



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:48 AM UTC

PDB ID : 5X3E / pdb_00005x3e
Title : kinesin 6
Authors : Chen, Z.; Guan, R.; Zhang, L.
Deposited on : 2017-02-04
Resolution : 2.61 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

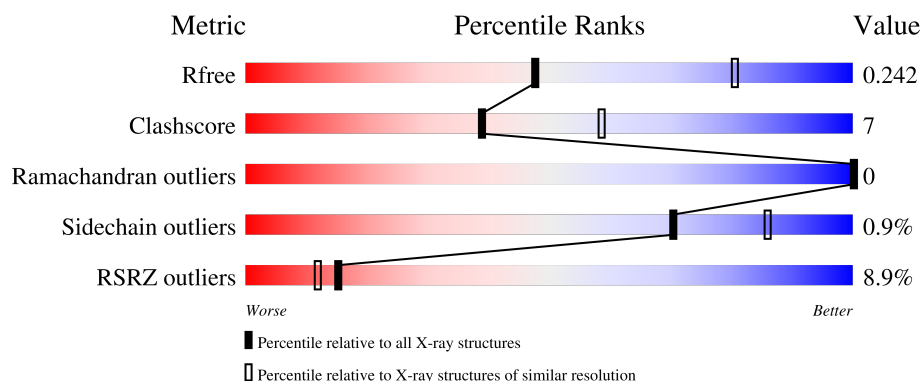
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	449	8% 69% 14% 16%
1	B	449	6% 67% 13% 20%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6159 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 Kinesin-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	1	0
			2972	1852	516	584	20			
1	B	358	Total	C	N	O	S	0	1	0
			2842	1774	490	558	20			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP G5EG83
A	-6	HIS	-	expression tag	UNP G5EG83
A	-5	MET	-	expression tag	UNP G5EG83
A	-4	GLY	-	expression tag	UNP G5EG83
A	-3	SER	-	expression tag	UNP G5EG83
A	-2	SER	-	expression tag	UNP G5EG83
A	-1	GLY	-	expression tag	UNP G5EG83
A	0	GLY	-	expression tag	UNP G5EG83
B	-7	GLY	-	expression tag	UNP G5EG83
B	-6	HIS	-	expression tag	UNP G5EG83
B	-5	MET	-	expression tag	UNP G5EG83
B	-4	GLY	-	expression tag	UNP G5EG83
B	-3	SER	-	expression tag	UNP G5EG83
B	-2	SER	-	expression tag	UNP G5EG83
B	-1	GLY	-	expression tag	UNP G5EG83
B	0	GLY	-	expression tag	UNP G5EG83

- 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	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
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	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
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		
2	B	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		
2	B	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		
2	B	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		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	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 IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	I	0	0
			4	4		
3	B	3	Total	I	0	0
			3	3		

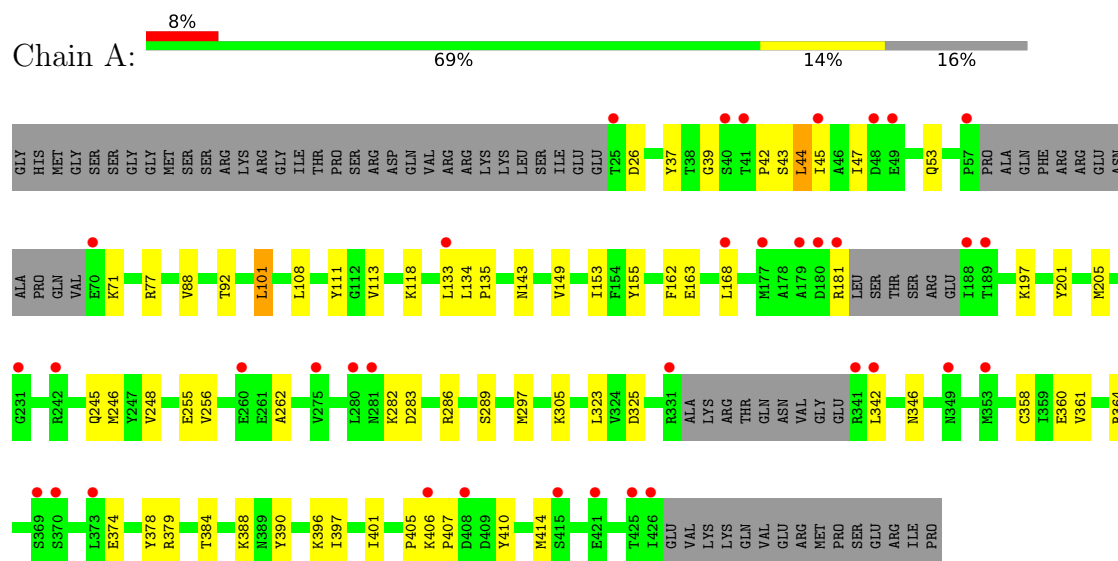
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	63	Total	O	0	0
			63	63		
4	B	85	Total	O	0	0
			85	85		

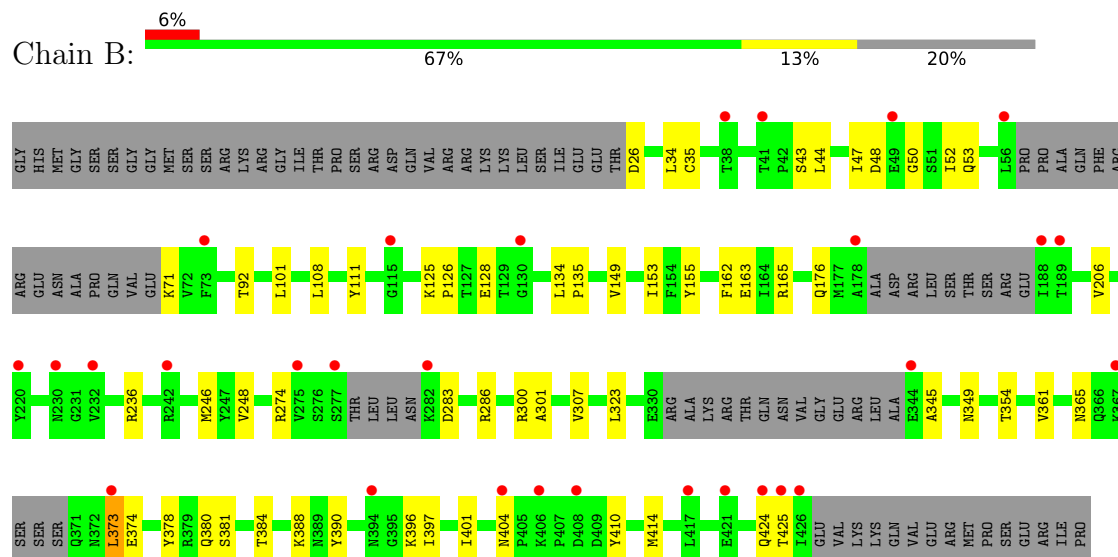
3 Residue-property plots [i](#)

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: Kinesin-like protein



• Molecule 1: Kinesin-like protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, α , β , γ	244.15Å 244.15Å 42.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.84 – 2.61 31.84 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.5 (31.84-2.61) 99.5 (31.84-2.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.209 , 0.240 0.211 , 0.242	Depositor DCC
R_{free} test set	2000 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å ²)	56.2	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 63.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.012 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6159	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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: IOD, 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	0.20	0/3016	0.44	0/4071
1	B	0.20	0/2880	0.43	0/3884
All	All	0.20	0/5896	0.43	0/7955

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	424	GLN	Peptide

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	2972	0	2958	42	0
1	B	2842	0	2817	37	0
2	A	95	0	0	6	0
2	B	95	0	0	7	0
3	A	4	0	0	0	0
3	B	3	0	0	0	0
4	A	63	0	0	2	1
4	B	85	0	0	3	1
All	All	6159	0	5775	80	1

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 (80) 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:B:246:MET:HE3	1:B:388:LYS:HD3	1.60	0.83
1:A:71:LYS:HD2	1:A:414:MET:HE1	1.65	0.77
1:A:246:MET:HE3	1:A:388:LYS:HD3	1.69	0.74
1:B:176:GLN:NE2	4:B:603:HOH:O	2.20	0.73
1:A:282:LYS:O	4:A:601:HOH:O	2.06	0.71
1:B:47:ILE:HD11	1:B:53:GLN:HB2	1.72	0.71
1:A:47:ILE:HD11	1:A:53:GLN:HB2	1.74	0.69
1:B:26:ASP:HB2	1:B:396:LYS:HD3	1.73	0.69
1:B:361:VAL:O	1:B:365:ASN:ND2	2.26	0.68
1:A:26:ASP:HB2	1:A:396:LYS:HD3	1.75	0.67
1:B:71:LYS:HD2	1:B:414:MET:HE1	1.76	0.67
1:A:305:LYS:HG2	2:A:502:SO4:O1	1.97	0.64
1:A:245:GLN:NE2	2:A:517:SO4:O1	2.33	0.61
1:A:379:ARG:NH1	2:A:511:SO4:O3	2.36	0.58
1:B:236:ARG:NH2	2:B:516:SO4:O4	2.29	0.57
1:B:155:TYR:CZ	1:B:163:GLU:HB2	2.39	0.56
2:B:508:SO4:O2	4:B:601:HOH:O	2.17	0.56
1:B:108:LEU:HB3	1:B:323:LEU:HD23	1.88	0.55
1:A:77:ARG:NH1	2:A:515:SO4:O1	2.39	0.55
1:A:181:ARG:NH2	1:A:255:GLU:O	2.37	0.55
1:B:381:SER:OG	1:B:384:THR:HG22	2.07	0.55
1:B:165:ARG:NH2	2:B:517:SO4:O4	2.34	0.54
1:A:92:THR:CG2	1:A:108:LEU:HD11	2.38	0.54
1:B:274:ARG:NH1	2:B:519:SO4:S	2.70	0.54
1:B:301:ALA:O	4:B:602:HOH:O	2.18	0.53
1:A:205:MET:HE3	1:A:297:MET:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:TYR:O	1:B:384:THR:HG23	2.09	0.52
1:A:248:VAL:N	2:A:501:SO4:O3	2.30	0.52
1:B:373:LEU:H	1:B:373:LEU:HD13	1.74	0.51
1:B:283:ASP:H	1:B:286:ARG:HD3	1.75	0.51
1:A:43:SER:HB3	1:A:407:PRO:HA	1.93	0.50
1:A:155:TYR:CZ	1:A:163:GLU:HB2	2.47	0.50
1:B:365:ASN:OD1	1:B:373:LEU:HB2	2.12	0.50
1:A:342:LEU:O	1:A:346:ASN:ND2	2.45	0.50
1:A:88:VAL:HG12	1:A:133:LEU:HD21	1.93	0.49
1:B:128:GLU:N	2:B:513:SO4:O2	2.45	0.49
1:B:248:VAL:N	2:B:501:SO4:O2	2.21	0.48
1:A:37:TYR:CE1	1:A:406:LYS:HG3	2.48	0.48
1:B:134:LEU:HB3	1:B:135:PRO:HD3	1.95	0.48
1:A:42:PRO:HG3	1:A:45:ILE:HD11	1.96	0.48
1:A:358:CYS:SG	1:A:384:THR:HG21	2.54	0.48
1:A:378:TYR:CZ	1:A:388:LYS:HD2	2.49	0.48
1:A:118:LYS:HB2	1:A:118:LYS:HE3	1.76	0.48
1:A:162:PHE:N	2:A:505:SO4:O3	2.45	0.48
1:A:390:TYR:HB3	1:A:397:ILE:HD11	1.95	0.47
1:A:113:VAL:HG23	4:A:625:HOH:O	2.14	0.47
1:A:283:ASP:H	1:A:286:ARG:HD3	1.80	0.47
1:B:125:LYS:HG2	1:B:126:PRO:HD2	1.96	0.47
1:A:92:THR:HG22	1:A:108:LEU:HD11	1.97	0.46
1:A:289:SER:OG	1:A:325:ASP:HB3	2.15	0.46
1:A:256:VAL:HG11	1:A:262:ALA:HA	1.97	0.46
1:A:134:LEU:HB3	1:A:135:PRO:HD3	1.98	0.45
1:A:111:TYR:HB3	1:A:401:ILE:HD13	1.97	0.45
1:A:361:VAL:HG13	1:A:374:GLU:HG3	1.98	0.45
1:B:134:LEU:HD23	1:B:323:LEU:HD12	1.97	0.45
1:B:345:ALA:O	1:B:349:ASN:ND2	2.50	0.45
1:A:43:SER:HB2	1:A:410:TYR:HD1	1.81	0.45
1:B:48:ASP:C	1:B:50:GLY:H	2.23	0.45
1:B:149:VAL:HB	1:B:153:ILE:HD12	1.99	0.45
1:A:364:ARG:HD2	1:A:374:GLU:OE2	2.18	0.44
1:A:149:VAL:HB	1:A:153:ILE:HD12	1.99	0.44
1:B:390:TYR:HB3	1:B:397:ILE:HD11	2.00	0.44
1:A:143:ASN:HB3	1:A:197:LYS:HG2	1.99	0.43
1:B:354:THR:HG21	1:B:380:GLN:HB2	2.00	0.43
1:A:108:LEU:HB3	1:A:323:LEU:HD23	2.00	0.43
1:A:406:LYS:HG2	1:A:407:PRO:HD2	2.01	0.43
1:A:37:TYR:CZ	1:A:39:GLY:HA3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:CYS:SG	1:B:404:ASN:HA	2.60	0.42
1:B:206:VAL:HG23	1:B:300:ARG:HB2	2.02	0.42
1:A:360:GLU:O	1:A:364:ARG:HG3	2.20	0.42
1:B:43:SER:HB2	1:B:410:TYR:HD1	1.84	0.42
1:A:101:LEU:HD12	1:A:201:TYR:HD2	1.85	0.41
1:B:71:LYS:HA	1:B:425:THR:O	2.21	0.41
1:B:111:TYR:HB3	1:B:401:ILE:HD13	2.02	0.41
1:B:162:PHE:N	2:B:502:SO4:O3	2.52	0.41
1:B:361:VAL:HG13	1:B:374:GLU:HG3	2.02	0.41
1:B:92:THR:HG23	1:B:108:LEU:HD21	2.03	0.41
1:B:34:LEU:HD11	1:B:52:ILE:HD11	2.02	0.40
1:B:149:VAL:HG12	1:B:307:VAL:O	2.22	0.40
1:A:44:LEU:HD13	1:A:405:PRO:HA	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:614:HOH:O	4:B:602:HOH:O[6_575]	2.12	0.08

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	368/449 (82%)	358 (97%)	10 (3%)	0	100	100
1	B	347/449 (77%)	340 (98%)	7 (2%)	0	100	100
All	All	715/898 (80%)	698 (98%)	17 (2%)	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	339/403 (84%)	336 (99%)	3 (1%)	70	86
1	B	324/403 (80%)	321 (99%)	3 (1%)	70	86
All	All	663/806 (82%)	657 (99%)	6 (1%)	70	86

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	101	LEU
1	A	168	LEU
1	B	44	LEU
1	B	101	LEU
1	B	373	LEU

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

Mol	Chain	Res	Type
1	A	243	GLN
1	A	245	GLN
1	A	375	GLN
1	B	146	ASN
1	B	365	ASN
1	B	375	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

Of 45 ligands modelled in this entry, 7 are monoatomic - leaving 38 for Mogul analysis.

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	502	-	4,4,4	0.23	0	6,6,6	0.30	0
2	SO4	A	505	-	4,4,4	0.23	0	6,6,6	0.13	0
2	SO4	A	509	-	4,4,4	0.25	0	6,6,6	0.11	0
2	SO4	B	512	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	B	504	-	4,4,4	0.26	0	6,6,6	0.09	0
2	SO4	B	517	-	4,4,4	0.23	0	6,6,6	0.10	0
2	SO4	B	518	-	4,4,4	0.22	0	6,6,6	0.08	0
2	SO4	A	512	-	4,4,4	0.27	0	6,6,6	0.14	0
2	SO4	B	501	-	4,4,4	0.19	0	6,6,6	0.18	0
2	SO4	A	510	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	B	511	-	4,4,4	0.24	0	6,6,6	0.10	0
2	SO4	B	507	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	A	514	-	4,4,4	0.25	0	6,6,6	0.13	0
2	SO4	B	519	-	4,4,4	0.25	0	6,6,6	0.07	0
2	SO4	B	508	-	4,4,4	0.23	0	6,6,6	0.06	0
2	SO4	B	515	-	4,4,4	0.24	0	6,6,6	0.10	0
2	SO4	A	504	-	4,4,4	0.22	0	6,6,6	0.18	0
2	SO4	A	516	-	4,4,4	0.24	0	6,6,6	0.04	0
2	SO4	A	517	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	B	510	-	4,4,4	0.23	0	6,6,6	0.06	0
2	SO4	A	513	-	4,4,4	0.26	0	6,6,6	0.04	0
2	SO4	B	513	-	4,4,4	0.24	0	6,6,6	0.10	0
2	SO4	A	508	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	A	501	-	4,4,4	0.28	0	6,6,6	0.09	0
2	SO4	B	509	-	4,4,4	0.23	0	6,6,6	0.11	0
2	SO4	A	511	-	4,4,4	0.25	0	6,6,6	0.14	0
2	SO4	B	516	-	4,4,4	0.23	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	518	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	A	507	-	4,4,4	0.22	0	6,6,6	0.12	0
2	SO4	B	514	-	4,4,4	0.24	0	6,6,6	0.10	0
2	SO4	A	519	-	4,4,4	0.24	0	6,6,6	0.06	0
2	SO4	B	502	-	4,4,4	0.23	0	6,6,6	0.14	0
2	SO4	A	503	-	4,4,4	0.24	0	6,6,6	0.06	0
2	SO4	A	506	-	4,4,4	0.24	0	6,6,6	0.10	0
2	SO4	A	515	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	B	506	-	4,4,4	0.25	0	6,6,6	0.07	0
2	SO4	B	503	-	4,4,4	0.24	0	6,6,6	0.05	0
2	SO4	B	505	-	4,4,4	0.24	0	6,6,6	0.11	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.

13 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	502	SO4	1	0
2	A	505	SO4	1	0
2	B	517	SO4	1	0
2	B	501	SO4	1	0
2	B	519	SO4	1	0
2	B	508	SO4	1	0
2	A	517	SO4	1	0
2	B	513	SO4	1	0
2	A	501	SO4	1	0
2	A	511	SO4	1	0
2	B	516	SO4	1	0
2	B	502	SO4	1	0
2	A	515	SO4	1	0

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	375/449 (83%)	0.53	36 (9%) 13 10	39, 68, 124, 140	1 (0%)
1	B	358/449 (79%)	0.54	29 (8%) 18 14	23, 72, 130, 146	1 (0%)
All	All	733/898 (81%)	0.53	65 (8%) 15 12	23, 69, 128, 146	2 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	426	ILE	6.6
1	B	188	ILE	6.3
1	A	342	LEU	5.9
1	B	56	LEU	5.7
1	B	178	ALA	4.9
1	A	188	ILE	4.6
1	A	426	ILE	4.5
1	B	406	LYS	4.4
1	A	168	LEU	4.1
1	B	275	VAL	3.9
1	A	40	SER	3.7
1	B	282	LYS	3.6
1	B	408	ASP	3.5
1	B	425	THR	3.5
1	B	230	ASN	3.3
1	B	367	LYS	3.3
1	A	49	GLU	3.3
1	A	189	THR	3.2
1	A	57	PRO	3.2
1	A	280	LEU	3.1
1	A	25	THR	3.1
1	B	242	ARG	3.0
1	B	73	PHE	3.0
1	B	421	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	181	ARG	2.9
1	A	406	LYS	2.9
1	A	369	SER	2.9
1	A	425	THR	2.9
1	B	49	GLU	2.9
1	B	41	THR	2.9
1	B	38	THR	2.8
1	B	373	LEU	2.8
1	A	177[A]	MET	2.8
1	B	344	GLU	2.8
1	A	275	VAL	2.7
1	A	242	ARG	2.7
1	A	331	ARG	2.7
1	A	260	GLU	2.7
1	B	277	SER	2.7
1	A	70	GLU	2.6
1	A	179	ALA	2.6
1	A	408	ASP	2.6
1	B	424	GLN	2.5
1	B	220	TYR	2.5
1	B	115	GLY	2.5
1	A	370	SER	2.5
1	A	281	ASN	2.4
1	B	417	LEU	2.4
1	A	180	ASP	2.4
1	A	341	ARG	2.4
1	A	421	GLU	2.4
1	A	41	THR	2.4
1	A	48	ASP	2.3
1	A	133	LEU	2.3
1	A	373	LEU	2.3
1	B	404	ASN	2.3
1	A	231	GLY	2.3
1	B	232	VAL	2.3
1	B	130	GLY	2.2
1	B	189	THR	2.1
1	A	45	ILE	2.1
1	A	415	SER	2.1
1	A	353	MET	2.1
1	A	349	ASN	2.0
1	B	394	ASN	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
2	SO4	B	514	5/5	0.67	0.18	136,138,146,153	0
2	SO4	B	518	5/5	0.67	0.15	143,148,152,159	0
2	SO4	A	513	5/5	0.70	0.23	148,155,159,164	0
2	SO4	B	516	5/5	0.72	0.10	159,166,169,170	0
2	SO4	A	517	5/5	0.72	0.15	173,174,175,176	0
2	SO4	B	507	5/5	0.73	0.17	127,130,137,144	0
2	SO4	A	515	5/5	0.73	0.14	113,127,138,140	0
3	IOD	B	522	1/1	0.73	0.26	254,254,254,254	0
2	SO4	A	511	5/5	0.75	0.19	99,104,132,141	0
2	SO4	B	515	5/5	0.76	0.14	119,132,137,143	0
2	SO4	B	513	5/5	0.77	0.14	146,147,149,154	0
2	SO4	B	512	5/5	0.78	0.12	129,133,136,138	0
2	SO4	B	508	5/5	0.79	0.17	113,128,130,136	0
3	IOD	A	523	1/1	0.79	0.28	251,251,251,251	0
2	SO4	A	516	5/5	0.79	0.17	131,136,151,156	0
2	SO4	B	519	5/5	0.81	0.12	108,116,124,136	0
2	SO4	A	509	5/5	0.82	0.13	95,117,118,123	0
2	SO4	B	517	5/5	0.83	0.14	144,148,153,160	0
2	SO4	B	510	5/5	0.85	0.18	83,100,114,117	0
2	SO4	B	511	5/5	0.85	0.14	121,124,133,135	0
2	SO4	A	519	5/5	0.85	0.17	101,132,139,140	0
2	SO4	A	512	5/5	0.86	0.27	51,109,125,125	0
2	SO4	A	507	5/5	0.86	0.15	101,116,119,132	0
3	IOD	B	521	1/1	0.87	0.25	165,165,165,165	0
2	SO4	A	518	5/5	0.87	0.10	118,122,133,134	0
2	SO4	A	514	5/5	0.88	0.26	86,102,114,122	0
2	SO4	B	509	5/5	0.89	0.14	77,97,110,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	510	5/5	0.89	0.20	87,88,90,112	0
3	IOD	A	522	1/1	0.90	0.26	168,168,168,168	0
2	SO4	B	506	5/5	0.91	0.11	109,119,126,127	0
2	SO4	B	504	5/5	0.92	0.18	60,85,107,116	0
2	SO4	B	505	5/5	0.93	0.21	82,95,103,111	0
2	SO4	B	503	5/5	0.93	0.12	61,90,100,105	0
2	SO4	A	508	5/5	0.93	0.17	76,94,102,107	0
3	IOD	A	521	1/1	0.93	0.18	171,171,171,171	0
2	SO4	B	501	5/5	0.94	0.18	67,72,81,91	0
2	SO4	B	502	5/5	0.94	0.22	54,54,85,90	0
2	SO4	A	503	5/5	0.95	0.11	58,59,79,94	0
2	SO4	A	504	5/5	0.95	0.12	45,66,90,93	0
2	SO4	A	505	5/5	0.95	0.15	39,50,101,103	0
2	SO4	A	501	5/5	0.95	0.25	47,54,86,87	0
3	IOD	B	520	1/1	0.97	0.05	69,69,69,69	0
2	SO4	A	506	5/5	0.97	0.10	58,70,89,91	0
2	SO4	A	502	5/5	0.97	0.10	42,46,71,85	0
3	IOD	A	520	1/1	0.99	0.04	66,66,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.