



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:39 PM UTC

PDB ID : 5LT3 / pdb_00005lt3
Title : nucleotide-free kinesin-1 motor domain T87A mutant, P1 crystal form
Authors : Cao, L.; Gigant, B.
Deposited on : 2016-09-06
Resolution : 2.59 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

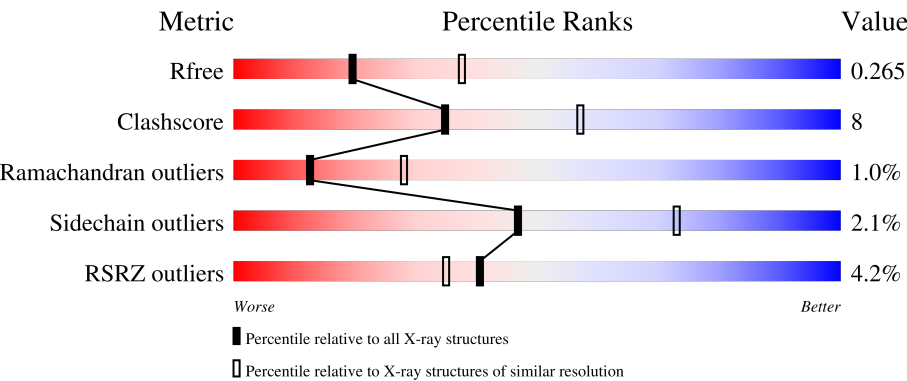
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	3% 79%14%6%
1	B	325	7% 78%14%6%
1	C	325	2% 74%18%8%
1	D	325	2% 78%17%. .
1	E	325	6% 78%16%5%

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Mol	Chain	Length	Quality of chain
1	K	325	4% 75% 20% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14006 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-1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	1	0
			2334	1455	402	468	9			
1	B	305	Total	C	N	O	S	0	0	0
			2251	1411	384	447	9			
1	C	300	Total	C	N	O	S	0	0	0
			2280	1427	391	453	9			
1	D	311	Total	C	N	O	S	0	0	0
			2335	1460	405	461	9			
1	E	308	Total	C	N	O	S	0	0	0
			2253	1412	388	444	9			
1	K	312	Total	C	N	O	S	0	0	0
			2313	1452	400	452	9			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	SER	CYS	engineered mutation	UNP P33176
A	65	ALA	CYS	engineered mutation	UNP P33176
A	87	ALA	THR	engineered mutation	UNP P33176
A	168	ALA	CYS	engineered mutation	UNP P33176
A	174	SER	CYS	engineered mutation	UNP P33176
A	294	ALA	CYS	engineered mutation	UNP P33176
B	7	SER	CYS	engineered mutation	UNP P33176
B	65	ALA	CYS	engineered mutation	UNP P33176
B	87	ALA	THR	engineered mutation	UNP P33176
B	168	ALA	CYS	engineered mutation	UNP P33176
B	174	SER	CYS	engineered mutation	UNP P33176
B	294	ALA	CYS	engineered mutation	UNP P33176
C	7	SER	CYS	engineered mutation	UNP P33176
C	65	ALA	CYS	engineered mutation	UNP P33176
C	87	ALA	THR	engineered mutation	UNP P33176
C	168	ALA	CYS	engineered mutation	UNP P33176
C	174	SER	CYS	engineered mutation	UNP P33176

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Chain	Residue	Modelled	Actual	Comment	Reference
C	294	ALA	CYS	engineered mutation	UNP P33176
D	7	SER	CYS	engineered mutation	UNP P33176
D	65	ALA	CYS	engineered mutation	UNP P33176
D	87	ALA	THR	engineered mutation	UNP P33176
D	168	ALA	CYS	engineered mutation	UNP P33176
D	174	SER	CYS	engineered mutation	UNP P33176
D	294	ALA	CYS	engineered mutation	UNP P33176
E	7	SER	CYS	engineered mutation	UNP P33176
E	65	ALA	CYS	engineered mutation	UNP P33176
E	87	ALA	THR	engineered mutation	UNP P33176
E	168	ALA	CYS	engineered mutation	UNP P33176
E	174	SER	CYS	engineered mutation	UNP P33176
E	294	ALA	CYS	engineered mutation	UNP P33176
K	7	SER	CYS	engineered mutation	UNP P33176
K	65	ALA	CYS	engineered mutation	UNP P33176
K	87	ALA	THR	engineered mutation	UNP P33176
K	168	ALA	CYS	engineered mutation	UNP P33176
K	174	SER	CYS	engineered mutation	UNP P33176
K	294	ALA	CYS	engineered mutation	UNP P33176

- 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		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	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	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		

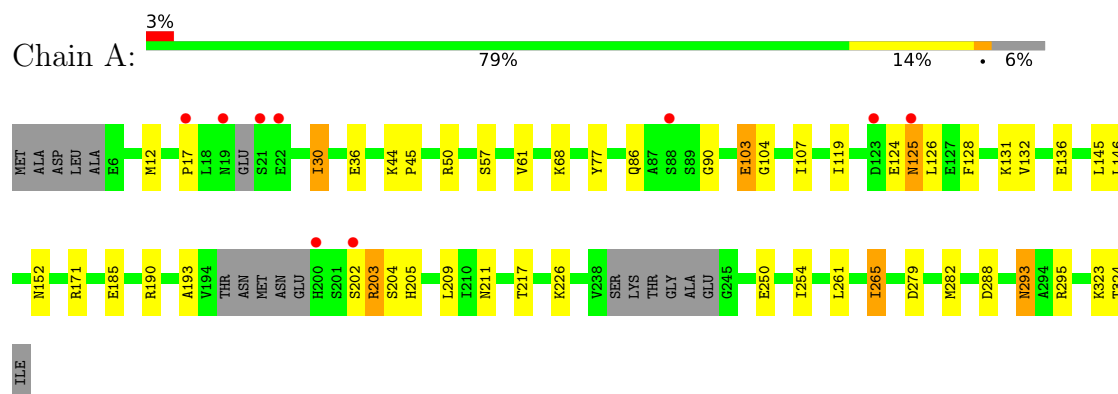
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	45	Total	O	0	0
			45	45		
3	B	28	Total	O	0	0
			28	28		
3	C	36	Total	O	0	0
			36	36		
3	D	40	Total	O	0	0
			40	40		
3	E	27	Total	O	0	0
			27	27		
3	K	24	Total	O	0	0
			24	24		

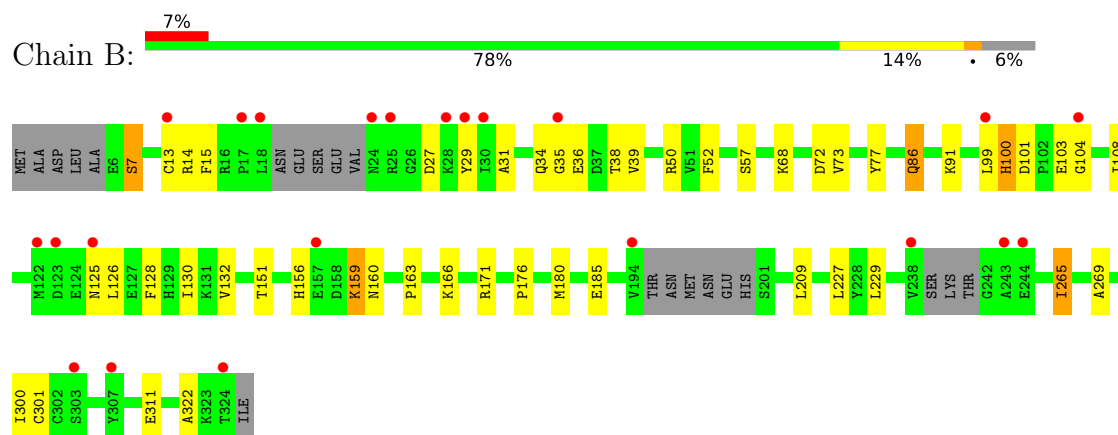
3 Residue-property plots [i](#)

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.

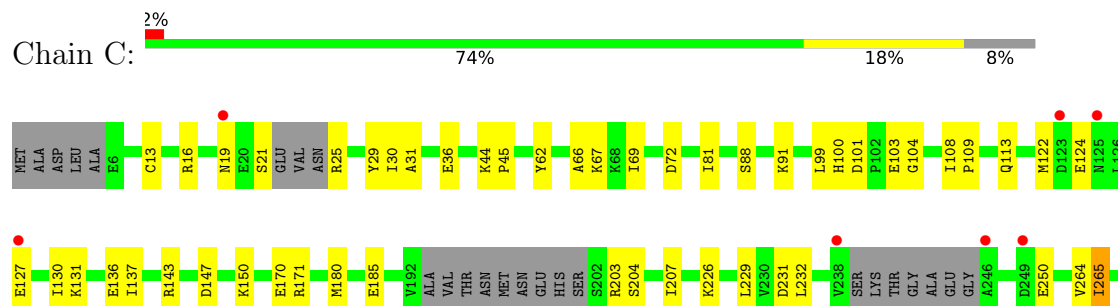
• Molecule 1: Kinesin-1 heavy chain



• Molecule 1: Kinesin-1 heavy chain

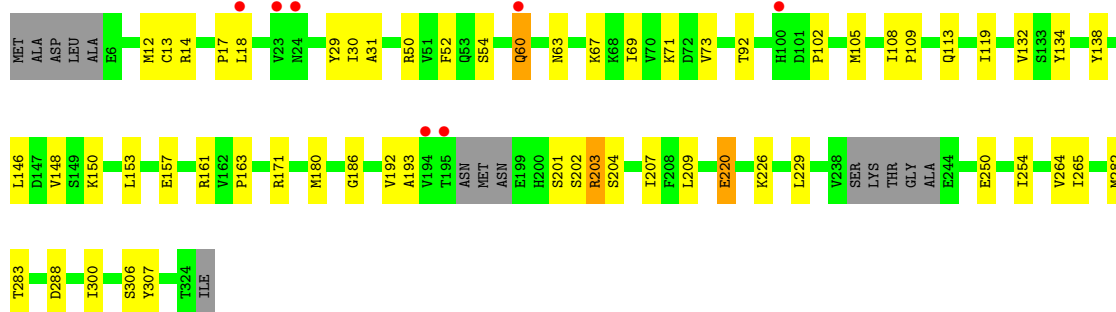
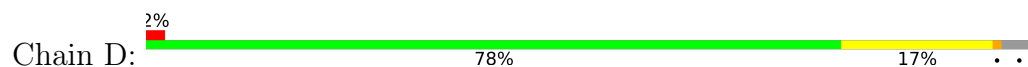


• Molecule 1: Kinesin-1 heavy chain

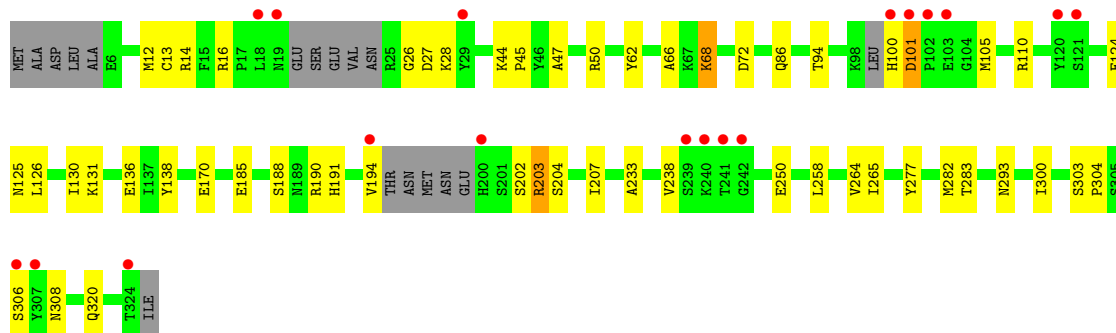
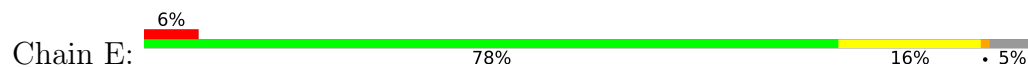




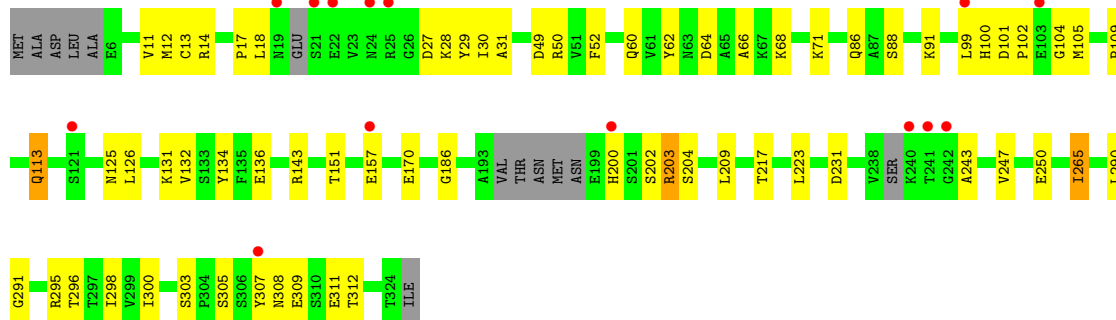
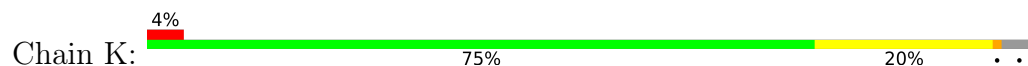
- Molecule 1: Kinesin-1 heavy chain



- Molecule 1: Kinesin-1 heavy chain



- Molecule 1: Kinesin-1 heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	56.67Å 101.30Å 101.53Å 119.57° 91.91° 91.75°	Depositor
Resolution (Å)	33.18 – 2.59 33.18 – 2.59	Depositor EDS
% Data completeness (in resolution range)	97.2 (33.18-2.59) 92.3 (33.18-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.21 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.203 , 0.263 0.208 , 0.265	Depositor DCC
R_{free} test set	2926 reflections (4.34%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.567	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 61.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.025 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14006	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.53% 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	0.68	0/2368	1.01	2/3200 (0.1%)
1	B	0.59	0/2286	0.97	2/3098 (0.1%)
1	C	0.64	0/2315	0.97	1/3129 (0.0%)
1	D	0.63	0/2370	0.96	0/3205
1	E	0.60	0/2287	0.96	5/3103 (0.2%)
1	K	0.62	0/2348	1.00	4/3180 (0.1%)
All	All	0.63	0/13974	0.98	14/18915 (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	1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	309	GLU	N-CA-C	-6.76	103.98	111.82
1	E	238	VAL	N-CA-C	6.29	116.77	110.23
1	B	151	THR	N-CA-C	6.10	119.20	111.69
1	A	103	GLU	N-CA-C	5.94	121.97	114.31
1	E	303	SER	N-CA-C	-5.84	102.41	109.83
1	K	17	PRO	CA-C-O	-5.67	115.09	122.12
1	E	101	ASP	CA-C-N	5.29	139.69	127.00
1	E	101	ASP	C-N-CA	5.29	139.69	127.00
1	B	7	SER	N-CA-C	5.17	117.81	111.82
1	C	67	LYS	N-CA-C	5.15	117.28	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	203	ARG	N-CA-C	5.14	121.75	110.80
1	A	30	ILE	N-CA-C	5.02	119.79	109.34
1	K	17	PRO	CA-C-N	5.02	130.74	121.70
1	K	17	PRO	C-N-CA	5.02	130.74	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	17	PRO	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	2334	0	2216	37	0
1	B	2251	0	2098	36	0
1	C	2280	0	2165	33	0
1	D	2335	0	2219	34	0
1	E	2253	0	2064	28	0
1	K	2313	0	2170	35	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	15	0	0	0	0
2	E	5	0	0	0	0
2	K	5	0	0	0	0
3	A	45	0	0	4	0
3	B	28	0	0	0	0
3	C	36	0	0	4	0
3	D	40	0	0	6	0
3	E	27	0	0	3	0
3	K	24	0	0	1	0
All	All	14006	0	12932	201	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 8.

All (201) 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:12:MET:HG2	1:A:50:ARG:HB2	1.51	0.91
1:C:16:ARG:NH1	1:C:88:SER:O	2.18	0.76
1:A:202:SER:O	1:A:204:SER:N	2.21	0.74
1:D:226:LYS:NZ	1:D:288:ASP:OD2	2.19	0.74
1:C:69:ILE:HG21	3:C:521:HOH:O	1.86	0.73
1:E:202:SER:O	1:E:204:SER:N	2.20	0.73
1:B:86:GLN:HG2	1:B:311:GLU:HB2	1.71	0.73
1:B:29:TYR:CZ	1:B:31:ALA:HB3	2.23	0.73
1:D:12:MET:HG2	1:D:50:ARG:HB2	1.72	0.72
1:D:220:GLU:OE2	3:D:501:HOH:O	2.06	0.72
1:E:190:ARG:O	3:E:501:HOH:O	2.08	0.71
1:C:103:GLU:H	1:C:104:GLY:HA3	1.58	0.69
1:A:12:MET:HE2	1:A:50:ARG:HG3	1.74	0.68
1:D:157:GLU:OE1	1:D:161:ARG:NH2	2.27	0.67
1:B:156:HIS:CE1	1:B:166:LYS:HD3	2.30	0.67
1:K:101:ASP:OD2	1:K:104:GLY:N	2.27	0.66
1:D:203:ARG:HA	1:D:254:ILE:HD11	1.78	0.65
1:E:13:CYS:HA	1:E:300:ILE:HG13	1.79	0.65
1:A:103:GLU:N	1:A:104:GLY:HA3	2.12	0.65
1:D:119:ILE:O	3:D:502:HOH:O	2.14	0.64
1:A:226:LYS:NZ	1:A:288:ASP:OD2	2.27	0.64
1:B:34:GLN:OE1	1:B:36:GLU:N	2.31	0.64
1:C:113:GLN:NE2	3:C:502:HOH:O	2.30	0.63
1:K:12:MET:HG2	1:K:50:ARG:HB2	1.81	0.62
1:C:109:PRO:HA	1:C:180:MET:HE1	1.81	0.61
1:K:13:CYS:HA	1:K:300:ILE:HG13	1.84	0.60
1:A:103:GLU:H	1:A:104:GLY:HA3	1.65	0.59
1:A:132:VAL:HG23	3:A:518:HOH:O	2.02	0.59
1:K:68:LYS:NZ	1:K:295:ARG:HH11	2.00	0.59
1:E:293:ASN:ND2	3:E:503:HOH:O	2.35	0.58
1:E:185:GLU:O	1:E:188:SER:OG	2.21	0.58
1:E:131:LYS:HD2	1:E:170:GLU:HB3	1.86	0.57
1:K:60:GLN:NE2	1:K:64:ASP:OD2	2.36	0.57
1:E:207:ILE:HD11	1:E:282:MET:HE2	1.86	0.57
1:D:17:PRO:HB3	1:D:54:SER:HB3	1.85	0.57
1:C:293:ASN:OD1	3:C:501:HOH:O	2.17	0.56
1:K:202:SER:O	1:K:204:SER:N	2.38	0.56
1:K:243:ALA:HB1	1:K:247:VAL:HG23	1.87	0.56
1:E:14:ARG:NH2	1:E:94:THR:OG1	2.33	0.56
1:D:113:GLN:HG2	3:D:540:HOH:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:99:LEU:HD13	1:K:100:HIS:ND1	2.21	0.55
1:C:108:ILE:HG12	1:C:229:LEU:HD13	1.87	0.55
1:B:156:HIS:HE1	1:B:166:LYS:HD3	1.71	0.55
1:D:60:GLN:NE2	1:D:63:ASN:HD22	2.04	0.55
1:D:17:PRO:HD3	1:D:54:SER:HA	1.90	0.54
1:K:303:SER:O	1:K:312:THR:HG21	2.08	0.53
1:E:190:ARG:CZ	1:E:202:SER:HB2	2.39	0.53
1:A:211:ASN:HD22	1:A:226:LYS:HG2	1.74	0.53
1:D:14:ARG:HG3	1:D:52:PHE:HB2	1.91	0.52
1:B:73:VAL:HG21	1:B:227:LEU:HB2	1.92	0.52
1:K:91:LYS:HE3	1:K:231:ASP:OD2	2.10	0.52
1:B:108:ILE:HG12	1:B:229:LEU:HD13	1.91	0.52
1:E:68:LYS:NZ	1:E:72:ASP:OD2	2.35	0.52
1:C:147:ASP:OD2	1:C:150:LYS:HG3	2.11	0.51
1:E:26:GLY:O	1:E:28:LYS:N	2.33	0.51
1:D:264:VAL:HG21	1:D:283:THR:HG21	1.93	0.51
1:B:29:TYR:CE2	1:B:31:ALA:HB3	2.46	0.51
1:D:202:SER:O	1:D:204:SER:N	2.44	0.50
1:B:34:GLN:OE1	1:B:35:GLY:N	2.44	0.50
1:E:12:MET:HE2	1:E:50:ARG:HH11	1.77	0.50
1:A:57:SER:HB3	1:B:57:SER:HB3	1.94	0.50
1:B:265:ILE:HG23	1:B:322:ALA:HB2	1.93	0.50
1:A:203:ARG:HD3	1:A:250:GLU:OE1	2.11	0.49
1:D:67:LYS:HG2	1:D:71:LYS:HE2	1.93	0.49
1:A:68:LYS:NZ	1:A:295:ARG:HH11	2.10	0.49
1:D:69:ILE:O	1:D:73:VAL:HG23	2.13	0.49
1:E:264:VAL:HG21	1:E:283:THR:HG21	1.95	0.48
1:K:307:TYR:CG	1:K:308:ASN:N	2.81	0.48
1:C:207:ILE:HD11	1:C:282:MET:HE2	1.95	0.48
1:A:125:ASN:HA	1:A:217:THR:HB	1.96	0.48
1:C:130:ILE:HD12	1:C:130:ILE:N	2.29	0.48
1:C:131:LYS:HD2	1:C:170:GLU:HB3	1.94	0.48
1:E:16:ARG:O	1:E:304:PRO:HG3	2.13	0.48
1:B:7:SER:HB3	1:B:269:ALA:HA	1.95	0.48
1:B:34:GLN:CB	1:B:38:THR:HB	2.43	0.48
1:E:306:SER:C	1:E:308:ASN:H	2.20	0.48
1:A:36:GLU:HB3	1:A:50:ARG:HH21	1.77	0.48
1:B:13:CYS:HA	1:B:300:ILE:HG13	1.95	0.48
1:C:72:ASP:OD2	1:C:295:ARG:HG3	2.13	0.48
1:K:307:TYR:CD1	1:K:308:ASN:N	2.81	0.48
1:B:99:LEU:O	1:B:100:HIS:ND1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:TYR:HE1	1:A:293:ASN:HD22	1.60	0.47
1:B:101:ASP:C	1:B:103:GLU:H	2.22	0.47
1:C:171:ARG:HH12	1:C:185:GLU:CD	2.22	0.47
1:C:226:LYS:NZ	1:C:288:ASP:OD2	2.39	0.47
1:K:62:TYR:CD1	1:K:66:ALA:HB3	2.50	0.47
1:A:125:ASN:O	1:A:126:LEU:HD12	2.15	0.47
1:C:264:VAL:HG21	1:C:283:THR:HG21	1.97	0.47
1:D:207:ILE:HD11	1:D:282:MET:HE2	1.96	0.47
1:B:159:LYS:HE2	1:B:160:ASN:OD1	2.14	0.47
1:C:277:TYR:O	1:C:283:THR:OG1	2.25	0.47
1:K:132:VAL:HA	1:K:209:LEU:O	2.15	0.47
1:C:21:SER:HA	1:C:25:ARG:N	2.30	0.46
1:B:126:LEU:HB3	1:B:128:PHE:CE1	2.51	0.46
1:D:109:PRO:HA	1:D:180:MET:HE1	1.97	0.46
1:A:132:VAL:HA	1:A:209:LEU:O	2.15	0.46
1:A:211:ASN:ND2	1:A:226:LYS:CG	2.79	0.46
1:E:105:MET:O	1:E:110:ARG:NH1	2.44	0.46
1:C:99:LEU:C	1:C:101:ASP:H	2.23	0.46
1:K:88:SER:O	1:K:88:SER:OG	2.27	0.46
1:A:202:SER:C	1:A:204:SER:H	2.20	0.46
1:C:29:TYR:O	1:C:31:ALA:N	2.49	0.46
1:K:68:LYS:HZ3	1:K:295:ARG:HH11	1.63	0.46
1:B:171:ARG:HH12	1:B:185:GLU:CD	2.23	0.46
1:D:134:TYR:CD2	1:D:186:GLY:HA3	2.51	0.45
1:K:105:MET:HB2	1:K:109:PRO:HG2	1.98	0.45
1:E:277:TYR:O	1:E:283:THR:OG1	2.28	0.45
1:K:68:LYS:HZ3	1:K:295:ARG:HG3	1.80	0.45
1:E:130:ILE:HD12	1:E:130:ILE:N	2.32	0.45
1:B:91:LYS:HA	1:B:301:CYS:SG	2.56	0.45
1:C:81:ILE:HG13	3:C:521:HOH:O	2.16	0.45
1:A:211:ASN:HD22	1:A:226:LYS:CG	2.29	0.45
1:A:261:LEU:HG	1:A:265:ILE:HD12	1.99	0.45
1:B:29:TYR:HD1	1:B:29:TYR:HA	1.63	0.45
1:B:103:GLU:H	1:B:104:GLY:HA3	1.81	0.45
1:E:47:ALA:O	1:E:320:GLN:NE2	2.45	0.45
1:K:134:TYR:CD2	1:K:186:GLY:HA3	2.52	0.45
1:A:152:ASN:OD1	1:D:171:ARG:NH2	2.44	0.45
1:B:99:LEU:O	1:B:100:HIS:HB3	2.16	0.45
1:B:130:ILE:HD12	1:B:130:ILE:N	2.32	0.45
1:D:102:PRO:HA	1:D:105:MET:HE2	1.97	0.45
1:K:131:LYS:HD2	1:K:170:GLU:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:GLU:OE2	1:C:143:ARG:NH1	2.50	0.45
1:D:138:TYR:OH	1:D:250:GLU:OE2	2.30	0.45
1:A:279:ASP:HB2	3:A:522:HOH:O	2.17	0.44
1:K:14:ARG:HG3	1:K:52:PHE:HB2	2.00	0.44
1:A:171:ARG:NH1	1:A:185:GLU:OE1	2.40	0.44
1:B:99:LEU:O	1:B:99:LEU:HD12	2.18	0.44
1:D:163:PRO:HD2	1:D:288:ASP:HB3	2.00	0.44
1:B:99:LEU:O	1:B:100:HIS:CB	2.64	0.44
1:E:62:TYR:CD1	1:E:66:ALA:HB3	2.53	0.43
1:E:264:VAL:HG23	3:E:505:HOH:O	2.17	0.43
1:A:205:HIS:CB	1:A:282:MET:HE1	2.48	0.43
1:A:324:THR:HG23	3:A:515:HOH:O	2.18	0.43
1:K:102:PRO:HA	1:K:105:MET:HE2	2.01	0.43
1:K:308:ASN:HB3	1:K:311:GLU:CB	2.48	0.43
1:D:92:THR:HA	3:D:537:HOH:O	2.17	0.43
1:A:131:LYS:NZ	3:A:504:HOH:O	2.40	0.43
1:A:190:ARG:CZ	1:A:202:SER:HB3	2.48	0.43
1:D:148:VAL:HG22	3:D:526:HOH:O	2.19	0.43
1:E:138:TYR:CE1	1:E:250:GLU:HG2	2.54	0.43
1:K:28:LYS:O	1:K:305:SER:HA	2.18	0.43
1:K:203:ARG:HD3	1:K:250:GLU:OE1	2.18	0.43
1:K:290:LEU:HD13	1:K:296:THR:HG21	2.00	0.43
1:B:99:LEU:C	1:B:100:HIS:HD1	2.27	0.43
1:C:91:LYS:NZ	1:C:232:LEU:O	2.42	0.43
1:K:29:TYR:O	1:K:31:ALA:N	2.51	0.43
1:D:150:LYS:HB3	1:D:153:LEU:HD21	2.00	0.43
1:A:44:LYS:HA	1:A:45:PRO:HD3	1.91	0.43
1:C:62:TYR:CD1	1:C:66:ALA:HB3	2.54	0.43
1:D:13:CYS:HA	1:D:300:ILE:HG13	2.01	0.43
1:D:17:PRO:HA	1:D:18:LEU:HA	1.80	0.42
1:E:125:ASN:O	1:E:126:LEU:HD12	2.19	0.42
1:K:136:GLU:OE2	1:K:143:ARG:NH1	2.52	0.42
1:B:125:ASN:O	1:B:126:LEU:HD12	2.19	0.42
1:E:136:GLU:OE2	1:E:191:HIS:ND1	2.40	0.42
1:K:265:ILE:HD13	1:K:298:ILE:HD11	2.01	0.42
1:A:211:ASN:ND2	1:A:226:LYS:HG3	2.34	0.42
1:B:159:LYS:HE2	1:B:159:LYS:HB3	1.65	0.42
1:D:193:ALA:HB3	1:D:203:ARG:HD2	2.01	0.42
1:B:156:HIS:O	1:B:163:PRO:HA	2.19	0.42
1:E:233:ALA:O	1:E:258:LEU:HD11	2.19	0.42
1:K:125:ASN:HA	1:K:217:THR:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:ASP:HB3	1:B:77:TYR:HB2	2.02	0.42
1:C:91:LYS:HE3	1:C:231:ASP:OD1	2.20	0.42
1:C:203:ARG:HD3	1:C:250:GLU:OE1	2.20	0.42
1:D:226:LYS:NZ	3:D:504:HOH:O	2.46	0.42
1:K:125:ASN:O	1:K:126:LEU:HD12	2.19	0.42
1:B:132:VAL:HA	1:B:209:LEU:O	2.20	0.42
1:C:103:GLU:N	1:C:104:GLY:HA3	2.26	0.42
1:D:108:ILE:HG12	1:D:229:LEU:HD13	2.01	0.42
1:D:29:TYR:O	1:D:31:ALA:N	2.53	0.41
1:E:50:ARG:HH11	1:E:50:ARG:HG3	1.85	0.41
1:K:49:ASP:O	1:K:50:ARG:HG2	2.20	0.41
1:A:61:VAL:HG12	1:A:107:ILE:HD11	2.01	0.41
1:A:323:LYS:HA	1:A:323:LYS:HD2	1.86	0.41
1:E:44:LYS:HA	1:E:45:PRO:HD3	1.97	0.41
1:B:265:ILE:CG2	1:B:322:ALA:HB2	2.50	0.41
1:C:44:LYS:HA	1:C:45:PRO:HD3	1.93	0.41
1:A:136:GLU:HG2	1:A:145:LEU:HD21	2.00	0.41
1:C:109:PRO:HA	1:C:180:MET:CE	2.49	0.41
1:K:291:GLY:N	3:K:501:HOH:O	2.34	0.41
1:D:132:VAL:HA	1:D:209:LEU:O	2.21	0.41
1:D:192:VAL:HG13	1:D:201:SER:O	2.21	0.41
1:E:100:HIS:O	1:E:100:HIS:ND1	2.53	0.41
1:B:176:PRO:O	1:B:180:MET:HG2	2.21	0.41
1:K:105:MET:HE1	1:K:113:GLN:HE22	1.86	0.41
1:A:146:LEU:HD23	1:A:146:LEU:HA	1.88	0.41
1:C:137:ILE:O	1:C:204:SER:HB2	2.20	0.41
1:C:265:ILE:HD13	1:C:298:ILE:HD11	2.03	0.41
1:B:15:PHE:CE2	1:B:39:VAL:HG21	2.56	0.41
1:C:122:MET:C	1:C:124:GLU:H	2.29	0.41
1:A:90:GLY:N	2:A:401:SO4:O4	2.36	0.40
1:K:223:LEU:HA	1:K:223:LEU:HD23	1.73	0.40
1:C:13:CYS:HA	1:C:300:ILE:HG13	2.02	0.40
1:D:146:LEU:HD23	1:D:146:LEU:HA	1.91	0.40
1:A:193:ALA:HB3	1:A:203:ARG:HD2	2.02	0.40
1:B:14:ARG:HG3	1:B:52:PHE:HB2	2.03	0.40
1:C:171:ARG:NH1	1:C:185:GLU:OE1	2.49	0.40
1:A:119:ILE:HG12	1:A:128:PHE:CD1	2.57	0.40
1:A:203:ARG:HA	1:A:254:ILE:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	300/325 (92%)	290 (97%)	6 (2%)	4 (1%)	9	21
1	B	297/325 (91%)	282 (95%)	14 (5%)	1 (0%)	36	58
1	C	292/325 (90%)	280 (96%)	9 (3%)	3 (1%)	12	28
1	D	305/325 (94%)	292 (96%)	10 (3%)	3 (1%)	12	28
1	E	300/325 (92%)	284 (95%)	13 (4%)	3 (1%)	12	28
1	K	304/325 (94%)	292 (96%)	8 (3%)	4 (1%)	9	21
All	All	1798/1950 (92%)	1720 (96%)	60 (3%)	18 (1%)	12	28

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	ILE
1	A	124	GLU
1	A	203	ARG
1	D	30	ILE
1	D	203	ARG
1	E	203	ARG
1	K	203	ARG
1	A	125	ASN
1	B	100	HIS
1	D	307	TYR
1	E	27	ASP
1	K	18	LEU
1	C	30	ILE
1	C	100	HIS
1	K	30	ILE
1	C	19	ASN
1	E	101	ASP
1	K	200	HIS

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	248/285 (87%)	245 (99%)	3 (1%)	63	83
1	B	230/285 (81%)	224 (97%)	6 (3%)	40	68
1	C	241/285 (85%)	237 (98%)	4 (2%)	53	78
1	D	244/285 (86%)	240 (98%)	4 (2%)	55	79
1	E	221/285 (78%)	216 (98%)	5 (2%)	44	71
1	K	234/285 (82%)	226 (97%)	8 (3%)	32	60
All	All	1418/1710 (83%)	1388 (98%)	30 (2%)	47	73

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	GLN
1	A	265	ILE
1	A	293	ASN
1	B	27	ASP
1	B	50	ARG
1	B	68	LYS
1	B	86	GLN
1	B	159	LYS
1	B	265	ILE
1	C	36	GLU
1	C	127	GLU
1	C	265	ILE
1	C	323	LYS
1	D	60	GLN
1	D	220	GLU
1	D	265	ILE
1	D	306	SER
1	E	68	LYS
1	E	86	GLN
1	E	124	GLU
1	E	194	VAL
1	E	265	ILE

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Mol	Chain	Res	Type
1	K	11	VAL
1	K	27	ASP
1	K	71	LYS
1	K	86	GLN
1	K	113	GLN
1	K	151	THR
1	K	157	GLU
1	K	265	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	GLN
1	A	189	ASN
1	A	211	ASN
1	A	293	ASN
1	B	53	GLN
1	B	86	GLN
1	B	93	HIS
1	B	308	ASN
1	C	113	GLN
1	C	189	ASN
1	C	293	ASN
1	D	60	GLN
1	D	189	ASN
1	E	86	GLN
1	E	293	ASN
1	K	58	GLN
1	K	86	GLN
1	K	113	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	A	401	-	4,4,4	0.27	0	6,6,6	0.16	0
2	SO4	D	402	-	4,4,4	0.28	0	6,6,6	0.25	0
2	SO4	C	401	-	4,4,4	0.29	0	6,6,6	0.27	0
2	SO4	D	403	-	4,4,4	0.39	0	6,6,6	0.16	0
2	SO4	B	401	-	4,4,4	0.26	0	6,6,6	0.20	0
2	SO4	D	401	-	4,4,4	0.24	0	6,6,6	0.23	0
2	SO4	K	401	-	4,4,4	0.26	0	6,6,6	0.40	0
2	SO4	E	401	-	4,4,4	0.27	0	6,6,6	0.16	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	SO4	1	0

5.7 Other polymers [i](#)

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	307/325 (94%)	0.19	9 (2%) 53 48	15, 36, 71, 95	1 (0%)
1	B	305/325 (93%)	0.57	22 (7%) 21 17	28, 54, 90, 117	0
1	C	300/325 (92%)	0.29	7 (2%) 61 55	19, 40, 71, 90	0
1	D	311/325 (95%)	0.28	7 (2%) 61 55	22, 41, 72, 100	0
1	E	308/325 (94%)	0.48	18 (5%) 29 23	24, 51, 88, 117	0
1	K	312/325 (96%)	0.35	14 (4%) 38 32	23, 48, 88, 108	0
All	All	1843/1950 (94%)	0.36	77 (4%) 40 35	15, 45, 84, 117	1 (0%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	239	SER	4.4
1	C	19	ASN	4.0
1	B	29	TYR	3.8
1	E	240	LYS	3.7
1	K	24	ASN	3.6
1	K	19	ASN	3.6
1	B	35	GLY	3.6
1	B	18	LEU	3.5
1	K	307	TYR	3.3
1	K	21	SER	3.3
1	A	21	SER	3.3
1	E	103	GLU	3.3
1	B	24	ASN	3.2
1	E	102	PRO	3.2
1	E	241	THR	3.2
1	E	19	ASN	3.1
1	B	30	ILE	3.1
1	D	60	GLN	3.1
1	A	19	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	202	SER	3.0
1	K	99	LEU	3.0
1	B	125	ASN	3.0
1	E	18	LEU	2.9
1	B	99	LEU	2.9
1	C	125	ASN	2.9
1	B	303	SER	2.8
1	B	13	CYS	2.8
1	B	324	THR	2.8
1	A	200	HIS	2.7
1	K	157	GLU	2.6
1	B	194	VAL	2.6
1	K	121	SER	2.6
1	B	104	GLY	2.5
1	K	103	GLU	2.5
1	C	249	ASP	2.5
1	B	122	MET	2.5
1	E	200	HIS	2.5
1	B	243	ALA	2.5
1	D	23	VAL	2.5
1	D	24	ASN	2.5
1	E	194	VAL	2.5
1	E	101	ASP	2.4
1	B	123	ASP	2.4
1	E	100	HIS	2.4
1	K	241	THR	2.4
1	K	200	HIS	2.4
1	C	127	GLU	2.4
1	B	28	LYS	2.3
1	D	195	THR	2.3
1	E	29	TYR	2.3
1	K	22	GLU	2.3
1	B	307	TYR	2.3
1	A	125	ASN	2.3
1	A	17	PRO	2.2
1	D	100	HIS	2.2
1	E	242	GLY	2.2
1	B	244	GLU	2.2
1	C	238	VAL	2.2
1	E	120	TYR	2.2
1	E	121	SER	2.2
1	A	123	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	123	ASP	2.2
1	A	88	SER	2.1
1	E	306	SER	2.1
1	B	17	PRO	2.1
1	K	240	LYS	2.1
1	D	18	LEU	2.1
1	K	242	GLY	2.1
1	E	307	TYR	2.1
1	K	25	ARG	2.1
1	D	194	VAL	2.1
1	C	246	ALA	2.1
1	A	22	GLU	2.1
1	B	25	ARG	2.0
1	B	238	VAL	2.0
1	B	157	GLU	2.0
1	E	324	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 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	403	5/5	0.73	0.27	60,63,64,64	0
2	SO4	D	402	5/5	0.77	0.20	63,63,66,71	0
2	SO4	K	401	5/5	0.86	0.10	61,65,68,68	0
2	SO4	B	401	5/5	0.89	0.09	68,68,71,78	0
2	SO4	E	401	5/5	0.90	0.10	68,69,77,78	0
2	SO4	A	401	5/5	0.92	0.08	49,54,56,58	0
2	SO4	C	401	5/5	0.94	0.08	38,58,62,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	D	401	5/5	0.94	0.09	44,47,53,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.