B:171:TYR:CE1	1:B:173[A]:CYS:SG	3.10	0.44
1:B:238:ARG:HA	4:B:409:EDO:H11	1.99	0.44
1:A:292:ALA:O	1:A:310[A]:ARG:NH1	2.51	0.44
1:B:156:ARG:NH1	4:B:406:EDO:C1	2.81	0.44
1:A:136:ALA:O	1:A:139:GLN:HB3	2.18	0.43
1:B:117:TRP:HB2	1:B:120:HIS:CE1	2.54	0.43
1:B:232:GLU:HG3	1:B:273:TRP:CD1	2.54	0.43
1:A:133:TYR:CD1	4:A:410:EDO:H21	2.54	0.42
1:A:301:ASP:O	1:A:302:HIS:HB2	2.20	0.42
1:B:156:ARG:NH1	4:B:406:EDO:O1	2.52	0.42
1:A:181:HIS:HE1	1:A:249:ASP:OD2	2.03	0.42
1:A:10:TYR:CE1	1:A:310[A]:ARG:HD3	2.55	0.42
1:B:156:ARG:HH12	4:B:406:EDO:C1	2.31	0.41
1:A:139:GLN:HE22	1:A:144:MET:HG3	1.85	0.41
1:A:181:HIS:HD2	6:A:801:HOH:O	2.04	0.41
1:B:21:LEU:HD12	1:B:23:MET:HE3	2.02	0.41
1:B:289:ARG:HG2	4:B:416:EDO:H21	2.02	0.41
4:A:421:EDO:H22	6:B:722:HOH:O	2.20	0.41
1:B:158:LEU:HG	1:B:214:VAL:HG21	2.03	0.41
1:A:136:ALA:O	1:A:139:GLN:CB	2.69	0.41
1:A:171:TYR:CD1	1:A:171:TYR:C	2.98	0.41
1:A:192:VAL:HG13	1:A:195:PRO:HD3	2.03	0.40
1:A:228[A]:ILE:HG22	6:A:652:HOH:O	2.20	0.40
4:A:409:EDO:H12	6:A:621:HOH:O	2.21	0.40
1:B:104[A]:SER:OG	1:B:108:ARG:CZ	2.69	0.40
1:B:147:LYS:HG2	3:B:403:PG4:H62	2.03	0.40
1:A:286:LEU:N	1:A:287:PRO:CD	2.84	0.40
1:B:278:ARG:HB3	1:B:279:PRO:HD3	2.02	0.40
1:B:308:ARG:HH22	4:B:407:EDO:H21	1.86	0.40

There are no symmetry-related clashes.

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	310/312 (99%)	302 (97%)	7 (2%)	1 (0%)	36	25
1	B	288/312 (92%)	284 (99%)	4 (1%)	0	100	100
All	All	598/624 (96%)	586 (98%)	11 (2%)	1 (0%)	43	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	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	266/269 (99%)	252 (95%)	14 (5%)	20	9
1	B	250/269 (93%)	245 (98%)	5 (2%)	48	38
All	All	516/538 (96%)	497 (96%)	19 (4%)	29	18

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LEU
1	A	76	GLU
1	A	78	LEU
1	A	80	GLU
1	A	82	GLN

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Mol	Chain	Res	Type
1	A	110	LEU
1	A	119	HIS
1	A	139	GLN
1	A	142	ASN
1	A	211	THR
1	A	214	VAL
1	A	217	LEU
1	A	229	GLU
1	A	240	LEU
1	B	37	LEU
1	B	54	LEU
1	B	59	LEU
1	B	214	VAL
1	B	217	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	139	GLN
1	A	181	HIS
1	B	82	GLN
1	B	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 ⓘ

47 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	$\# Z > 2$
4	EDO	A	422	-	3,3,3	0.47	0	2,2,2	1.19	0
4	EDO	B	404	-	3,3,3	0.15	0	2,2,2	1.49	0
4	EDO	B	411	-	3,3,3	0.46	0	2,2,2	0.43	0
4	EDO	A	416	-	3,3,3	0.42	0	2,2,2	0.54	0
4	EDO	A	411	-	3,3,3	0.45	0	2,2,2	0.67	0
4	EDO	A	407	-	3,3,3	0.51	0	2,2,2	0.11	0
4	EDO	B	414	-	3,3,3	0.71	0	2,2,2	0.12	0
4	EDO	B	418	-	3,3,3	0.81	0	2,2,2	0.16	0
4	EDO	B	420	-	3,3,3	0.66	0	2,2,2	0.35	0
4	EDO	B	422	-	3,3,3	0.32	0	2,2,2	0.93	0
2	SO4	B	402	-	4,4,4	0.50	0	6,6,6	0.98	0
4	EDO	A	405	-	3,3,3	0.28	0	2,2,2	1.28	0
3	PG4	A	403	-	12,12,12	0.72	0	11,11,11	0.64	0
4	EDO	A	410	-	3,3,3	0.47	0	2,2,2	0.35	0
4	EDO	A	413	-	3,3,3	0.43	0	2,2,2	0.50	0
4	EDO	A	408	-	3,3,3	0.60	0	2,2,2	0.50	0
4	EDO	A	412	-	3,3,3	0.46	0	2,2,2	0.59	0
4	EDO	A	421	-	3,3,3	1.18	0	2,2,2	0.80	0
5	GOL	A	424	-	5,5,5	0.86	0	5,5,5	1.17	0
3	PG4	B	403	-	12,12,12	0.70	0	11,11,11	1.67	3 (27%)
4	EDO	B	407	-	3,3,3	0.50	0	2,2,2	0.63	0
2	SO4	B	401	-	4,4,4	0.17	0	6,6,6	0.32	0
4	EDO	B	413	-	3,3,3	0.43	0	2,2,2	0.38	0
4	EDO	A	404	-	3,3,3	0.33	0	2,2,2	1.30	0
4	EDO	A	419	-	3,3,3	0.38	0	2,2,2	0.97	0
4	EDO	B	421	-	3,3,3	0.47	0	2,2,2	0.36	0
4	EDO	A	420	-	3,3,3	0.60	0	2,2,2	0.93	0
4	EDO	A	406	-	3,3,3	0.43	0	2,2,2	0.87	0
4	EDO	B	415	-	3,3,3	0.37	0	2,2,2	0.67	0
2	SO4	A	402	-	4,4,4	0.46	0	6,6,6	0.60	0
4	EDO	A	409	-	3,3,3	0.23	0	2,2,2	0.72	0
2	SO4	A	401	-	4,4,4	0.39	0	6,6,6	0.46	0
4	EDO	B	417	-	3,3,3	0.24	0	2,2,2	0.89	0
4	EDO	A	414	-	3,3,3	0.68	0	2,2,2	0.11	0
4	EDO	B	405	-	3,3,3	0.25	0	2,2,2	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	A	423	-	5,5,5	0.51	0	5,5,5	0.85	0
4	EDO	B	406	-	3,3,3	0.21	0	2,2,2	0.99	0
4	EDO	A	415	-	3,3,3	0.58	0	2,2,2	0.22	0
4	EDO	B	416	-	3,3,3	0.55	0	2,2,2	0.19	0
4	EDO	A	417	-	3,3,3	0.90	0	2,2,2	0.49	0
4	EDO	B	408	-	3,3,3	0.55	0	2,2,2	0.43	0
4	EDO	B	409	-	3,3,3	0.27	0	2,2,2	1.03	0
5	GOL	B	423	-	5,5,5	0.85	0	5,5,5	0.94	0
4	EDO	B	410	-	3,3,3	0.57	0	2,2,2	0.15	0
4	EDO	B	412	-	3,3,3	0.49	0	2,2,2	0.56	0
4	EDO	B	419	-	3,3,3	0.33	0	2,2,2	0.79	0
4	EDO	A	418	-	3,3,3	0.80	0	2,2,2	0.35	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
4	EDO	A	422	-	-	1/1/1/1	-
4	EDO	B	404	-	-	0/1/1/1	-
4	EDO	B	411	-	-	1/1/1/1	-
4	EDO	A	416	-	-	1/1/1/1	-
4	EDO	A	411	-	-	1/1/1/1	-
4	EDO	A	407	-	-	1/1/1/1	-
4	EDO	B	414	-	-	1/1/1/1	-
4	EDO	B	418	-	-	0/1/1/1	-
4	EDO	B	420	-	-	1/1/1/1	-
4	EDO	B	422	-	-	1/1/1/1	-
4	EDO	A	405	-	-	1/1/1/1	-
3	PG4	A	403	-	-	2/10/10/10	-
4	EDO	A	410	-	-	0/1/1/1	-
4	EDO	A	413	-	-	1/1/1/1	-
4	EDO	A	408	-	-	1/1/1/1	-
4	EDO	A	412	-	-	1/1/1/1	-
4	EDO	A	421	-	-	1/1/1/1	-
5	GOL	A	424	-	-	3/4/4/4	-
3	PG4	B	403	-	-	5/10/10/10	-
4	EDO	B	407	-	-	0/1/1/1	-
4	EDO	B	413	-	-	0/1/1/1	-
4	EDO	A	404	-	-	1/1/1/1	-
4	EDO	A	419	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	421	-	-	1/1/1/1	-
4	EDO	A	420	-	-	1/1/1/1	-
4	EDO	A	406	-	-	1/1/1/1	-
4	EDO	B	415	-	-	1/1/1/1	-
4	EDO	A	409	-	-	1/1/1/1	-
4	EDO	B	417	-	-	1/1/1/1	-
4	EDO	A	414	-	-	0/1/1/1	-
4	EDO	B	405	-	-	0/1/1/1	-
5	GOL	A	423	-	-	2/4/4/4	-
4	EDO	B	406	-	-	1/1/1/1	-
4	EDO	A	415	-	-	1/1/1/1	-
4	EDO	B	416	-	-	0/1/1/1	-
4	EDO	A	417	-	-	1/1/1/1	-
4	EDO	B	408	-	-	1/1/1/1	-
4	EDO	B	409	-	-	1/1/1/1	-
5	GOL	B	423	-	-	2/4/4/4	-
4	EDO	B	410	-	-	0/1/1/1	-
4	EDO	B	412	-	-	0/1/1/1	-
4	EDO	B	419	-	-	0/1/1/1	-
4	EDO	A	418	-	-	1/1/1/1	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	403	PG4	C5-O3-C4	3.71	129.49	113.26
3	B	403	PG4	O1-C1-C2	-2.99	94.21	111.82
3	B	403	PG4	C3-O2-C2	-2.05	104.29	113.26

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	423	GOL	C1-C2-C3-O3
5	A	423	GOL	O2-C2-C3-O3
5	A	424	GOL	C1-C2-C3-O3
5	B	423	GOL	O1-C1-C2-C3
5	A	424	GOL	O2-C2-C3-O3
3	B	403	PG4	O2-C3-C4-O3
5	A	424	GOL	O1-C1-C2-C3
5	B	423	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	409	EDO	O1-C1-C2-O2
4	A	411	EDO	O1-C1-C2-O2
4	A	415	EDO	O1-C1-C2-O2
4	B	409	EDO	O1-C1-C2-O2
3	A	403	PG4	O3-C5-C6-O4
4	A	404	EDO	O1-C1-C2-O2
4	A	407	EDO	O1-C1-C2-O2
4	A	408	EDO	O1-C1-C2-O2
4	A	412	EDO	O1-C1-C2-O2
4	A	413	EDO	O1-C1-C2-O2
4	A	416	EDO	O1-C1-C2-O2
4	A	417	EDO	O1-C1-C2-O2
4	A	418	EDO	O1-C1-C2-O2
4	A	419	EDO	O1-C1-C2-O2
4	A	420	EDO	O1-C1-C2-O2
4	B	406	EDO	O1-C1-C2-O2
4	B	408	EDO	O1-C1-C2-O2
4	B	421	EDO	O1-C1-C2-O2
4	A	421	EDO	O1-C1-C2-O2
3	B	403	PG4	C4-C3-O2-C2
3	B	403	PG4	C1-C2-O2-C3
4	A	406	EDO	O1-C1-C2-O2
4	B	417	EDO	O1-C1-C2-O2
3	A	403	PG4	C8-C7-O4-C6
4	A	422	EDO	O1-C1-C2-O2
4	B	414	EDO	O1-C1-C2-O2
4	B	415	EDO	O1-C1-C2-O2
4	B	422	EDO	O1-C1-C2-O2
4	B	420	EDO	O1-C1-C2-O2
3	B	403	PG4	C3-C4-O3-C5
4	A	405	EDO	O1-C1-C2-O2
4	B	411	EDO	O1-C1-C2-O2
3	B	403	PG4	O3-C5-C6-O4

There are no ring outliers.

27 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	422	EDO	1	0
4	B	404	EDO	1	0
4	B	411	EDO	1	0
4	A	416	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	411	EDO	1	0
4	A	407	EDO	1	0
4	B	418	EDO	1	0
4	B	422	EDO	1	0
4	A	405	EDO	3	0
3	A	403	PG4	1	0
4	A	410	EDO	1	0
4	A	421	EDO	2	0
5	A	424	GOL	1	0
3	B	403	PG4	6	0
4	B	407	EDO	1	0
4	B	413	EDO	4	0
4	A	420	EDO	2	0
4	B	415	EDO	3	0
4	A	409	EDO	1	0
4	B	417	EDO	2	0
4	A	414	EDO	1	0
4	B	405	EDO	1	0
5	A	423	GOL	2	0
4	B	406	EDO	7	0
4	B	416	EDO	1	0
4	B	409	EDO	1	0
4	B	412	EDO	3	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, 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	306/312 (98%)	-0.30	11 (3%) 46 46	12, 21, 43, 86	6 (1%)
1	B	288/312 (92%)	-0.37	12 (4%) 40 40	8, 20, 43, 57	5 (1%)
All	All	594/624 (95%)	-0.33	23 (3%) 43 43	8, 21, 43, 86	11 (1%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	119	HIS	4.8
1	A	25	THR	4.8
1	A	27	LEU	4.3
1	A	10	TYR	4.0
1	A	211	THR	3.8
1	B	41	GLY	3.7
1	B	28	ALA	3.7
1	A	26	PRO	3.7
1	A	7	PRO	3.5
1	B	211	THR	2.9
1	A	212	LEU	2.9
1	B	7	PRO	2.7
1	B	10	TYR	2.7
1	B	43	GLN	2.6
1	A	140	ARG	2.4
1	A	24	SER	2.4
1	A	210	PRO	2.4
1	B	27	LEU	2.3
1	A	139	GLN	2.2
1	B	210	PRO	2.2
1	B	242	MET	2.1
1	B	42	GLU	2.1
1	B	212	LEU	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($\text{\AA}^2$)	Q<0.9
4	EDO	B	420	4/4	0.50	0.30	60,75,76,77	0
4	EDO	A	418	4/4	0.66	0.30	50,56,59,64	0
4	EDO	B	419	4/4	0.68	0.17	65,66,67,74	0
4	EDO	A	408	4/4	0.76	0.20	52,54,54,57	0
4	EDO	B	414	4/4	0.80	0.20	47,52,56,56	0
4	EDO	B	422	4/4	0.80	0.17	48,50,52,72	0
4	EDO	A	417	4/4	0.81	0.22	43,54,55,56	0
4	EDO	A	421	4/4	0.82	0.20	42,42,42,46	0
4	EDO	B	404	4/4	0.82	0.17	41,42,43,55	0
4	EDO	A	410	4/4	0.83	0.20	43,47,49,60	0
5	GOL	B	423	6/6	0.83	0.14	36,47,52,54	0
4	EDO	A	420	4/4	0.84	0.19	44,47,49,51	0
4	EDO	A	412	4/4	0.84	0.17	57,61,62,66	0
4	EDO	B	409	4/4	0.85	0.22	37,45,49,59	0
5	GOL	A	424	6/6	0.85	0.14	41,44,47,56	0
4	EDO	B	415	4/4	0.85	0.15	49,57,58,59	0
4	EDO	B	408	4/4	0.86	0.21	40,42,46,46	0
4	EDO	A	415	4/4	0.86	0.17	52,52,54,54	0
4	EDO	A	407	4/4	0.86	0.21	42,42,47,48	0
4	EDO	B	407	4/4	0.86	0.13	53,54,55,59	0
4	EDO	B	416	4/4	0.86	0.16	46,47,53,54	0
4	EDO	A	422	4/4	0.87	0.18	52,54,61,67	0
4	EDO	A	411	4/4	0.87	0.20	40,47,49,52	0
4	EDO	B	421	4/4	0.87	0.18	53,56,58,60	0
4	EDO	A	416	4/4	0.87	0.13	51,53,54,56	0
4	EDO	A	409	4/4	0.87	0.23	29,40,45,51	0
4	EDO	B	418	4/4	0.87	0.20	31,41,49,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	A	405	4/4	0.88	0.14	51,53,54,58	0
4	EDO	B	406	4/4	0.89	0.14	47,48,50,50	0
4	EDO	B	411	4/4	0.89	0.13	53,55,55,58	0
4	EDO	A	414	4/4	0.89	0.15	39,43,51,52	0
4	EDO	A	419	4/4	0.89	0.15	39,42,45,50	0
3	PG4	B	403	13/13	0.91	0.11	25,27,33,34	0
5	GOL	A	423	6/6	0.91	0.14	31,50,54,58	0
4	EDO	B	405	4/4	0.92	0.14	42,45,45,49	0
4	EDO	B	412	4/4	0.92	0.15	29,38,44,47	0
4	EDO	B	413	4/4	0.92	0.17	47,50,51,53	0
4	EDO	B	417	4/4	0.92	0.19	39,39,46,50	0
4	EDO	B	410	4/4	0.93	0.14	34,42,45,47	0
2	SO4	B	402	5/5	0.93	0.11	37,39,50,52	0
4	EDO	A	406	4/4	0.93	0.14	31,34,41,42	0
4	EDO	A	413	4/4	0.93	0.14	40,42,45,55	0
4	EDO	A	404	4/4	0.94	0.13	27,37,39,54	0
3	PG4	A	403	13/13	0.95	0.08	24,28,35,36	0
2	SO4	A	402	5/5	0.96	0.12	33,39,44,51	0
2	SO4	A	401	5/5	1.00	0.02	16,16,18,18	0
2	SO4	B	401	5/5	1.00	0.02	14,15,15,16	0

6.5 Other polymers

There are no such residues in this entry.