Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 10:14 PM BST

PDB ID	:	5X3E
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 following versions of software and data (see references ⓘ) were used in the production of this report:

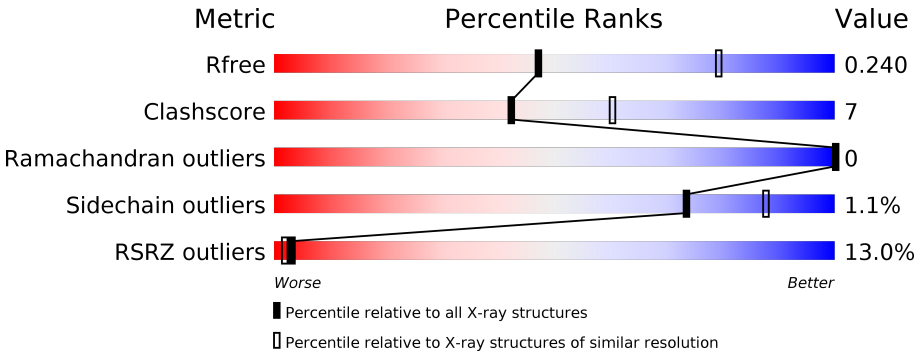
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	449	10% 68% 15% 16%
1	B	449	11% 67% 12% 20%

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
2	SO4	A	517	-	-	-	X
2	SO4	B	516	-	-	-	X
2	SO4	B	517	-	-	-	X
3	IOD	A	523	-	-	-	X

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.

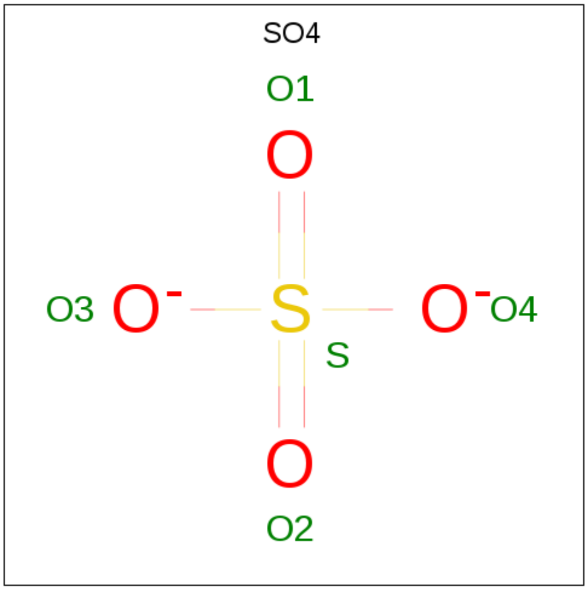
- Molecule 1 is a protein called Kinesin-like protein.

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 (three-letter code: SO4) (formula: O_4S).



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

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

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

- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

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

- Molecule 4 is water.

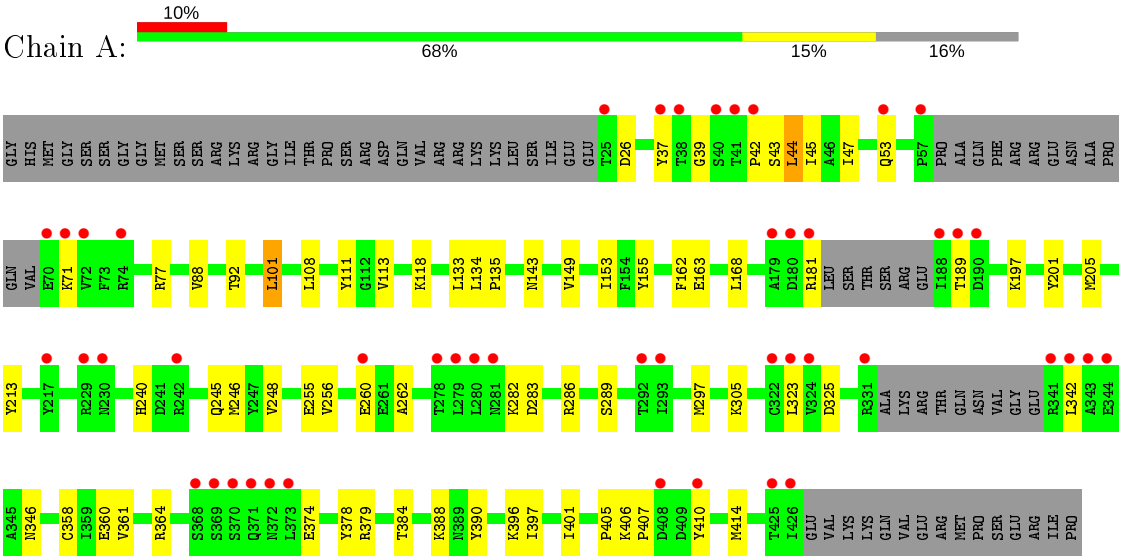
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	63	Total O 63 63	0	0
4	B	85	Total O 85 85	0	0

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.

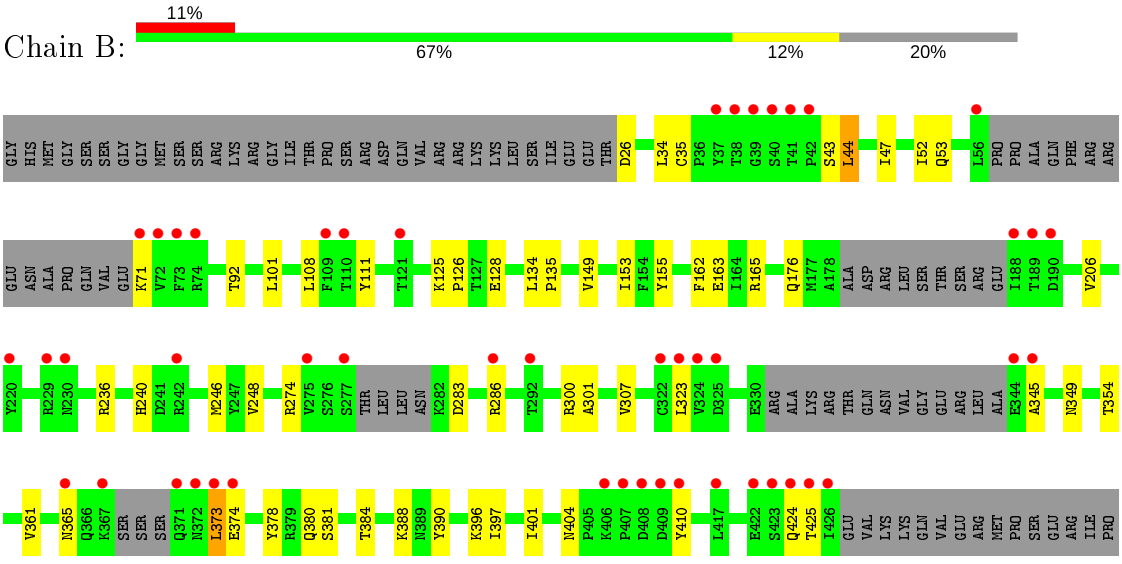
- Molecule 1: Kinesin-like protein

Chain A:



- Molecule 1: Kinesin-like protein

Chain B:



4 Data and refinement statistics (i)

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 31.85 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.5 (31.84-2.61) 99.5 (31.85-2.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.209 , 0.240 0.210 , 0.240	Depositor DCC
R_{free} test set	1999 reflections (4.49%)	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 , 63.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.31	0/3016	0.50	0/4071
1	B	0.31	0/2880	0.51	1/3884 (0.0%)
All	All	0.31	0/5896	0.50	1/7955 (0.0%)

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.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	44	LEU	CA-CB-CG	5.41	127.75	115.30

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

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	44	0
1	B	2842	0	2817	36	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	81	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 (81) 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: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:A:305:LYS:HG2	2:A:502:SO4:O1	1.97	0.64
1:B:246:MET:HE3	1:B:388:LYS:HD3	1.80	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:A:240:HIS:HB3	1:A:246:MET:HE2	1.90	0.54
1:B:240:HIS:HB3	1:B:246:MET:HE2	1.89	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

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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:A:71:LYS:HD2	1:A:414:MET:HE1	1.93	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:A:205:MET:HE3	1:A:297:MET:HB3	1.94	0.48
1:B:134:LEU:HB3	1:B:135:PRO:HD3	1.95	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:42:PRO:HG3	1:A:45:ILE:HD11	1.96	0.48
1:A:118:LYS:HE3	1:A:118:LYS:HB2	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: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:246:MET:HE3	1:A:388:LYS:HD3	2.00	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:189:THR:OG1	1:A:260:GLU:OE2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	335 (99%)	4 (1%)	71	86
1	B	324/403 (80%)	321 (99%)	3 (1%)	78	90
All	All	663/806 (82%)	656 (99%)	7 (1%)	73	88

All (7) 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	A	213	TYR
1	B	44	LEU
1	B	101	LEU
1	B	373	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	511	-	4,4,4	0.15	0	6,6,6	0.12	0
2	SO4	A	502	-	4,4,4	0.19	0	6,6,6	0.32	0
2	SO4	B	511	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	A	517	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	507	-	4,4,4	0.12	0	6,6,6	0.11	0
2	SO4	B	509	-	4,4,4	0.13	0	6,6,6	0.09	0
2	SO4	A	508	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	B	517	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	A	509	-	4,4,4	0.15	0	6,6,6	0.08	0
2	SO4	B	507	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	A	503	-	4,4,4	0.15	0	6,6,6	0.07	0
2	SO4	B	514	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	B	513	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	A	504	-	4,4,4	0.13	0	6,6,6	0.15	0
2	SO4	B	515	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	B	505	-	4,4,4	0.15	0	6,6,6	0.09	0
2	SO4	A	505	-	4,4,4	0.14	0	6,6,6	0.14	0
2	SO4	B	516	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	A	501	-	4,4,4	0.19	0	6,6,6	0.08	0
2	SO4	B	518	-	4,4,4	0.12	0	6,6,6	0.08	0
2	SO4	A	506	-	4,4,4	0.16	0	6,6,6	0.07	0
2	SO4	A	515	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	B	519	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	B	506	-	4,4,4	0.15	0	6,6,6	0.07	0
2	SO4	A	510	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	A	518	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	B	510	-	4,4,4	0.13	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	514	-	4,4,4	0.15	0	6,6,6	0.10	0
2	SO4	A	519	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	B	503	-	4,4,4	0.15	0	6,6,6	0.09	0
2	SO4	B	504	-	4,4,4	0.15	0	6,6,6	0.11	0
2	SO4	A	513	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	B	502	-	4,4,4	0.14	0	6,6,6	0.16	0
2	SO4	B	508	-	4,4,4	0.13	0	6,6,6	0.07	0
2	SO4	B	512	-	4,4,4	0.13	0	6,6,6	0.07	0
2	SO4	A	512	-	4,4,4	0.16	0	6,6,6	0.18	0
2	SO4	B	501	-	4,4,4	0.11	0	6,6,6	0.19	0
2	SO4	A	516	-	4,4,4	0.14	0	6,6,6	0.05	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	511	SO4	1	0
2	A	502	SO4	1	0
2	A	517	SO4	1	0
2	B	517	SO4	1	0
2	B	513	SO4	1	0
2	A	505	SO4	1	0
2	B	516	SO4	1	0
2	A	501	SO4	1	0
2	A	515	SO4	1	0
2	B	519	SO4	1	0
2	B	502	SO4	1	0
2	B	508	SO4	1	0
2	B	501	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, 95^{th} 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%)	0.48	47 (12%)	3	2	39, 68, 125, 140	0
1	B	358/449 (79%)	0.50	48 (13%)	3	2	36, 72, 130, 146	0
All	All	733/898 (81%)	0.49	95 (12%)	3	2	36, 70, 128, 146	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	188	ILE	12.9
1	A	370	SER	7.7
1	A	188	ILE	7.4
1	B	373	LEU	7.2
1	B	230	ASN	7.1
1	A	368	SER	6.1
1	A	342	LEU	5.8
1	B	41	THR	5.6
1	B	408	ASP	5.5
1	A	373	LEU	5.3
1	A	40	SER	5.3
1	B	425	THR	5.1
1	A	189	THR	5.1
1	A	70	GLU	5.1
1	B	38	THR	5.0
1	B	426	ILE	4.7
1	A	372	ASN	4.7
1	A	71	LYS	4.7
1	B	190	ASP	4.6
1	A	425	THR	4.6
1	A	281	ASN	4.6
1	A	280	LEU	4.6
1	A	426	ILE	4.5
1	A	331	ARG	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	73	PHE	4.3
1	B	71	LYS	4.3
1	A	369	SER	4.2
1	A	278	THR	4.1
1	B	372	ASN	4.1
1	B	189	THR	4.1
1	A	179	ALA	4.0
1	A	292	THR	3.9
1	B	422	GLU	3.9
1	A	371	GLN	3.8
1	B	229	ARG	3.7
1	B	40	SER	3.7
1	B	406	LYS	3.7
1	A	230	ASN	3.6
1	A	180	ASP	3.6
1	B	344	GLU	3.5
1	B	424	GLN	3.5
1	B	42	PRO	3.5
1	A	190	ASP	3.5
1	B	409	ASP	3.5
1	A	74	ARG	3.4
1	B	56	LEU	3.4
1	A	229	ARG	3.3
1	B	371	GLN	3.3
1	A	324	VAL	3.3
1	B	74	ARG	3.3
1	A	242	ARG	3.1
1	B	407	PRO	3.1
1	B	242	ARG	3.1
1	A	41	THR	3.0
1	A	322	CYS	3.0
1	B	39	GLY	3.0
1	A	38	THR	3.0
1	B	367	LYS	3.0
1	A	341	ARG	2.9
1	B	72	VAL	2.9
1	A	181	ARG	2.9
1	A	323	LEU	2.8
1	B	345	ALA	2.8
1	B	323	LEU	2.8
1	A	37	TYR	2.7
1	A	25	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	417	LEU	2.6
1	B	109	PHE	2.6
1	B	374	GLU	2.6
1	A	57	PRO	2.5
1	A	217	TYR	2.5
1	B	286	ARG	2.5
1	B	37	TYR	2.5
1	A	293	ILE	2.4
1	B	423	SER	2.4
1	B	365	ASN	2.4
1	B	324	VAL	2.4
1	A	344	GLU	2.4
1	A	260	GLU	2.4
1	A	72	VAL	2.3
1	A	279	LEU	2.3
1	A	343	ALA	2.3
1	A	408	ASP	2.3
1	B	121	THR	2.2
1	B	325	ASP	2.2
1	A	53	GLN	2.2
1	B	275	VAL	2.2
1	B	220	TYR	2.2
1	A	42	PRO	2.1
1	B	277	SER	2.1
1	B	410	TYR	2.1
1	A	410	TYR	2.1
1	B	322[A]	CYS	2.1
1	B	110	THR	2.0
1	B	292	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	B	518	5/5	0.57	0.36	143,148,152,159	0
2	SO4	A	516	5/5	0.70	0.30	131,136,151,156	0
2	SO4	B	517	5/5	0.71	0.43	144,148,153,160	0
2	SO4	B	514	5/5	0.71	0.27	136,138,146,153	0
2	SO4	B	515	5/5	0.72	0.25	119,132,137,143	0
2	SO4	A	517	5/5	0.75	0.46	173,174,175,176	0
2	SO4	B	516	5/5	0.75	0.42	159,166,169,170	0
2	SO4	A	513	5/5	0.78	0.25	148,155,159,164	0
3	IOD	A	523	1/1	0.79	0.51	251,251,251,251	0
2	SO4	A	519	5/5	0.81	0.39	101,132,139,140	0
2	SO4	A	515	5/5	0.82	0.19	113,127,138,140	0
3	IOD	A	521	1/1	0.82	0.08	171,171,171,171	0
2	SO4	A	511	5/5	0.83	0.18	99,104,132,141	0
3	IOD	A	522	1/1	0.84	0.17	168,168,168,168	0
2	SO4	A	512	5/5	0.85	0.32	51,109,125,125	0
2	SO4	A	507	5/5	0.85	0.26	101,116,119,132	0
2	SO4	B	512	5/5	0.86	0.20	129,133,136,138	0
2	SO4	A	509	5/5	0.87	0.17	95,117,118,123	0
2	SO4	B	507	5/5	0.88	0.34	127,130,137,144	0
2	SO4	B	508	5/5	0.89	0.24	113,128,130,136	0
2	SO4	A	518	5/5	0.89	0.27	118,122,133,134	0
2	SO4	B	513	5/5	0.90	0.58	146,147,149,154	0
2	SO4	B	506	5/5	0.91	0.16	109,119,126,127	0
2	SO4	B	504	5/5	0.92	0.19	60,85,107,116	0
2	SO4	B	511	5/5	0.92	0.25	121,124,133,135	0
3	IOD	B	521	1/1	0.92	0.11	165,165,165,165	0
2	SO4	B	509	5/5	0.94	0.21	77,97,110,120	0
2	SO4	B	519	5/5	0.94	0.17	108,116,124,136	0
2	SO4	A	514	5/5	0.95	0.35	86,102,114,122	0
2	SO4	A	510	5/5	0.95	0.20	87,88,90,112	0
2	SO4	A	505	5/5	0.96	0.15	39,50,101,103	0
2	SO4	B	503	5/5	0.96	0.21	61,90,100,105	0
2	SO4	B	510	5/5	0.96	0.19	83,100,114,117	0
2	SO4	A	501	5/5	0.96	0.18	47,54,86,87	0
2	SO4	A	504	5/5	0.97	0.12	45,66,90,93	0
2	SO4	B	505	5/5	0.97	0.26	82,95,103,111	0
3	IOD	B	522	1/1	0.97	0.55	254,254,254,254	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	B	502	5/5	0.98	0.19	54,54,85,90	0
2	SO4	A	508	5/5	0.98	0.14	76,94,102,107	0
2	SO4	A	503	5/5	0.98	0.12	58,59,79,94	0
3	IOD	B	520	1/1	0.98	0.08	69,69,69,69	0
2	SO4	B	501	5/5	0.98	0.13	67,72,81,91	0
2	SO4	A	502	5/5	0.98	0.17	42,46,71,85	0
3	IOD	A	520	1/1	0.99	0.10	66,66,66,66	0
2	SO4	A	506	5/5	0.99	0.15	58,70,89,91	0

6.5 Other polymers (i)

There are no such residues in this entry.