



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:14 AM UTC

PDB ID : 5LT2 / pdb_00005lt2
Title : nucleotide-free kinesin-1 motor domain, P1 crystal form
Authors : Cao, L.; Gigant, B.
Deposited on : 2016-09-06
Resolution : 2.60 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:

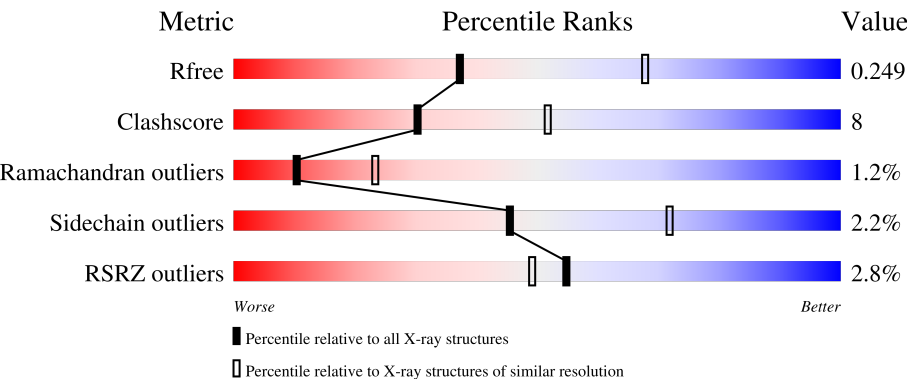
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	325	2% 81% 13% • •
1	B	325	5% 78% 14% • 6%
1	C	325	2% 77% 16% • 5%
1	D	325	3% 75% 20% • •
1	E	325	2% 80% 13% • 6%

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Mol	Chain	Length	Quality of chain
1	K	325	2% 73% 19% • 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14214 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	314	Total	C	N	O	S	0	0	0
			2362	1473	405	475	9			
1	B	307	Total	C	N	O	S	0	0	0
			2260	1418	387	446	9			
1	C	308	Total	C	N	O	S	0	0	0
			2335	1460	402	464	9			
1	D	313	Total	C	N	O	S	0	0	0
			2339	1463	403	464	9			
1	E	307	Total	C	N	O	S	0	0	0
			2256	1411	384	452	9			
1	K	307	Total	C	N	O	S	0	0	0
			2288	1435	392	452	9			

There are 30 discrepancies between the modelled and reference sequences:

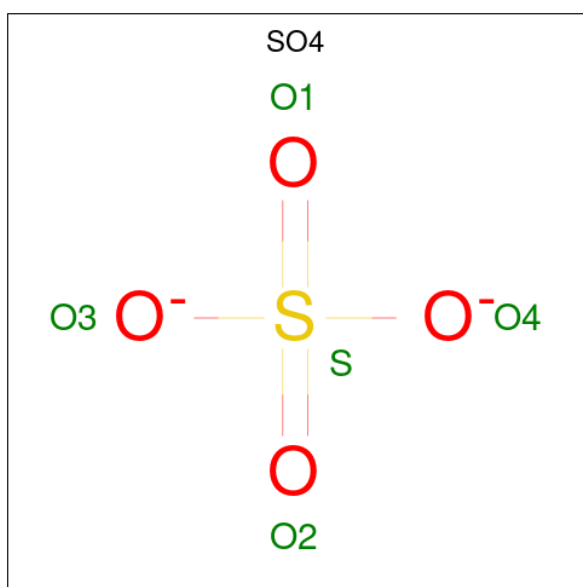
Chain	Residue	Modelled	Actual	Comment	Reference
A	7	SER	CYS	engineered mutation	UNP Q6P164
A	65	ALA	CYS	engineered mutation	UNP Q6P164
A	168	ALA	CYS	engineered mutation	UNP Q6P164
A	174	SER	CYS	engineered mutation	UNP Q6P164
A	294	ALA	CYS	engineered mutation	UNP Q6P164
B	7	SER	CYS	engineered mutation	UNP Q6P164
B	65	ALA	CYS	engineered mutation	UNP Q6P164
B	168	ALA	CYS	engineered mutation	UNP Q6P164
B	174	SER	CYS	engineered mutation	UNP Q6P164
B	294	ALA	CYS	engineered mutation	UNP Q6P164
C	7	SER	CYS	engineered mutation	UNP Q6P164
C	65	ALA	CYS	engineered mutation	UNP Q6P164
C	168	ALA	CYS	engineered mutation	UNP Q6P164
C	174	SER	CYS	engineered mutation	UNP Q6P164
C	294	ALA	CYS	engineered mutation	UNP Q6P164
D	7	SER	CYS	engineered mutation	UNP Q6P164
D	65	ALA	CYS	engineered mutation	UNP Q6P164

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Chain	Residue	Modelled	Actual	Comment	Reference
D	168	ALA	CYS	engineered mutation	UNP Q6P164
D	174	SER	CYS	engineered mutation	UNP Q6P164
D	294	ALA	CYS	engineered mutation	UNP Q6P164
E	7	SER	CYS	engineered mutation	UNP Q6P164
E	65	ALA	CYS	engineered mutation	UNP Q6P164
E	168	ALA	CYS	engineered mutation	UNP Q6P164
E	174	SER	CYS	engineered mutation	UNP Q6P164
E	294	ALA	CYS	engineered mutation	UNP Q6P164
K	7	SER	CYS	engineered mutation	UNP Q6P164
K	65	ALA	CYS	engineered mutation	UNP Q6P164
K	168	ALA	CYS	engineered mutation	UNP Q6P164
K	174	SER	CYS	engineered mutation	UNP Q6P164
K	294	ALA	CYS	engineered mutation	UNP Q6P164

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



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

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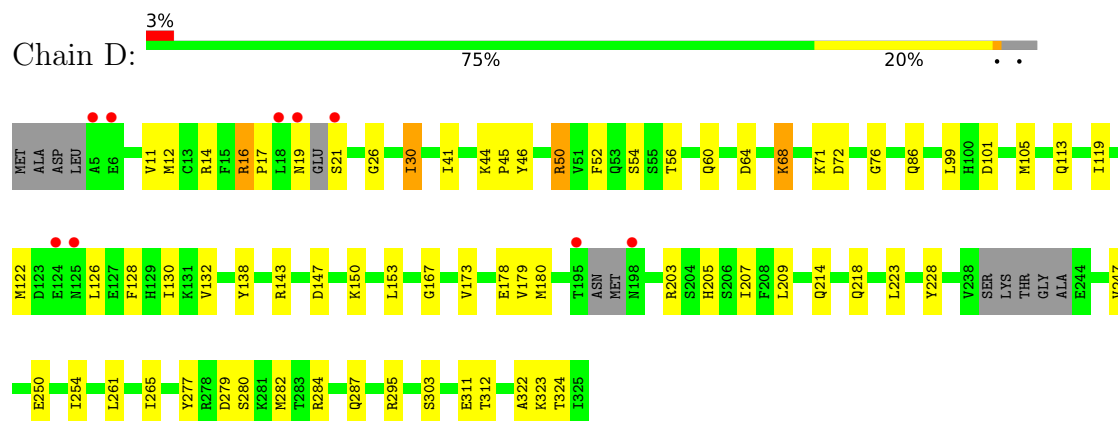
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		

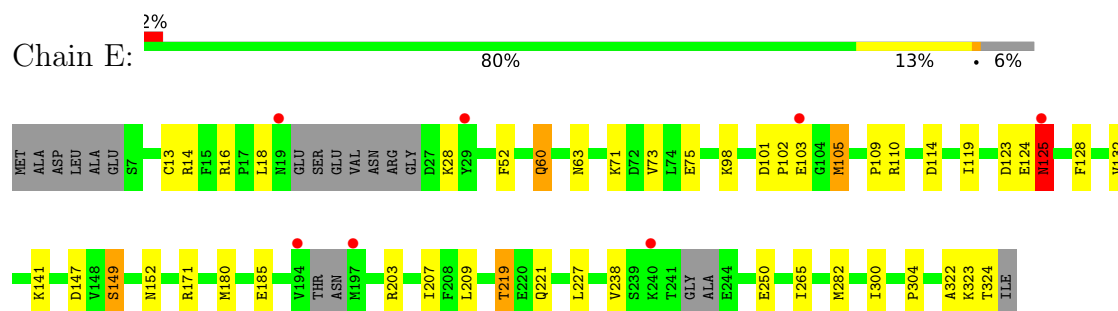
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	77	Total	O	0	0
			77	77		
3	B	21	Total	O	0	0
			21	21		
3	C	74	Total	O	0	0
			74	74		
3	D	57	Total	O	0	0
			57	57		
3	E	47	Total	O	0	0
			47	47		
3	K	43	Total	O	0	0
			43	43		

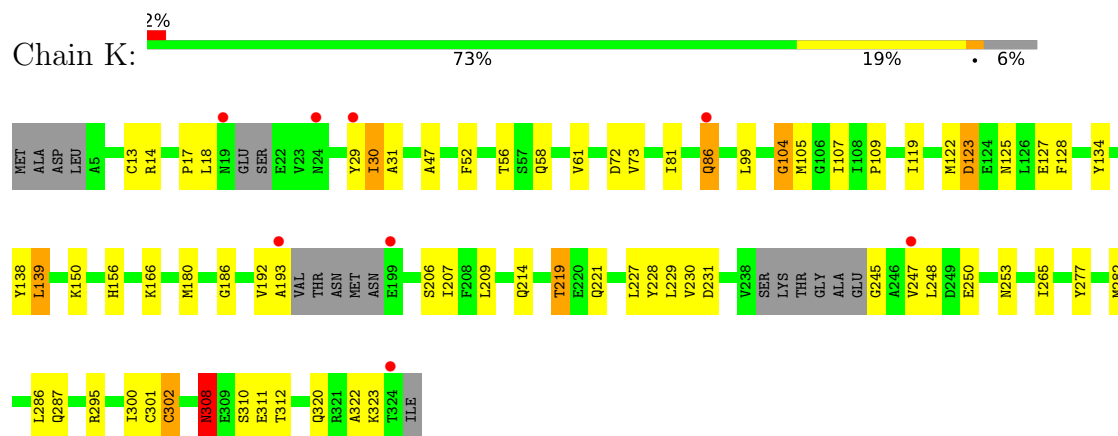
- Molecule 1: Kinesin-like protein



- Molecule 1: Kinesin-like protein



- Molecule 1: Kinesin-like protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	56.74Å 101.45Å 101.59Å 119.24° 91.96° 91.93°	Depositor
Resolution (Å)	38.40 – 2.60 38.40 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.0 (38.40-2.60) 92.4 (38.40-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.9_1692, BUSTER	Depositor
R, R_{free}	0.193 , 0.249 0.198 , 0.249	Depositor DCC
R_{free} test set	2016 reflections (3.32%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.743	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 65.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14214	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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

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	0.67	0/2398	1.04	10/3247 (0.3%)
1	B	0.65	3/2295 (0.1%)	0.97	1/3114 (0.0%)
1	C	0.65	0/2370	1.01	8/3204 (0.2%)
1	D	0.63	0/2373	1.00	2/3212 (0.1%)
1	E	0.62	0/2289	1.00	3/3107 (0.1%)
1	K	0.63	0/2322	1.02	8/3144 (0.3%)
All	All	0.64	3/14047 (0.0%)	1.01	32/19028 (0.2%)

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	K	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	156	HIS	CE1-NE2	7.03	1.39	1.32
1	B	156	HIS	ND1-CE1	-5.07	1.27	1.32
1	B	154	SER	CB-OG	5.01	1.52	1.42

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	17	PRO	CA-C-N	6.92	134.15	121.70
1	C	17	PRO	C-N-CA	6.92	134.15	121.70
1	A	17	PRO	CA-C-N	6.89	134.09	121.70
1	A	17	PRO	C-N-CA	6.89	134.09	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	125	ASN	N-CA-C	6.70	119.42	111.71
1	A	17	PRO	CA-C-O	-6.47	114.04	122.19
1	K	308	ASN	N-CA-C	6.44	119.12	111.33
1	A	159	LYS	CA-C-N	-6.42	112.94	122.83
1	A	159	LYS	C-N-CA	-6.42	112.94	122.83
1	A	107	ILE	N-CA-C	6.36	116.53	110.42
1	K	30	ILE	N-CA-C	6.02	121.86	109.34
1	C	18	LEU	N-CA-C	-6.00	94.20	111.00
1	K	302	CYS	N-CA-C	5.90	119.10	109.24
1	A	103	GLU	N-CA-C	5.86	121.09	113.88
1	C	195	THR	N-CA-C	-5.76	106.23	113.72
1	K	17	PRO	CA-C-O	-5.67	114.95	121.86
1	A	30	ILE	N-CA-C	5.58	120.94	109.34
1	C	107	ILE	N-CA-C	5.58	115.77	110.42
1	E	125	ASN	N-CA-C	5.50	118.20	111.82
1	C	17	PRO	CA-C-O	-5.48	115.33	122.12
1	D	50	ARG	N-CA-C	5.41	117.31	108.55
1	C	103	GLU	N-CA-C	5.38	120.09	112.93
1	K	125	ASN	N-CA-C	5.26	117.76	111.71
1	A	19	ASN	N-CA-C	5.26	122.00	110.80
1	D	30	ILE	N-CA-C	5.23	120.23	109.34
1	K	17	PRO	CA-C-N	5.21	131.08	121.70
1	K	17	PRO	C-N-CA	5.21	131.08	121.70
1	K	107	ILE	N-CA-C	5.17	115.38	110.42
1	B	85	GLY	N-CA-C	5.12	125.31	113.18
1	E	101	ASP	CA-C-N	-5.12	114.81	119.82
1	E	101	ASP	C-N-CA	-5.12	114.81	119.82
1	A	309	GLU	N-CA-C	5.11	117.52	111.33

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	K	308	ASN	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	2362	0	2229	32	0
1	B	2260	0	2080	31	0
1	C	2335	0	2225	37	0
1	D	2339	0	2215	55	0
1	E	2256	0	2065	33	0
1	K	2288	0	2156	42	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
2	C	15	0	0	0	0
2	D	15	0	0	1	0
2	E	5	0	0	0	0
2	K	10	0	0	0	0
3	A	77	0	0	3	0
3	B	21	0	0	0	0
3	C	74	0	0	5	2
3	D	57	0	0	6	0
3	E	47	0	0	3	1
3	K	43	0	0	5	1
All	All	14214	0	12970	226	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (226) 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:K:86:GLN:NE2	3:K:501:HOH:O	1.94	0.98
1:C:30:ILE:HD11	1:C:306:SER:HA	1.56	0.87
1:D:86:GLN:HG3	1:D:311:GLU:HG2	1.56	0.85
1:D:323:LYS:HD2	1:D:324:THR:H	1.41	0.85
1:D:323:LYS:HD2	1:D:324:THR:N	1.92	0.85
1:A:218:GLN:OE1	3:A:501:HOH:O	1.96	0.82
1:K:14:ARG:HG3	1:K:52:PHE:HB2	1.63	0.81
1:D:12:MET:HG2	1:D:50:ARG:HB3	1.63	0.77
1:A:159:LYS:HG3	1:A:160:ASN:OD1	1.86	0.75
1:D:50:ARG:HD3	1:D:52:PHE:CE1	2.22	0.75
1:A:125:ASN:ND2	1:A:125:ASN:H	1.85	0.74
1:C:193:ALA:O	1:C:195:THR:N	2.20	0.74
1:K:301:CYS:O	3:K:501:HOH:O	2.05	0.73
1:D:203:ARG:HH12	1:D:247:VAL:HG23	1.55	0.72
1:K:86:GLN:HG3	1:K:311:GLU:HB3	1.71	0.71
1:D:99:LEU:HD21	1:D:180:MET:HE2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:86:GLN:N	1:K:86:GLN:OE1	2.25	0.69
1:K:99:LEU:HD21	1:K:180:MET:HE2	1.74	0.68
1:A:213:LYS:NZ	3:A:502:HOH:O	2.22	0.66
2:D:403:SO4:O3	3:D:501:HOH:O	2.14	0.65
1:D:60:GLN:NE2	1:D:64:ASP:OD2	2.28	0.65
1:A:122:MET:O	1:A:125:ASN:ND2	2.31	0.64
1:K:58:GLN:HG3	1:K:104:GLY:HA2	1.79	0.64
1:K:86:GLN:CD	1:K:86:GLN:H	2.04	0.64
1:K:72:ASP:OD2	1:K:295:ARG:HD2	1.97	0.63
1:E:71:LYS:NZ	1:E:75:GLU:OE2	2.30	0.63
1:A:16:ARG:HG2	1:A:17:PRO:O	1.99	0.62
1:A:203:ARG:HD3	1:A:250:GLU:OE1	1.98	0.62
1:B:16:ARG:HH12	1:B:18:LEU:HA	1.64	0.62
1:D:113:GLN:HG2	3:D:557:HOH:O	1.99	0.62
1:D:150:LYS:NZ	1:D:167:GLY:O	2.23	0.62
1:C:213:LYS:NZ	3:C:504:HOH:O	2.32	0.61
1:K:138:TYR:OH	1:K:250:GLU:OE2	2.06	0.60
1:A:103:GLU:N	1:A:104:GLY:HA3	2.17	0.60
1:C:219:THR:HG23	1:C:221:GLN:HG2	1.83	0.59
1:E:73:VAL:HG21	1:E:227:LEU:HB2	1.84	0.59
1:C:152:ASN:O	3:C:501:HOH:O	2.16	0.59
1:E:102:PRO:O	1:E:103:GLU:HG2	2.02	0.59
1:B:278:ARG:HA	1:B:284:ARG:HD2	1.84	0.59
1:E:219:THR:CG2	1:E:221:GLN:HG2	2.34	0.58
1:B:138:TYR:OH	1:B:250:GLU:OE1	2.16	0.57
1:K:219:THR:CG2	1:K:221:GLN:HG2	2.35	0.57
1:A:303:SER:O	1:A:312:THR:HG21	2.05	0.57
1:D:72:ASP:OD2	1:D:295:ARG:HD2	2.04	0.57
1:D:203:ARG:NH1	1:D:247:VAL:HG23	2.20	0.57
1:B:154:SER:H	1:B:166:LYS:HE3	1.69	0.56
1:B:155:VAL:HG21	1:B:285:ILE:HG13	1.86	0.56
1:E:105:MET:HB3	1:E:110:ARG:NH1	2.21	0.56
1:B:137:ILE:HD13	1:B:142:ILE:HG12	1.88	0.56
1:E:171:ARG:NH1	1:E:185:GLU:OE1	2.31	0.55
1:E:16:ARG:NH1	1:E:18:LEU:HA	2.22	0.55
1:D:44:LYS:HD2	1:D:45:PRO:HD2	1.87	0.55
1:E:18:LEU:HB3	1:E:304:PRO:HG2	1.89	0.55
1:E:105:MET:O	1:E:110:ARG:NH1	2.38	0.55
1:C:310:SER:O	1:C:313:LYS:HG2	2.07	0.54
1:D:16:ARG:HG2	1:D:17:PRO:N	2.22	0.54
1:D:50:ARG:NH1	1:D:64:ASP:OD2	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:TYR:O	1:A:31:ALA:N	2.40	0.54
1:D:19:ASN:O	1:D:21:SER:HA	2.07	0.54
1:E:114:ASP:OD1	3:E:501:HOH:O	2.19	0.54
1:C:303:SER:O	1:C:312:THR:HG21	2.07	0.54
1:E:203:ARG:HD3	1:E:250:GLU:OE1	2.08	0.54
1:E:207:ILE:HD11	1:E:282:MET:HE2	1.90	0.54
1:B:153:LEU:HD22	1:B:166:LYS:O	2.07	0.53
1:C:292:GLY:HA3	3:C:552:HOH:O	2.07	0.53
1:A:103:GLU:H	1:A:104:GLY:HA3	1.73	0.53
1:A:147:ASP:HB2	1:C:152:ASN:HD21	1.73	0.53
1:B:154:SER:N	1:B:166:LYS:HE3	2.23	0.53
1:B:105:MET:HB2	1:B:109:PRO:HG2	1.91	0.53
1:K:14:ARG:HD2	1:K:61:VAL:HG21	1.90	0.53
1:B:158:ASP:HB3	1:B:164:TYR:HE2	1.73	0.52
1:C:207:ILE:HD11	1:C:282:MET:HE2	1.92	0.52
1:D:44:LYS:HG3	1:D:46:TYR:CZ	2.44	0.52
1:C:41:ILE:HD12	1:C:316:LEU:HD11	1.91	0.52
1:C:219:THR:HG22	1:C:221:GLN:H	1.75	0.52
1:D:150:LYS:HB3	1:D:153:LEU:HD21	1.92	0.51
1:D:207:ILE:HD11	1:D:282:MET:HE2	1.91	0.51
1:A:80:THR:OG1	1:A:289:SER:O	2.23	0.51
1:C:119:ILE:HG12	1:C:128:PHE:CG	2.46	0.51
1:A:101:ASP:O	1:A:105:MET:N	2.33	0.51
1:K:29:TYR:O	1:K:31:ALA:N	2.44	0.51
1:C:30:ILE:HD12	1:C:309:GLU:HB2	1.93	0.50
1:E:141:LYS:HE3	1:E:152:ASN:ND2	2.26	0.50
1:A:166:LYS:HE2	1:D:178:GLU:OE2	2.11	0.50
1:K:156:HIS:CE1	1:K:166:LYS:HD2	2.46	0.50
1:D:138:TYR:OH	1:D:250:GLU:OE2	2.16	0.50
1:D:205:HIS:HB3	1:D:282:MET:HE1	1.94	0.50
1:A:125:ASN:ND2	1:A:125:ASN:N	2.56	0.50
1:C:219:THR:CG2	1:C:221:GLN:HG2	2.43	0.49
1:D:105:MET:HE1	3:D:557:HOH:O	2.11	0.49
1:C:90:GLY:HA2	3:C:532:HOH:O	2.12	0.49
1:K:209:LEU:HD13	1:K:228:TYR:CZ	2.47	0.49
1:B:303:SER:O	1:B:312:THR:HG21	2.12	0.49
1:C:80:THR:OG1	1:C:289:SER:O	2.26	0.49
1:E:16:ARG:HH12	1:E:18:LEU:HA	1.76	0.49
1:B:109:PRO:HA	1:B:180:MET:HE1	1.93	0.49
1:D:14:ARG:HA	1:D:52:PHE:HB2	1.95	0.49
1:E:219:THR:HG22	1:E:221:GLN:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:GLU:N	1:B:104:GLY:HA3	2.28	0.49
1:K:56:THR:HB	3:K:504:HOH:O	2.13	0.49
1:D:205:HIS:CB	1:D:282:MET:HE1	2.42	0.48
1:D:209:LEU:HD13	1:D:228:TYR:CE1	2.48	0.48
1:C:30:ILE:CD1	1:C:309:GLU:HB2	2.43	0.48
1:C:216:ASN:OD1	1:C:219:THR:HB	2.14	0.48
1:K:277:TYR:CG	1:K:287:GLN:HG3	2.47	0.48
1:E:147:ASP:OD1	1:E:149:SER:HB3	2.12	0.48
1:C:60:GLN:O	1:C:60:GLN:HG2	2.13	0.48
1:D:119:ILE:HD11	1:D:130:ILE:HD11	1.96	0.48
1:K:207:ILE:HD11	1:K:282:MET:HE2	1.95	0.48
1:A:199:GLU:O	1:A:200:HIS:C	2.56	0.48
1:E:265:ILE:HG21	3:E:547:HOH:O	2.13	0.48
1:K:310:SER:OG	3:K:502:HOH:O	2.20	0.47
1:B:18:LEU:HD12	1:B:19:ASN:H	1.78	0.47
1:D:16:ARG:HG2	1:D:17:PRO:O	2.15	0.47
1:C:103:GLU:H	1:C:104:GLY:HA3	1.80	0.47
1:C:153:LEU:HD22	1:C:166:LYS:O	2.15	0.47
1:E:13:CYS:HA	1:E:300:ILE:HG13	1.96	0.47
1:D:203:ARG:HA	1:D:254:ILE:HD11	1.96	0.47
1:E:60:GLN:OE1	1:E:63:ASN:HB2	2.15	0.47
1:B:11:VAL:HG21	1:B:322:ALA:HB3	1.97	0.47
1:B:76:GLY:HA3	1:B:223:LEU:HD22	1.96	0.47
1:C:102:PRO:HA	1:C:105:MET:HE2	1.97	0.47
1:D:17:PRO:HG3	1:D:54:SER:HB3	1.96	0.47
1:K:156:HIS:HE1	1:K:166:LYS:HD2	1.78	0.47
1:K:308:ASN:HB3	1:K:312:THR:HG23	1.96	0.47
1:D:50:ARG:NH1	1:D:64:ASP:CG	2.73	0.46
1:A:160:ASN:OD1	1:A:160:ASN:N	2.47	0.46
1:C:119:ILE:HG12	1:C:128:PHE:CD1	2.50	0.46
1:E:119:ILE:HG12	1:E:128:PHE:CG	2.51	0.46
1:B:116:PHE:HA	1:B:119:ILE:HD12	1.98	0.46
1:E:60:GLN:OE1	1:E:60:GLN:HA	2.16	0.46
1:K:209:LEU:HD13	1:K:228:TYR:CE1	2.51	0.46
1:K:122:MET:O	1:K:123:ASP:C	2.59	0.46
1:K:134:TYR:CD2	1:K:186:GLY:HA3	2.51	0.46
1:A:164:TYR:OH	1:D:178:GLU:OE1	2.30	0.46
1:D:122:MET:HB3	1:D:126:LEU:HD12	1.98	0.46
1:B:16:ARG:NH1	1:B:18:LEU:HA	2.29	0.46
1:B:58:GLN:HG3	1:B:104:GLY:H	1.81	0.46
1:K:13:CYS:HA	1:K:300:ILE:HG13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:308:ASN:O	1:K:310:SER:N	2.49	0.46
1:A:137:ILE:HG13	1:A:282:MET:HE3	1.97	0.46
1:B:308:ASN:OD1	1:B:308:ASN:N	2.49	0.46
1:C:173:VAL:HG21	1:C:179:VAL:HG22	1.98	0.46
1:E:125:ASN:OD1	1:E:125:ASN:N	2.44	0.46
1:K:47:ALA:O	1:K:320:GLN:NE2	2.49	0.46
1:D:86:GLN:CG	1:D:311:GLU:HG2	2.37	0.45
1:D:52:PHE:CD1	1:D:56:THR:HG21	2.51	0.45
1:A:226:LYS:NZ	1:A:288:ASP:OD2	2.32	0.45
1:D:261:LEU:O	1:D:265:ILE:HG12	2.16	0.45
1:D:11:VAL:HG21	1:D:322:ALA:HB3	1.98	0.45
1:D:128:PHE:CE2	1:D:214:GLN:HG2	2.51	0.45
1:E:105:MET:HG2	1:E:110:ARG:HG3	1.97	0.45
1:D:99:LEU:C	1:D:101:ASP:H	2.25	0.45
1:A:147:ASP:HB2	1:C:152:ASN:ND2	2.32	0.45
1:C:126:LEU:HD23	1:C:216:ASN:HA	1.98	0.45
1:B:87:THR:O	1:B:88:SER:OG	2.29	0.45
1:C:128:PHE:CE2	1:C:214:GLN:HG2	2.51	0.45
1:D:41:ILE:O	1:D:44:LYS:HB3	2.17	0.45
1:K:105:MET:HB2	1:K:109:PRO:HG2	1.98	0.45
1:D:280:SER:O	1:D:284:ARG:HG3	2.16	0.45
1:K:128:PHE:CE2	1:K:214:GLN:HG2	2.52	0.44
1:A:119:ILE:HG12	1:A:128:PHE:CD1	2.53	0.44
1:C:86:GLN:HG3	1:C:311:GLU:HB3	2.00	0.44
1:C:141:LYS:HG3	3:C:540:HOH:O	2.17	0.44
1:D:11:VAL:CG2	1:D:322:ALA:HB3	2.48	0.44
1:A:91:LYS:N	2:A:401:SO4:O1	2.48	0.44
1:B:52:PHE:CD1	1:B:56:THR:HG21	2.52	0.44
1:K:119:ILE:HG12	1:K:128:PHE:CG	2.53	0.44
1:K:302:CYS:HA	3:K:501:HOH:O	2.16	0.44
1:C:106:GLY:O	1:C:110:ARG:HG3	2.18	0.44
1:K:192:VAL:HG12	1:K:193:ALA:H	1.83	0.44
1:D:16:ARG:NH2	1:D:303:SER:HB2	2.33	0.44
1:E:323:LYS:HG2	1:E:324:THR:H	1.83	0.43
1:C:105:MET:HB2	1:C:109:PRO:HG2	1.99	0.43
1:B:278:ARG:HA	1:B:284:ARG:CD	2.49	0.43
1:D:132:VAL:HA	1:D:209:LEU:O	2.19	0.43
1:E:219:THR:HG23	1:E:221:GLN:HG2	2.00	0.43
1:K:14:ARG:HG3	1:K:52:PHE:CB	2.42	0.43
1:K:81:ILE:HB	1:K:229:LEU:HD23	1.99	0.43
1:B:122:MET:O	1:B:123:ASP:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:LYS:H	1:E:105:MET:H	1.65	0.43
1:E:123:ASP:OD1	1:E:124:GLU:N	2.49	0.43
1:B:174:SER:N	1:B:178:GLU:OE1	2.50	0.43
1:K:14:ARG:CG	1:K:52:PHE:HB2	2.43	0.43
1:E:109:PRO:HA	1:E:180:MET:HE1	2.01	0.42
1:C:103:GLU:N	1:C:104:GLY:HA3	2.34	0.42
1:A:119:ILE:HG12	1:A:128:PHE:CG	2.54	0.42
1:E:324:THR:HG23	3:E:536:HOH:O	2.20	0.42
1:K:139:LEU:HD12	1:K:253:ASN:OD1	2.19	0.42
1:K:230:VAL:HG21	1:K:286:LEU:HD11	2.02	0.42
1:B:190:ARG:O	1:B:192:VAL:HG23	2.19	0.42
1:D:16:ARG:HH21	1:D:303:SER:HA	1.84	0.42
1:A:205:HIS:CB	1:A:282:MET:HE1	2.50	0.42
1:A:207:ILE:HD11	1:A:282:MET:HE2	2.02	0.42
1:A:105:MET:HB2	1:A:109:PRO:HG2	2.00	0.42
1:E:132:VAL:HA	1:E:209:LEU:O	2.20	0.42
1:D:76:GLY:HA3	1:D:223:LEU:HD22	2.01	0.42
1:D:143:ARG:NE	3:D:513:HOH:O	2.53	0.42
1:K:73:VAL:HG21	1:K:227:LEU:HB2	2.02	0.41
1:A:136:GLU:OE2	1:A:143:ARG:HD3	2.20	0.41
1:B:219:THR:O	1:B:221:GLN:NE2	2.33	0.41
1:D:279:ASP:HB2	3:D:516:HOH:O	2.19	0.41
1:A:312:THR:HG22	3:A:568:HOH:O	2.20	0.41
1:E:14:ARG:HG3	1:E:52:PHE:HB2	2.01	0.41
1:K:245:GLY:O	1:K:248:LEU:HB3	2.20	0.41
1:C:13:CYS:HA	1:C:300:ILE:HG13	2.03	0.41
1:C:87:THR:O	1:C:88:SER:OG	2.35	0.41
1:K:219:THR:HG23	1:K:221:GLN:HG2	2.02	0.41
1:A:44:LYS:HA	1:A:45:PRO:HD3	1.96	0.41
1:B:124:GLU:HA	1:B:126:LEU:N	2.35	0.41
1:C:323:LYS:HB3	1:C:323:LYS:HE2	1.83	0.41
1:D:303:SER:O	1:D:312:THR:HG21	2.21	0.41
1:D:173:VAL:HG21	1:D:179:VAL:HG22	2.02	0.41
1:D:71:LYS:HG3	3:D:546:HOH:O	2.21	0.41
1:D:16:ARG:HE	1:D:16:ARG:HB3	1.52	0.40
1:D:277:TYR:CG	1:D:287:GLN:HG3	2.56	0.40
1:A:141:LYS:HD3	1:D:147:ASP:OD1	2.22	0.40
1:D:68:LYS:HG2	1:D:295:ARG:NH1	2.36	0.40
1:E:265:ILE:CG2	1:E:322:ALA:HB2	2.51	0.40
1:K:265:ILE:HG21	1:K:322:ALA:HB2	2.02	0.40
1:C:223:LEU:HD23	1:C:223:LEU:HA	1.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:219:THR:HG22	1:E:221:GLN:HG2	2.03	0.40
1:B:84:TYR:O	1:B:85:GLY:O	2.40	0.40
1:B:131:LYS:NZ	1:B:170:GLU:OE1	2.31	0.40
1:B:312:THR:O	1:B:316:LEU:HG	2.22	0.40
1:K:206:SER:OG	1:K:231:ASP:HB3	2.22	0.40

All (2) 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)
3:C:551:HOH:O	3:K:528:HOH:O[1_665]	2.19	0.01
3:C:573:HOH:O	3:E:512:HOH:O[1_655]	2.19	0.01

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	308/325 (95%)	289 (94%)	12 (4%)	7 (2%)	5	9
1	B	299/325 (92%)	286 (96%)	11 (4%)	2 (1%)	18	38
1	C	300/325 (92%)	287 (96%)	10 (3%)	3 (1%)	12	28
1	D	305/325 (94%)	290 (95%)	13 (4%)	2 (1%)	18	38
1	E	299/325 (92%)	288 (96%)	8 (3%)	3 (1%)	12	28
1	K	299/325 (92%)	289 (97%)	6 (2%)	4 (1%)	9	21
All	All	1810/1950 (93%)	1729 (96%)	60 (3%)	21 (1%)	10	23

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	30	ILE

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Mol	Chain	Res	Type
1	A	99	LEU
1	B	85	GLY
1	B	123	ASP
1	C	18	LEU
1	C	194	VAL
1	D	30	ILE
1	K	30	ILE
1	K	123	ASP
1	A	18	LEU
1	A	198	ASN
1	A	200	HIS
1	E	238	VAL
1	K	18	LEU
1	C	123	ASP
1	A	123	ASP
1	E	105	MET
1	K	104	GLY
1	E	28	LYS
1	D	26	GLY

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	250/286 (87%)	244 (98%)	6 (2%)	43	70
1	B	226/286 (79%)	221 (98%)	5 (2%)	45	72
1	C	247/286 (86%)	241 (98%)	6 (2%)	43	70
1	D	245/286 (86%)	242 (99%)	3 (1%)	63	83
1	E	226/286 (79%)	222 (98%)	4 (2%)	51	76
1	K	236/286 (82%)	229 (97%)	7 (3%)	36	64
All	All	1430/1716 (83%)	1399 (98%)	31 (2%)	45	72

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	GLN
1	A	125	ASN
1	A	160	ASN
1	A	166	LYS
1	A	247	VAL
1	A	320	GLN
1	B	99	LEU
1	B	166	LYS
1	B	192	VAL
1	B	308	ASN
1	B	320	GLN
1	C	30	ILE
1	C	39	VAL
1	C	50	ARG
1	C	215	GLU
1	C	219	THR
1	C	273	THR
1	D	16	ARG
1	D	68	LYS
1	D	218	GLN
1	E	60	GLN
1	E	125	ASN
1	E	149	SER
1	E	219	THR
1	K	86	GLN
1	K	127	GLU
1	K	139	LEU
1	K	150	LYS
1	K	219	THR
1	K	247	VAL
1	K	323	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	125	ASN
1	B	320	GLN
1	C	53	GLN
1	C	125	ASN
1	C	214	GLN
1	E	156	HIS

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 ⓘ

11 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	D	403	-	4,4,4	0.37	0	6,6,6	0.38	0
2	SO4	K	402	-	4,4,4	0.43	0	6,6,6	0.20	0
2	SO4	C	403	-	4,4,4	0.27	0	6,6,6	0.12	0
2	SO4	D	402	-	4,4,4	0.38	0	6,6,6	0.21	0
2	SO4	D	401	-	4,4,4	0.23	0	6,6,6	0.42	0
2	SO4	B	401	-	4,4,4	0.26	0	6,6,6	0.07	0
2	SO4	C	401	-	4,4,4	0.32	0	6,6,6	0.29	0
2	SO4	K	401	-	4,4,4	0.30	0	6,6,6	0.18	0
2	SO4	E	401	-	4,4,4	0.24	0	6,6,6	0.23	0
2	SO4	C	402	-	4,4,4	0.35	0	6,6,6	0.28	0
2	SO4	A	401	-	4,4,4	0.28	0	6,6,6	0.47	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	403	SO4	1	0
2	A	401	SO4	1	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	314/325 (96%)	-0.13	5 (1%) 70 66	23, 44, 84, 103	0
1	B	307/325 (94%)	0.41	16 (5%) 33 27	39, 71, 110, 149	0
1	C	308/325 (94%)	-0.10	7 (2%) 61 55	25, 46, 83, 115	0
1	D	313/325 (96%)	0.02	9 (2%) 53 48	27, 49, 82, 116	0
1	E	307/325 (94%)	-0.05	7 (2%) 61 55	27, 51, 86, 113	0
1	K	307/325 (94%)	0.07	8 (2%) 57 51	28, 56, 93, 125	0
All	All	1856/1950 (95%)	0.04	52 (2%) 55 49	23, 52, 94, 149	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	19	ASN	4.1
1	C	200	HIS	3.4
1	D	21	SER	3.4
1	C	194	VAL	3.4
1	B	123	ASP	3.3
1	B	195	THR	3.0
1	A	197	MET	2.9
1	D	18	LEU	2.9
1	B	320	GLN	2.9
1	K	19	ASN	2.8
1	B	155	VAL	2.8
1	C	197	MET	2.7
1	E	29	TYR	2.7
1	K	199	GLU	2.7
1	D	125	ASN	2.7
1	B	99	LEU	2.6
1	C	98	LYS	2.5
1	E	240	LYS	2.5
1	B	156	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	124	GLU	2.5
1	K	86	GLN	2.4
1	B	26	GLY	2.4
1	A	307	TYR	2.4
1	D	195	THR	2.4
1	K	24	ASN	2.4
1	D	5	ALA	2.3
1	E	197	MET	2.3
1	B	7	SER	2.3
1	B	149	SER	2.3
1	B	22	GLU	2.3
1	C	196	ASN	2.2
1	A	243	ALA	2.2
1	K	193	ALA	2.2
1	A	125	ASN	2.2
1	B	24	ASN	2.2
1	E	125	ASN	2.2
1	B	28	LYS	2.2
1	K	324	THR	2.2
1	C	19	ASN	2.2
1	E	194	VAL	2.2
1	E	19	ASN	2.2
1	K	29	TYR	2.2
1	B	30	ILE	2.2
1	B	324	THR	2.1
1	B	154	SER	2.1
1	K	247	VAL	2.1
1	D	6	GLU	2.1
1	B	162	VAL	2.1
1	A	198	ASN	2.1
1	D	198	ASN	2.1
1	E	103	GLU	2.0
1	C	5	ALA	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 [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	D	402	5/5	0.64	0.26	76,77,79,81	0
2	SO4	K	402	5/5	0.70	0.21	75,76,77,78	0
2	SO4	B	401	5/5	0.82	0.13	81,91,92,95	0
2	SO4	C	403	5/5	0.82	0.17	76,77,77,79	0
2	SO4	D	403	5/5	0.83	0.21	75,76,77,78	0
2	SO4	K	401	5/5	0.86	0.10	73,75,78,79	0
2	SO4	E	401	5/5	0.88	0.12	60,69,73,78	0
2	SO4	D	401	5/5	0.89	0.11	54,64,66,68	0
2	SO4	C	402	5/5	0.89	0.22	61,66,69,70	0
2	SO4	C	401	5/5	0.92	0.10	54,57,69,76	0
2	SO4	A	401	5/5	0.93	0.07	55,57,62,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.