



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:57 AM UTC

PDB ID : 4O7O / pdb_00004o7o
Title : Crystal structure of Mycobacterium tuberculosis maltose kinase MaK
Authors : Li, J.; Guan, X.T.; Rao, Z.H.
Deposited on : 2013-12-26
Resolution : 2.40 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

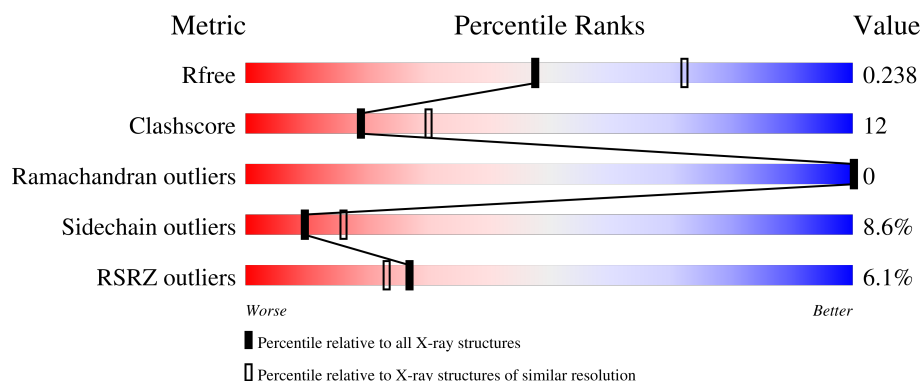
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	455	<div> <div>7%</div> <div>70%</div> <div>22%</div> <div>5%</div> </div>
1	B	455	<div> <div>5%</div> <div>78%</div> <div>20%</div> <div>..</div> </div>

2 Entry composition [i](#)

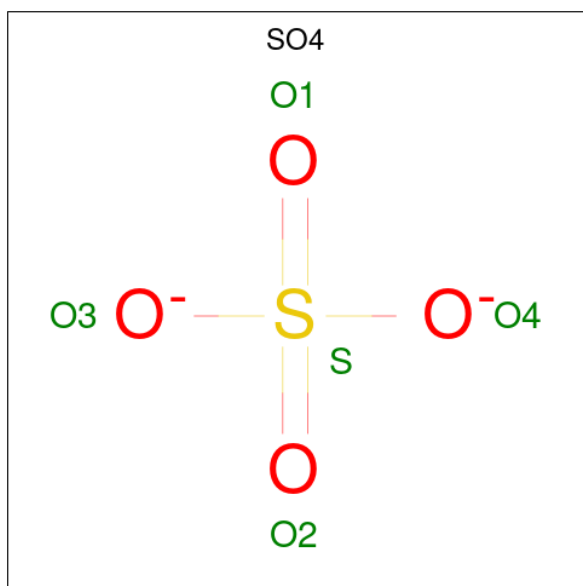
There are 3 unique types of molecules in this entry. The entry contains 6998 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Maltokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	0	0	0
			3349	2114	593	636	6			
1	B	451	Total	C	N	O	S	0	0	0
			3490	2199	618	667	6			

- 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		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	72	Total	O	0	0
			72	72		

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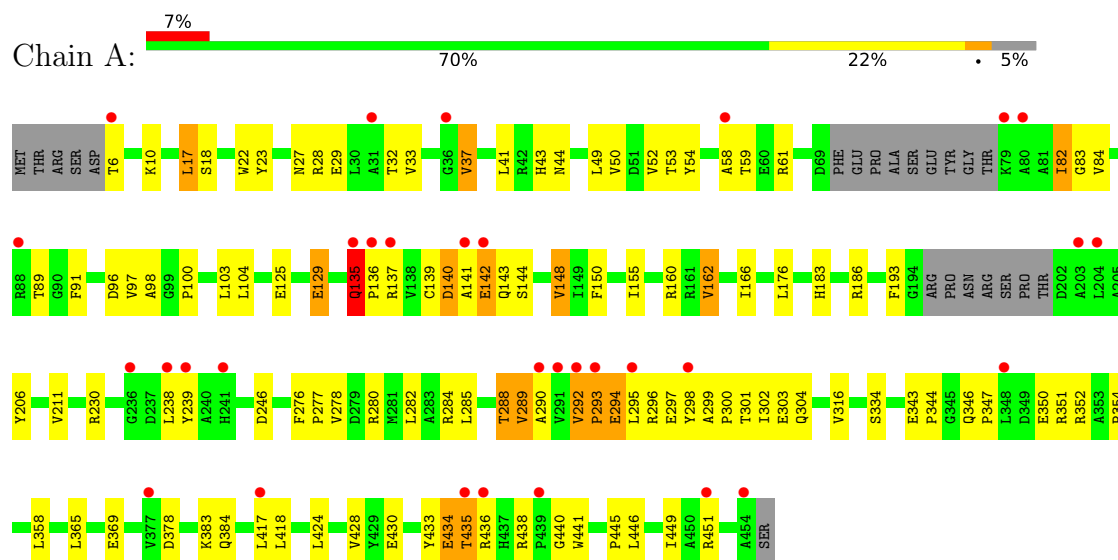
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	82	Total	O	0	0
			82	82		

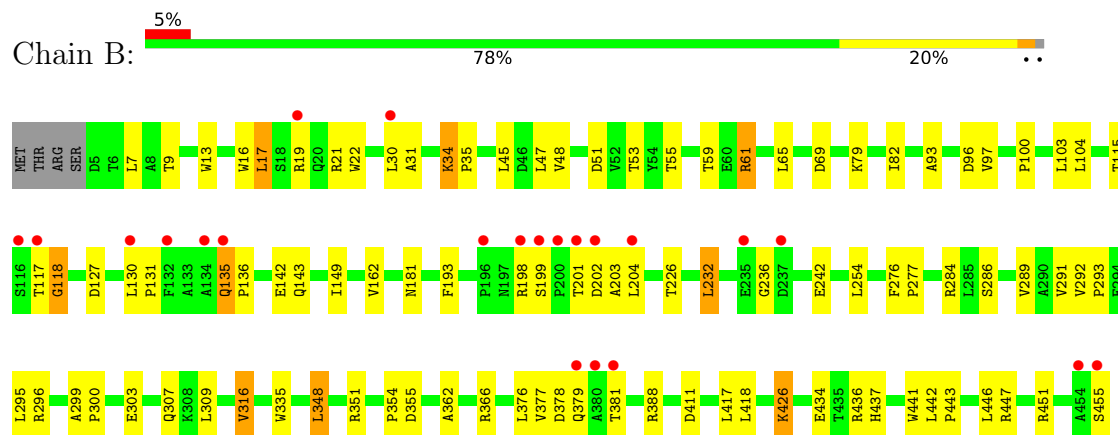
3 Residue-property plots [i](#)

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: Maltokinase



• Molecule 1: Maltokinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	96.61Å 96.61Å 459.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.31 – 2.40 38.31 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.3 (38.31-2.40) 99.9 (38.31-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.56 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.7_650	Depositor
R, R_{free}	0.207 , 0.244 0.204 , 0.238	Depositor DCC
R_{free} test set	2592 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	49.7	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6998	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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	0.57	0/3420	0.92	5/4661 (0.1%)
1	B	0.56	0/3568	0.90	5/4867 (0.1%)
All	All	0.57	0/6988	0.91	10/9528 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
All	All	0	4

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	135	GLN	CA-C-N	11.70	131.28	119.82
1	A	135	GLN	C-N-CA	11.70	131.28	119.82
1	A	383	LYS	N-CA-C	6.44	118.38	111.36
1	B	181	ASN	CA-C-N	5.70	125.80	119.87
1	B	181	ASN	C-N-CA	5.70	125.80	119.87
1	A	334	SER	N-CA-C	5.68	116.89	108.60
1	A	183	HIS	N-CA-C	5.61	119.82	112.92
1	B	118	GLY	N-CA-C	5.36	118.89	110.91
1	B	411	ASP	CA-C-N	5.32	125.38	119.32
1	B	411	ASP	C-N-CA	5.32	125.38	119.32

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	142	GLU	Peptide
1	A	293	PRO	Peptide
1	A	344	PRO	Peptide
1	B	115	THR	Peptide

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	3349	0	3283	99	0
1	B	3490	0	3409	72	0
2	A	5	0	0	0	0
3	A	72	0	0	4	0
3	B	82	0	0	1	0
All	All	6998	0	6692	159	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 12.

All (159) 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:96:ASP:O	1:A:100:PRO:HD3	1.61	1.01
1:B:96:ASP:O	1:B:100:PRO:HD2	1.63	0.96
1:A:238:LEU:HD12	1:A:239:TYR:H	1.29	0.96
1:A:238:LEU:HD12	1:A:239:TYR:N	1.84	0.92
1:A:135:GLN:HE22	1:B:100:PRO:HG2	1.34	0.90
1:A:136:PRO:HD3	1:B:97:VAL:HG22	1.55	0.88
1:B:198:ARG:HG2	1:B:204:LEU:HD13	1.56	0.88
1:A:142:GLU:HA	1:A:143:GLN:C	1.99	0.87
1:A:135:GLN:NE2	1:B:100:PRO:HG2	1.90	0.86
1:A:96:ASP:O	1:A:100:PRO:CD	2.26	0.83
1:A:294:GLU:OE1	1:A:295:LEU:HD12	1.80	0.82
1:B:236:GLY:HA3	1:B:388:ARG:NH1	1.96	0.81
1:A:136:PRO:O	1:A:137:ARG:HG3	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:ASP:OD1	1:A:440:GLY:HA3	1.83	0.77
1:B:293:PRO:HA	1:B:296:ARG:HH21	1.51	0.75
1:A:32:THR:HG22	1:A:53:THR:OG1	1.87	0.74
1:A:82:ILE:HG23	1:A:83:GLY:H	1.54	0.72
1:A:135:GLN:NE2	1:B:100:PRO:CG	2.53	0.71
1:A:129:GLU:OE1	1:B:69:ASP:OD2	2.08	0.71
1:A:294:GLU:OE1	1:A:294:GLU:C	2.36	0.69
1:A:438:ARG:HG2	1:A:441:TRP:CD1	2.28	0.68
1:A:97:VAL:C	1:A:100:PRO:HD2	2.21	0.66
1:B:198:ARG:CG	1:B:204:LEU:CD1	2.75	0.65
1:B:348:LEU:HD13	1:B:351:ARG:NH2	2.12	0.65
1:B:13:TRP:O	1:B:17:LEU:HB2	1.98	0.64
1:B:53:THR:HG23	1:B:59:THR:HG22	1.79	0.64
1:A:37:VAL:HG13	1:A:49:LEU:HB2	1.78	0.64
1:B:13:TRP:CD1	1:B:35:PRO:HG3	2.33	0.64
1:B:198:ARG:CG	1:B:204:LEU:HD13	2.27	0.64
1:A:162:VAL:CG1	1:A:206:TYR:HD1	2.12	0.63
1:B:47:LEU:C	1:B:47:LEU:HD23	2.24	0.63
1:A:277:PRO:HB2	1:A:280:ARG:HG2	1.80	0.63
1:B:198:ARG:HG2	1:B:204:LEU:CD1	2.28	0.63
1:B:201:THR:HG23	1:B:203:ALA:H	1.64	0.62
1:B:303:GLU:O	1:B:307:GLN:HG2	1.99	0.62
1:B:201:THR:O	1:B:202:ASP:HB2	1.99	0.62
1:B:232:LEU:HD13	1:B:388:ARG:HB3	1.82	0.62
1:B:348:LEU:HD13	1:B:351:ARG:HH22	1.65	0.61
1:A:384:GLN:NE2	3:A:655:HOH:O	2.33	0.60
1:B:96:ASP:O	1:B:100:PRO:CD	2.44	0.60
1:B:236:GLY:HA3	1:B:388:ARG:CZ	2.31	0.60
1:B:316:VAL:HG13	1:B:354:PRO:HB2	1.84	0.60
1:A:135:GLN:CD	1:A:136:PRO:HD2	2.28	0.59
1:A:144:SER:HB2	1:B:22:TRP:HB2	1.83	0.59
1:A:282:LEU:HD22	1:A:303:GLU:HG3	1.85	0.59
1:A:293:PRO:HB3	1:A:296:ARG:NH1	2.17	0.59
1:A:346:GLN:HG3	1:A:347:PRO:HD2	1.83	0.59
1:A:293:PRO:O	1:A:294:GLU:C	2.46	0.58
1:A:285:LEU:O	1:A:289:VAL:HG13	2.04	0.57
1:B:65:LEU:CD1	1:B:103:LEU:HD11	2.34	0.57
1:B:434:GLU:OE1	1:B:441:TRP:HB2	2.05	0.57
1:A:435:THR:HG22	1:A:436:ARG:N	2.20	0.57
1:A:141:ALA:O	1:A:144:SER:HA	2.06	0.56
1:A:18:SER:HA	1:A:23:TYR:CD2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ILE:HG23	1:A:83:GLY:N	2.19	0.56
1:B:51:ASP:OD1	1:B:61:ARG:HD2	2.06	0.55
1:A:104:LEU:HD12	1:A:211:VAL:HG21	1.87	0.55
1:B:426:LYS:HG3	3:B:545:HOH:O	2.05	0.55
1:A:433:TYR:O	1:A:434:GLU:C	2.49	0.55
1:B:199:SER:OG	1:B:201:THR:HG22	2.07	0.55
1:A:135:GLN:NE2	1:B:97:VAL:HA	2.21	0.54
1:B:299:ALA:HB3	1:B:300:PRO:HD3	1.88	0.54
1:A:445:PRO:O	1:A:449:ILE:HG12	2.07	0.54
1:A:53:THR:HG22	1:A:59:THR:HG22	1.89	0.54
1:A:316:VAL:CG1	1:A:354:PRO:HB2	2.38	0.53
1:B:198:ARG:O	1:B:199:SER:HB3	2.08	0.53
1:A:434:GLU:O	1:A:435:THR:C	2.51	0.53
1:B:130:LEU:HB3	1:B:131:PRO:HD2	1.90	0.53
1:A:238:LEU:HD12	1:A:239:TYR:CG	2.44	0.52
1:B:34:LYS:O	1:B:34:LYS:HG2	2.09	0.52
1:A:288:THR:HG21	1:A:428:VAL:CG1	2.39	0.52
1:B:376:LEU:HA	1:B:379:GLN:OE1	2.10	0.52
1:A:295:LEU:HD23	1:A:298:TYR:HE2	1.74	0.52
1:B:198:ARG:HG3	1:B:204:LEU:CD1	2.40	0.51
1:A:238:LEU:CD1	1:A:239:TYR:CD1	2.94	0.51
1:B:442:LEU:N	1:B:443:PRO:CD	2.73	0.51
1:A:22:TRP:CG	1:A:160:ARG:HG3	2.45	0.51
1:B:65:LEU:HD11	1:B:103:LEU:HD11	1.92	0.51
1:A:28:ARG:NH1	1:A:54:TYR:CD2	2.80	0.51
1:B:118:GLY:HA3	1:B:193:PHE:CZ	2.46	0.50
1:A:294:GLU:OE1	1:A:295:LEU:CD1	2.57	0.50
1:A:136:PRO:O	1:A:137:ARG:CG	2.57	0.49
1:A:238:LEU:CD1	1:A:239:TYR:CG	2.94	0.49
1:B:441:TRP:C	1:B:443:PRO:HD2	2.38	0.49
1:A:300:PRO:O	1:A:304:GLN:HG2	2.12	0.48
1:B:47:LEU:HD23	1:B:48:VAL:N	2.28	0.48
1:B:135:GLN:O	1:B:136:PRO:C	2.57	0.48
1:A:277:PRO:HB2	1:A:280:ARG:CG	2.43	0.48
1:A:288:THR:HG21	1:A:428:VAL:HG13	1.95	0.48
1:A:28:ARG:HH22	1:A:58:ALA:CB	2.27	0.48
1:A:288:THR:HG22	1:A:289:VAL:N	2.29	0.47
1:A:193:PHE:HB3	1:A:206:TYR:HB2	1.96	0.47
1:A:150:PHE:HZ	1:B:100:PRO:HB2	1.80	0.47
1:A:96:ASP:OD2	1:A:98:ALA:HB3	2.15	0.47
1:A:295:LEU:HD23	1:A:298:TYR:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:PRO:HG2	1:A:350:GLU:HB2	1.96	0.47
1:A:302:ILE:HG23	1:A:424:LEU:HD21	1.97	0.46
1:A:97:VAL:O	1:A:100:PRO:HD2	2.14	0.46
1:A:140:ASP:OD2	1:B:22:TRP:HD1	1.99	0.46
1:A:82:ILE:HG22	1:A:91:PHE:HA	1.98	0.46
1:A:343:GLU:O	1:A:351:ARG:HD3	2.17	0.45
1:A:142:GLU:HA	1:A:144:SER:N	2.31	0.45
1:A:144:SER:HB2	1:B:22:TRP:CB	2.47	0.45
1:A:292:VAL:HG22	1:A:292:VAL:O	2.16	0.45
1:B:377:VAL:O	1:B:378:ASP:C	2.60	0.45
1:A:358:LEU:HD12	1:A:418:LEU:HD23	1.99	0.45
1:B:377:VAL:HG12	1:B:378:ASP:N	2.32	0.44
1:A:17:LEU:HD13	1:A:23:TYR:CD1	2.52	0.44
1:A:186:ARG:HD2	3:A:667:HOH:O	2.18	0.44
1:B:135:GLN:H	1:B:135:GLN:HG2	1.53	0.44
1:B:434:GLU:HB2	1:B:442:LEU:HD12	1.99	0.44
1:A:135:GLN:OE1	1:A:148:VAL:CG2	2.66	0.44
1:B:16:TRP:CD1	1:B:82:ILE:HA	2.52	0.44
1:B:19:ARG:O	1:B:79:LYS:NZ	2.50	0.44
1:B:254:LEU:HD13	1:B:335:TRP:CD2	2.53	0.44
1:A:52:VAL:HG11	1:A:54:TYR:CZ	2.53	0.44
1:A:316:VAL:HG13	1:A:354:PRO:HB2	2.00	0.44
1:B:316:VAL:HG22	1:B:355:ASP:C	2.43	0.44
1:A:27:ASN:C	1:A:28:ARG:HG3	2.43	0.44
1:A:136:PRO:HB2	3:A:647:HOH:O	2.18	0.44
1:B:377:VAL:HG12	1:B:378:ASP:H	1.82	0.44
1:A:434:GLU:H	1:A:434:GLU:HG2	1.56	0.43
1:A:346:GLN:NE2	1:A:350:GLU:HG2	2.34	0.43
1:B:286:SER:O	1:B:289:VAL:HG12	2.17	0.43
1:B:316:VAL:HG22	1:B:355:ASP:CA	2.49	0.43
1:A:135:GLN:NE2	1:B:100:PRO:HG3	2.32	0.43
1:A:155:ILE:HD12	1:B:149:ILE:HG12	2.00	0.43
1:A:162:VAL:HG12	1:A:206:TYR:HD1	1.79	0.43
1:A:430:GLU:O	1:A:434:GLU:HG2	2.18	0.43
1:B:291:VAL:HG23	1:B:292:VAL:HG23	2.00	0.43
1:A:135:GLN:HA	1:A:136:PRO:HD3	1.60	0.43
1:A:96:ASP:OD1	1:A:97:VAL:N	2.52	0.43
1:A:346:GLN:HE21	1:A:350:GLU:HG2	1.83	0.43
1:A:346:GLN:HG3	1:A:347:PRO:CD	2.48	0.42
1:B:362:ALA:O	1:B:366:ARG:HG2	2.19	0.42
1:A:135:GLN:CG	1:A:136:PRO:HD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:THR:HA	1:B:35:PRO:HG2	2.01	0.42
1:A:277:PRO:HB2	1:A:280:ARG:CD	2.49	0.42
1:B:442:LEU:HG	1:B:446:LEU:HD11	2.01	0.42
1:A:297:GLU:O	1:A:300:PRO:HD2	2.20	0.42
1:B:65:LEU:HD13	1:B:103:LEU:HD11	2.02	0.42
1:A:28:ARG:NH1	1:A:54:TYR:CE2	2.88	0.42
1:A:295:LEU:CD2	1:A:298:TYR:HE2	2.33	0.42
1:A:43:HIS:O	1:A:44:ASN:HB2	2.18	0.41
1:A:299:ALA:N	1:A:300:PRO:HD2	2.35	0.41
1:A:288:THR:O	1:A:292:VAL:HG12	2.20	0.41
1:B:198:ARG:HG3	1:B:204:LEU:HD12	2.02	0.41
1:A:276:PHE:CD1	1:A:277:PRO:HD2	2.55	0.41
1:A:166:ILE:O	1:A:352:ARG:HD2	2.20	0.41
1:B:276:PHE:HA	1:B:277:PRO:HD3	1.83	0.41
1:A:49:LEU:HB3	1:A:61:ARG:HD3	2.03	0.41
1:A:84:VAL:HG12	1:A:89:THR:HG23	2.02	0.41
1:B:31:ALA:HB3	1:B:53:THR:O	2.21	0.41
1:B:289:VAL:HG23	1:B:295:LEU:HB3	2.03	0.41
1:A:125:GLU:HG3	3:A:616:HOH:O	2.20	0.41
1:A:290:ALA:HA	1:A:296:ARG:NH2	2.36	0.40
1:B:436:ARG:HB2	1:B:437:HIS:ND1	2.37	0.40
1:B:447:ARG:O	1:B:451:ARG:HG3	2.20	0.40
1:B:93:ALA:O	1:B:100:PRO:HD3	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	427/455 (94%)	407 (95%)	20 (5%)	0	100	100
1	B	449/455 (99%)	434 (97%)	15 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	876/910 (96%)	841 (96%)	35 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	342/362 (94%)	309 (90%)	33 (10%)	8	12
1	B	358/362 (99%)	331 (92%)	27 (8%)	12	21
All	All	700/724 (97%)	640 (91%)	60 (9%)	10	16

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	10	LYS
1	A	17	LEU
1	A	29	GLU
1	A	33	VAL
1	A	37	VAL
1	A	41	LEU
1	A	50	VAL
1	A	82	ILE
1	A	103	LEU
1	A	129	GLU
1	A	135	GLN
1	A	139	CYS
1	A	140	ASP
1	A	148	VAL
1	A	162	VAL
1	A	176	LEU
1	A	230	ARG
1	A	246	ASP
1	A	278	VAL

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Mol	Chain	Res	Type
1	A	284	ARG
1	A	288	THR
1	A	289	VAL
1	A	292	VAL
1	A	294	GLU
1	A	301	THR
1	A	365	LEU
1	A	369	GLU
1	A	417	LEU
1	A	434	GLU
1	A	435	THR
1	A	446	LEU
1	A	451	ARG
1	B	7	LEU
1	B	17	LEU
1	B	21	ARG
1	B	30	LEU
1	B	34	LYS
1	B	45	LEU
1	B	55	THR
1	B	61	ARG
1	B	104	LEU
1	B	117	THR
1	B	127	ASP
1	B	135	GLN
1	B	142	GLU
1	B	143	GLN
1	B	162	VAL
1	B	226	THR
1	B	232	LEU
1	B	242	GLU
1	B	284	ARG
1	B	309	LEU
1	B	316	VAL
1	B	348	LEU
1	B	381	THR
1	B	417	LEU
1	B	418	LEU
1	B	426	LYS
1	B	455	SER

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	135	GLN
1	A	273	GLN
1	B	43	HIS
1	B	63	GLN
1	B	305	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	A	501	-	4,4,4	0.32	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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	433/455 (95%)	0.28	32 (7%) 20 17	30, 61, 117, 154	0
1	B	451/455 (99%)	0.08	22 (4%) 35 31	28, 56, 113, 159	0
All	All	884/910 (97%)	0.18	54 (6%) 27 23	28, 58, 115, 159	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	136	PRO	6.8
1	A	204	LEU	5.4
1	B	200	PRO	5.0
1	B	130	LEU	4.9
1	A	454	ALA	4.3
1	A	239	TYR	4.1
1	A	291	VAL	4.1
1	A	6	THR	3.9
1	A	135	GLN	3.9
1	A	80	ALA	3.8
1	B	204	LEU	3.7
1	A	298	TYR	3.6
1	A	377	VAL	3.6
1	B	454	ALA	3.5
1	A	141	ALA	3.5
1	B	380	ALA	3.4
1	A	238	LEU	3.4
1	A	79	LYS	3.4
1	A	203	ALA	3.3
1	B	201	THR	3.2
1	B	132	PHE	3.2
1	A	295	LEU	3.1
1	B	199	SER	3.1
1	B	116	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	117	THR	2.9
1	A	137	ARG	2.9
1	A	293	PRO	2.9
1	B	455	SER	2.9
1	B	379	GLN	2.9
1	A	36	GLY	2.9
1	A	451	ARG	2.8
1	B	196	PRO	2.8
1	B	134	ALA	2.8
1	B	381	THR	2.8
1	B	30	LEU	2.7
1	A	31	ALA	2.7
1	A	241	HIS	2.7
1	A	439	PRO	2.5
1	A	236	GLY	2.5
1	A	436	ARG	2.3
1	A	88	ARG	2.3
1	B	237	ASP	2.3
1	A	292	VAL	2.3
1	A	348	LEU	2.2
1	B	235	GLU	2.2
1	A	290	ALA	2.2
1	A	417	LEU	2.2
1	A	58	ALA	2.1
1	B	19	ARG	2.1
1	B	198	ARG	2.1
1	A	142	GLU	2.1
1	B	202	ASP	2.1
1	A	435	THR	2.0
1	B	135	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

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	A	501	5/5	0.94	0.12	70,72,80,82	0

6.5 Other polymers

There are no such residues in this entry.