



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2017 – 05:58 PM EST

PDB ID : 5LT4
Title : nucleotide-free kinesin-1 motor domain T92V mutant, P1 crystal form
Authors : Cao, L.; Gigant, B.
Deposited on : 2016-09-06
Resolution : 2.88 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

<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

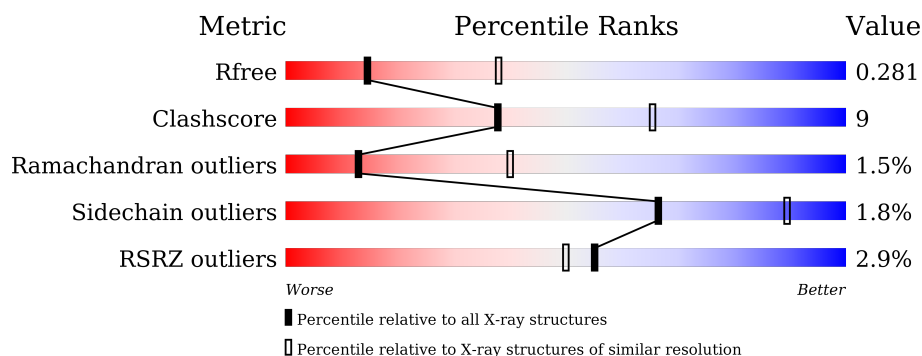
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 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}	91344	1945 (2.90-2.86)
Clashscore	102246	2202 (2.90-2.86)
Ramachandran outliers	100387	2149 (2.90-2.86)
Sidechain outliers	100360	2152 (2.90-2.86)
RSRZ outliers	91569	1950 (2.90-2.86)

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. 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	<div> <div>3%</div> <div>78% 17% . .</div> </div>
1	B	325	<div> <div>4%</div> <div>73% 20% . 5%</div> </div>
1	C	325	<div> <div>%</div> <div>73% 21% . 5%</div> </div>
1	D	325	<div> <div>2%</div> <div>82% 13% .</div> </div>
1	E	325	<div> <div>3%</div> <div>72% 21% . 6%</div> </div>
1	K	325	<div> <div>3%</div> <div>73% 21% . 6%</div> </div>

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	C	402	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14147 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	313	Total	C	N	O	S	0	0	0
			2362	1476	401	476	9			
1	B	308	Total	C	N	O	S	0	0	0
			2274	1425	390	450	9			
1	C	308	Total	C	N	O	S	0	0	0
			2322	1454	398	461	9			
1	D	311	Total	C	N	O	S	0	1	0
			2338	1466	399	464	9			
1	E	305	Total	C	N	O	S	0	0	0
			2244	1406	384	445	9			
1	K	307	Total	C	N	O	S	0	0	0
			2295	1439	393	454	9			

There are 36 discrepancies between the modelled and reference sequences:

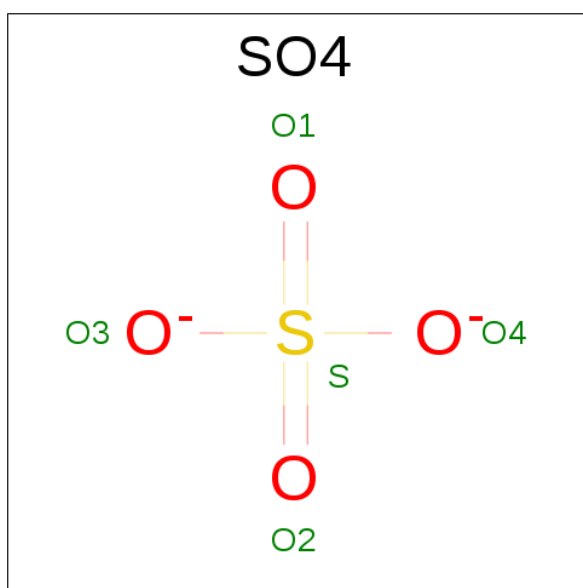
Chain	Residue	Modelled	Actual	Comment	Reference
A	7	SER	CYS	engineered mutation	UNP P33176
A	65	ALA	CYS	engineered mutation	UNP P33176
A	92	VAL	THR	engineered mutation	UNP P33176
A	168	ALA	CYS	engineered mutation	UNP P33176
A	174	SER	CYS	engineered mutation	UNP P33176
A	294	ALA	CYS	engineered mutation	UNP P33176
B	7	SER	CYS	engineered mutation	UNP P33176
B	65	ALA	CYS	engineered mutation	UNP P33176
B	92	VAL	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	92	VAL	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	92	VAL	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	92	VAL	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	92	VAL	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 (three-letter code: SO4) (formula: O₄S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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	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	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		

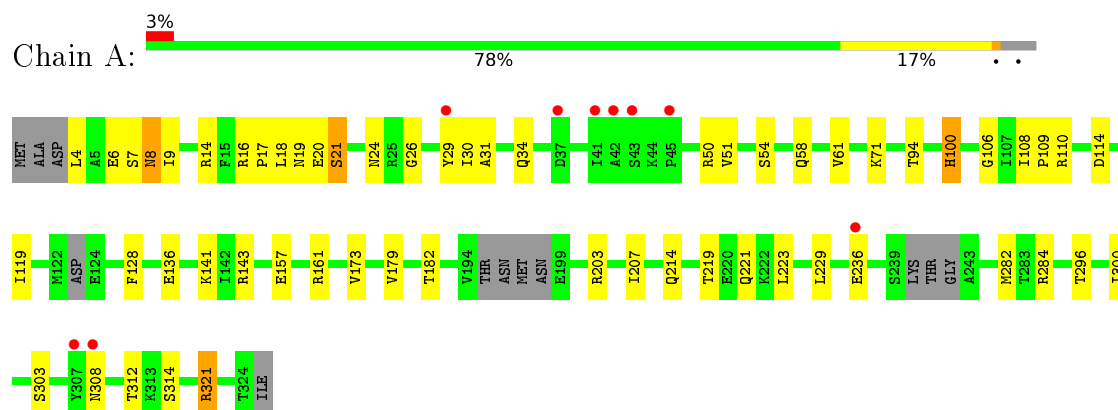
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	60	Total	O	0	0
			60	60		
3	B	16	Total	O	0	0
			16	16		
3	C	67	Total	O	0	0
			67	67		
3	D	43	Total	O	0	0
			43	43		
3	E	33	Total	O	0	0
			33	33		
3	K	33	Total	O	0	0
			33	33		

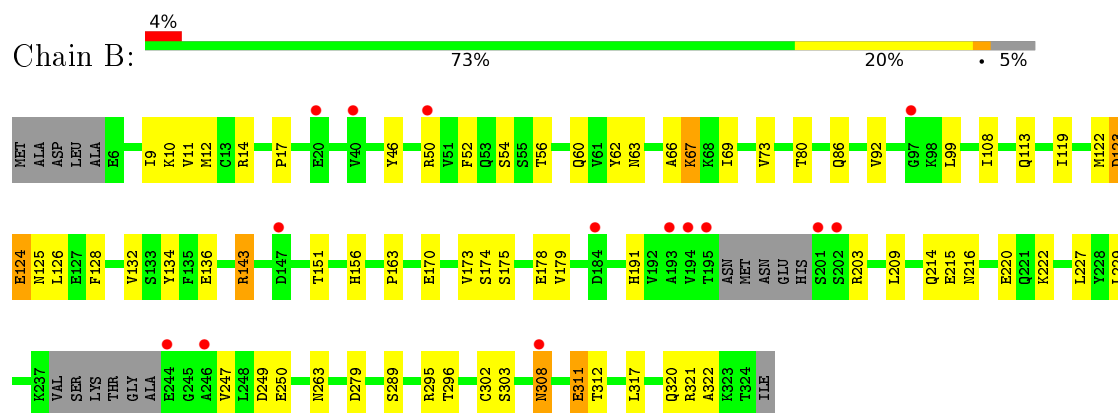
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

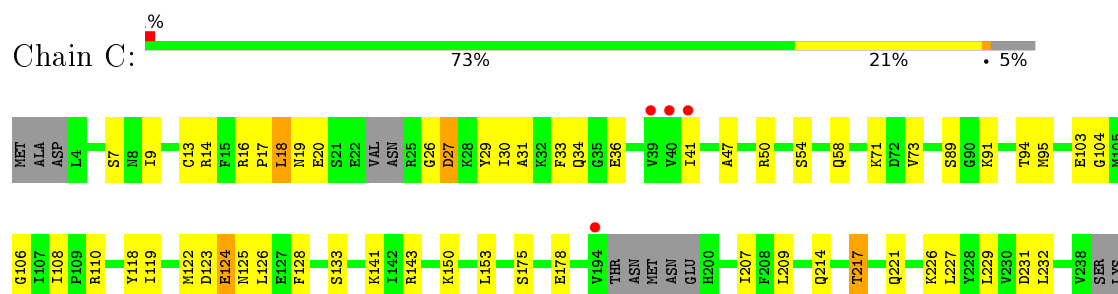
- Molecule 1: Kinesin-1 heavy chain



- Molecule 1: Kinesin-1 heavy chain

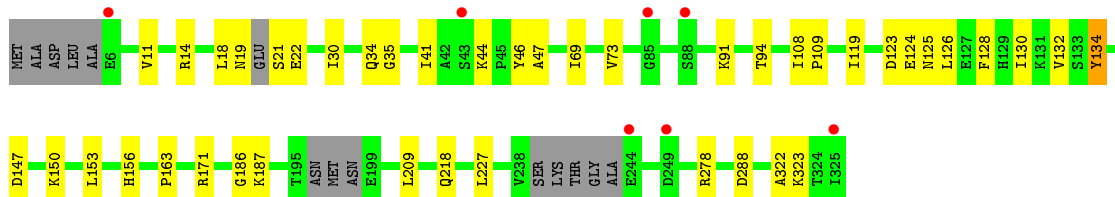
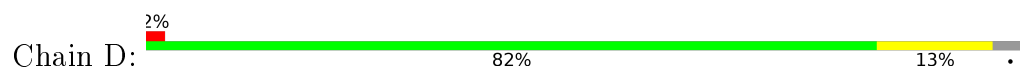


- Molecule 1: Kinesin-1 heavy chain

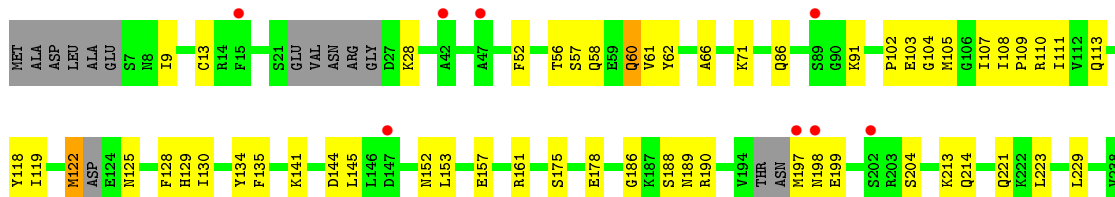
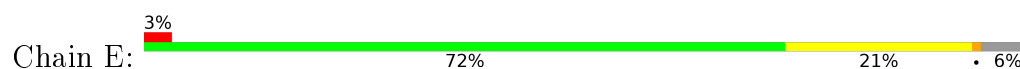




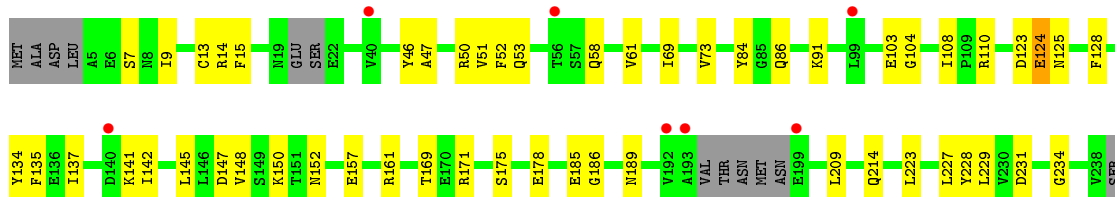
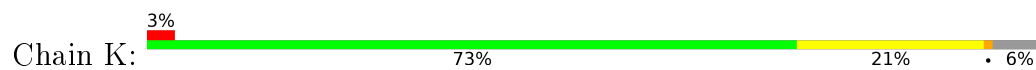
• Molecule 1: Kinesin-1 heavy chain



• 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	57.15Å 102.11Å 102.14Å 119.49° 91.95° 91.85°	Depositor
Resolution (Å)	49.28 – 2.88 49.28 – 2.87	Depositor EDS
% Data completeness (in resolution range)	97.1 (49.28-2.88) 75.3 (49.28-2.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.205 , 0.280 0.207 , 0.281	Depositor DCC
R_{free} test set	1882 reflections (4.59%)	DCC
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.472	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 62.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.008 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14147	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 3.87% 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	0.58	0/2397	0.74	1/3244 (0.0%)
1	B	0.53	0/2310	0.70	0/3136
1	C	0.54	0/2357	0.75	1/3188 (0.0%)
1	D	0.53	0/2373	0.70	0/3212
1	E	0.49	0/2277	0.67	0/3089
1	K	0.51	0/2329	0.71	0/3153
All	All	0.53	0/14043	0.71	2/19022 (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	A	0	1
1	K	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	18	LEU	N-CA-C	-7.09	91.87	111.00
1	A	16	ARG	C-N-CD	5.37	139.68	128.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	HIS	Peptide
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	2236	31	0
1	B	2274	0	2095	49	0
1	C	2322	0	2197	46	0
1	D	2338	0	2211	24	0
1	E	2244	0	2061	51	0
1	K	2295	0	2166	46	0
2	A	10	0	0	0	0
2	B	5	0	0	1	0
2	C	10	0	0	1	0
2	D	20	0	0	1	0
2	E	5	0	0	0	0
2	K	10	0	0	2	0
3	A	60	0	0	5	0
3	B	16	0	0	1	0
3	C	67	0	0	3	0
3	D	43	0	0	2	0
3	E	33	0	0	5	0
3	K	33	0	0	4	0
All	All	14147	0	12966	246	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 9.

All (246) 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:D:47:ALA:O	1:D:323:LYS:NZ	2.00	0.94
1:E:141:LYS:HE3	1:E:152:ASN:HB2	1.50	0.92
1:B:124:GLU:HG3	1:B:125:ASN:H	1.37	0.90
1:B:263:ASN:OD1	1:B:321:ARG:NH2	2.06	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:263:ASN:OD1	1:K:321:ARG:NH2	2.08	0.85
1:C:29:TYR:O	1:C:31:ALA:N	2.15	0.79
1:B:126:LEU:HD12	1:B:215:GLU:O	1.83	0.79
1:K:288:ASP:OD1	3:K:501:HOH:O	2.00	0.79
1:A:71:LYS:NZ	3:A:501:HOH:O	2.17	0.77
1:C:221:GLN:NE2	3:C:501:HOH:O	2.06	0.77
1:E:105:MET:O	1:E:110:ARG:NH1	2.17	0.76
1:E:86:GLN:OE1	3:E:501:HOH:O	2.03	0.75
1:K:305:SER:O	1:K:308:ASN:HB2	1.86	0.75
1:A:4:LEU:N	3:A:502:HOH:O	2.18	0.74
1:B:17:PRO:HG3	1:B:54:SER:HB3	1.70	0.74
1:A:157:GLU:OE1	1:A:161:ARG:NH2	2.19	0.73
1:A:203:ARG:NH2	1:A:236:GLU:OE2	2.22	0.72
1:E:190:ARG:NH2	1:E:204:SER:O	2.20	0.72
1:C:16:ARG:HH22	1:C:19:ASN:HA	1.55	0.72
1:K:157:GLU:HG2	1:K:161:ARG:HA	1.69	0.72
1:A:17:PRO:HG3	1:A:54:SER:HB3	1.72	0.70
1:K:69:ILE:HG12	1:K:295:ARG:HB3	1.74	0.67
1:E:57:SER:OG	1:E:60:GLN:HG2	1.94	0.67
1:A:321:ARG:HH21	1:K:272:SER:HB2	1.62	0.65
1:E:118:TYR:CZ	1:E:122:MET:HE2	2.32	0.64
1:B:173:VAL:HG21	1:B:179:VAL:HG22	1.80	0.64
2:C:402:SO4:O4	3:C:502:HOH:O	2.14	0.64
1:B:124:GLU:CG	1:B:125:ASN:H	2.03	0.63
1:D:44:LYS:HB2	1:D:46:TYR:CE2	2.33	0.63
1:D:41:ILE:O	1:D:44:LYS:HG3	1.98	0.63
1:K:305:SER:HB3	1:K:308:ASN:ND2	2.14	0.63
1:C:9:ILE:HG12	1:C:296:THR:HB	1.80	0.63
1:A:108:ILE:HG12	1:A:229:LEU:HD13	1.81	0.62
1:C:108:ILE:HG12	1:C:229:LEU:HD13	1.80	0.62
1:C:26:GLY:HA2	1:C:27:ASP:HB2	1.81	0.61
1:E:118:TYR:OH	1:E:122:MET:HE1	2.00	0.61
1:C:207:ILE:HD11	1:C:282:MET:HE2	1.80	0.61
1:C:321:ARG:HH21	1:E:272:SER:HB2	1.66	0.61
1:E:9:ILE:HG12	1:E:296:THR:HB	1.82	0.61
1:K:14:ARG:HG3	1:K:52:PHE:HB2	1.83	0.61
1:C:125:ASN:HB3	1:C:217:THR:OG1	2.00	0.61
1:C:274:TYR:OH	3:C:503:HOH:O	2.15	0.61
1:E:119:ILE:HD13	1:E:130:ILE:HD11	1.83	0.61
1:B:63:ASN:HA	1:B:67:LYS:HB3	1.83	0.60
1:D:14:ARG:NH1	1:D:94:THR:OG1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:169:THR:O	3:K:502:HOH:O	2.16	0.60
1:E:125:ASN:HA	3:E:504:HOH:O	2.02	0.60
1:B:9:ILE:HG12	1:B:296:THR:HB	1.84	0.59
2:K:401:SO4:O4	3:K:503:HOH:O	2.16	0.59
1:K:86:GLN:HG3	1:K:311:GLU:HG2	1.83	0.59
1:A:284:ARG:HG2	3:A:513:HOH:O	2.03	0.59
1:K:7:SER:HB3	1:K:291:GLY:HA2	1.83	0.59
1:C:91:LYS:HE3	1:C:231:ASP:OD2	2.03	0.59
1:K:128:PHE:CE1	1:K:214:GLN:HG2	2.38	0.59
1:B:80:THR:OG1	1:B:289:SER:O	2.21	0.58
1:B:11:VAL:HG21	1:B:322:ALA:HB3	1.85	0.58
1:C:14:ARG:NH1	1:C:58:GLN:OE1	2.34	0.58
2:K:402:SO4:O2	3:K:505:HOH:O	2.17	0.57
1:K:148:VAL:HG22	1:K:189:ASN:ND2	2.19	0.57
1:E:108:ILE:HG12	1:E:229:LEU:HD13	1.86	0.57
1:B:279:ASP:HB2	3:B:503:HOH:O	2.05	0.57
1:E:221:GLN:NE2	3:E:505:HOH:O	2.37	0.57
1:C:47:ALA:O	1:C:320:GLN:NE2	2.37	0.56
1:E:125:ASN:N	1:E:125:ASN:OD1	2.36	0.56
1:B:46:TYR:HB3	1:B:320:GLN:HE22	1.71	0.56
1:E:58:GLN:HG3	1:E:104:GLY:H	1.71	0.56
1:K:91:LYS:HE3	1:K:231:ASP:OD2	2.06	0.56
1:K:141:LYS:HD2	1:K:152:ASN:OD1	2.07	0.55
1:B:175:SER:HB3	1:B:178:GLU:HG2	1.89	0.54
1:A:9:ILE:HG12	1:A:296:THR:HB	1.89	0.54
1:B:124:GLU:CG	1:B:125:ASN:N	2.69	0.54
1:B:46:TYR:HB3	1:B:320:GLN:NE2	2.22	0.54
1:B:86:GLN:HG3	1:B:311:GLU:HB2	1.88	0.54
1:C:41:ILE:HD13	1:C:316:LEU:HD11	1.90	0.54
1:B:73:VAL:HG21	1:B:227:LEU:HB2	1.89	0.54
1:C:36:GLU:HB3	1:C:50:ARG:NH1	2.23	0.53
1:C:128:PHE:CE2	1:C:214:GLN:HG2	2.43	0.53
1:A:284:ARG:NH2	3:A:507:HOH:O	2.41	0.53
1:K:50:ARG:NH1	1:K:51:VAL:O	2.42	0.53
1:B:203:ARG:HH22	1:B:247:VAL:HA	1.73	0.53
1:K:46:TYR:HB3	1:K:320:GLN:HE21	1.74	0.53
1:E:109:PRO:O	1:E:113:GLN:HG3	2.08	0.52
1:E:157:GLU:HG2	1:E:161:ARG:HA	1.91	0.52
1:A:71:LYS:HE2	3:A:522:HOH:O	2.09	0.52
1:B:249:ASP:OD1	1:B:250:GLU:N	2.43	0.52
1:C:33:PHE:O	1:C:34:GLN:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:13:CYS:HA	1:E:300:ILE:HG13	1.90	0.52
1:E:323:LYS:O	1:E:323:LYS:HG2	2.09	0.52
1:E:103:GLU:N	1:E:104:GLY:HA3	2.25	0.52
1:B:136:GLU:OE2	1:B:191:HIS:ND1	2.31	0.52
1:D:19:ASN:CB	1:D:21:SER:HA	2.39	0.52
1:K:214:GLN:HB2	1:K:223:LEU:HB2	1.93	0.51
1:B:124:GLU:HG3	1:B:125:ASN:N	2.17	0.51
1:K:171:ARG:NH2	1:K:185:GLU:OE1	2.42	0.51
1:K:303:SER:OG	1:K:308:ASN:ND2	2.41	0.51
1:B:92:VAL:N	2:B:401:SO4:O1	2.41	0.51
1:C:318:PHE:O	1:C:321:ARG:HB2	2.11	0.51
1:E:197:MET:C	1:E:199:GLU:H	2.14	0.51
1:B:46:TYR:CA	1:B:320:GLN:HE22	2.24	0.51
1:E:134:TYR:CD2	1:E:186:GLY:HA3	2.45	0.51
1:D:288:ASP:OD1	3:D:501:HOH:O	2.19	0.51
1:E:145:LEU:O	1:E:189:ASN:ND2	2.39	0.51
1:D:134:TYR:CD2	1:D:186:GLY:HA3	2.46	0.50
1:C:303:SER:O	1:C:312:THR:HG21	2.11	0.50
1:C:26:GLY:HA2	1:C:27:ASP:CB	2.42	0.50
1:K:108:ILE:HG12	1:K:229:LEU:HD13	1.94	0.50
1:K:303:SER:HG	1:K:308:ASN:HD21	1.58	0.49
1:B:303:SER:O	1:B:312:THR:HG21	2.13	0.49
1:E:57:SER:O	1:E:61:VAL:HG13	2.12	0.49
1:C:94:THR:HG22	1:C:95:MET:HE2	1.94	0.49
1:D:34:GLN:HG3	1:D:35:GLY:N	2.28	0.49
1:C:91:LYS:NZ	1:C:232:LEU:O	2.45	0.49
1:E:129:HIS:HB2	1:E:213:LYS:HB2	1.95	0.49
1:A:207:ILE:HD11	1:A:282:MET:HE2	1.94	0.49
1:B:132:VAL:HA	1:B:209:LEU:O	2.13	0.48
1:K:148:VAL:HG22	1:K:189:ASN:HD21	1.78	0.48
1:K:84:TYR:CE1	1:K:234:GLY:HA2	2.48	0.48
1:C:119:ILE:HG12	1:C:128:PHE:CE2	2.49	0.48
1:C:150:LYS:HB3	1:C:153:LEU:HD21	1.95	0.48
1:A:303:SER:CB	1:A:308:ASN:HD22	2.27	0.48
1:K:175:SER:OG	1:K:178:GLU:HG3	2.14	0.48
1:E:52:PHE:CD1	1:E:56:THR:HG21	2.48	0.48
1:B:69:ILE:HG12	1:B:295:ARG:HB3	1.96	0.48
1:D:91:LYS:NZ	2:D:404:SO4:O2	2.38	0.48
1:K:303:SER:CB	1:K:308:ASN:HD21	2.26	0.48
1:B:14:ARG:HG2	1:B:52:PHE:HB2	1.96	0.47
1:D:126:LEU:HD22	1:D:128[A]:PHE:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:124:GLU:O	1:K:125:ASN:HB2	2.14	0.47
1:D:171:ARG:NH1	3:D:505:HOH:O	2.40	0.47
1:K:303:SER:CB	1:K:308:ASN:ND2	2.77	0.47
1:B:156:HIS:O	1:B:163:PRO:HA	2.14	0.47
1:E:118:TYR:OH	1:E:122:MET:CE	2.62	0.47
1:B:119:ILE:HG12	1:B:128:PHE:CE2	2.49	0.47
1:C:119:ILE:HG12	1:C:128:PHE:CD2	2.49	0.47
1:C:141:LYS:NZ	1:C:143:ARG:HH22	2.13	0.47
1:E:303:SER:O	1:E:312:THR:HG21	2.15	0.47
1:K:137:ILE:HD13	1:K:142:ILE:HG12	1.96	0.47
1:B:108:ILE:HG12	1:B:229:LEU:HD13	1.97	0.47
1:B:203:ARG:HH21	1:B:250:GLU:CB	2.28	0.47
1:C:175:SER:OG	1:C:178:GLU:HG3	2.14	0.47
1:D:156:HIS:O	1:D:163:PRO:HA	2.14	0.47
1:C:321:ARG:NH2	1:E:272:SER:HB2	2.30	0.47
1:K:128:PHE:HE1	1:K:214:GLN:HG2	1.78	0.47
1:E:118:TYR:CZ	1:E:122:MET:CE	2.97	0.47
1:E:71:LYS:HD2	1:E:71:LYS:HA	1.50	0.47
1:A:136:GLU:OE2	1:A:143:ARG:HD3	2.15	0.46
1:C:73:VAL:HG21	1:C:227:LEU:HB2	1.95	0.46
1:A:128:PHE:CE2	1:A:214:GLN:HG2	2.51	0.46
1:K:46:TYR:HB3	1:K:320:GLN:NE2	2.30	0.46
1:C:209:LEU:HD11	1:C:226:LYS:HG2	1.97	0.46
1:A:24:ASN:C	1:A:26:GLY:N	2.69	0.46
1:E:214:GLN:HB2	1:E:223:LEU:HB2	1.96	0.46
1:K:134:TYR:CD2	1:K:186:GLY:HA3	2.50	0.46
1:K:303:SER:O	1:K:312:THR:HG21	2.16	0.46
1:A:119:ILE:HG12	1:A:128:PHE:CD2	2.52	0.45
1:B:215:GLU:HG3	1:B:222:LYS:HG2	1.98	0.45
1:A:58:GLN:O	1:A:61:VAL:HG22	2.15	0.45
1:B:308:ASN:O	1:B:312:THR:HG23	2.16	0.45
1:C:128:PHE:CD2	1:C:214:GLN:HG2	2.51	0.45
1:B:62:TYR:CD1	1:B:66:ALA:HB3	2.51	0.45
1:D:132:VAL:HA	1:D:209:LEU:O	2.17	0.45
1:A:106:GLY:O	1:A:110:ARG:HG3	2.16	0.45
1:K:9:ILE:HG12	1:K:296:THR:HB	1.99	0.45
1:A:303:SER:O	1:A:312:THR:HG21	2.17	0.45
1:E:197:MET:O	1:E:199:GLU:N	2.49	0.44
1:C:124:GLU:OE2	1:C:125:ASN:ND2	2.50	0.44
1:K:13:CYS:HA	1:K:300:ILE:HG13	2.00	0.44
1:K:308:ASN:O	1:K:311:GLU:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:73:VAL:HG21	1:K:227:LEU:HB2	2.00	0.44
1:C:103:GLU:N	1:C:104:GLY:HA3	2.33	0.44
1:C:118:TYR:O	1:C:122:MET:HG2	2.17	0.44
1:C:16:ARG:O	1:C:304:PRO:HG3	2.17	0.44
1:E:316:LEU:O	1:E:320:GLN:HG2	2.18	0.44
1:K:103:GLU:HA	1:K:110:ARG:HH22	1.83	0.44
1:B:123:ASP:O	1:B:124:GLU:CB	2.66	0.43
1:B:126:LEU:HG	1:B:128:PHE:CE1	2.52	0.43
1:B:308:ASN:OD1	1:B:308:ASN:N	2.51	0.43
1:E:175:SER:OG	1:E:178:GLU:HG3	2.17	0.43
1:A:179:VAL:O	1:A:182:THR:OG1	2.34	0.43
1:B:174:SER:H	1:B:178:GLU:CD	2.21	0.43
1:D:187:LYS:HB3	1:D:187:LYS:HE2	1.78	0.43
1:C:141:LYS:HZ2	1:C:143:ARG:HH12	1.66	0.43
1:D:19:ASN:HA	1:D:22:GLU:H	1.83	0.43
1:E:119:ILE:HG12	1:E:128:PHE:CD1	2.53	0.43
1:E:278:ARG:HD2	1:E:284:ARG:HD2	1.99	0.43
1:K:141:LYS:HA	1:K:141:LYS:HD3	1.82	0.43
1:K:209:LEU:HD13	1:K:228:TYR:CE1	2.54	0.43
1:C:71:LYS:HD3	1:C:71:LYS:HA	1.67	0.43
1:C:13:CYS:HA	1:C:300:ILE:HG13	2.00	0.42
1:E:317:LEU:O	1:E:320:GLN:HB2	2.19	0.42
1:B:46:TYR:CB	1:B:320:GLN:HE22	2.32	0.42
1:B:52:PHE:CD1	1:B:56:THR:HG21	2.54	0.42
1:D:150:LYS:HB3	1:D:153:LEU:HD21	2.00	0.42
1:D:11:VAL:HG21	1:D:322:ALA:HB3	2.01	0.42
1:E:135:PHE:HA	1:E:145:LEU:HG	2.01	0.42
1:E:144:ASP:HB2	1:E:153:LEU:HD11	2.01	0.42
1:K:15:PHE:HA	1:K:302:CYS:O	2.20	0.42
1:A:14:ARG:HD3	1:A:94:THR:OG1	2.19	0.42
1:A:223:LEU:HA	1:A:223:LEU:HD23	1.84	0.42
1:C:91:LYS:HA	1:C:301:CYS:SG	2.60	0.42
1:D:125:ASN:ND2	1:D:218:GLN:HG2	2.35	0.42
1:E:107:ILE:O	1:E:111:ILE:HG13	2.19	0.42
1:D:108:ILE:HB	1:D:109:PRO:HD3	2.01	0.42
1:A:50:ARG:NH1	1:A:51:VAL:O	2.53	0.42
1:D:47:ALA:HB3	1:D:323:LYS:HE2	2.01	0.42
1:E:102:PRO:O	1:E:110:ARG:NH2	2.52	0.42
1:A:300:ILE:O	1:A:300:ILE:HG13	2.19	0.42
1:B:216:ASN:O	1:B:220:GLU:N	2.53	0.42
1:E:91:LYS:HA	1:E:301:CYS:SG	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:47:ALA:N	1:K:320:GLN:HE22	2.18	0.42
1:E:119:ILE:CD1	1:E:130:ILE:HD11	2.50	0.41
1:E:280:SER:O	1:E:284:ARG:HG3	2.20	0.41
1:B:175:SER:O	1:B:179:VAL:HG23	2.20	0.41
1:C:133:SER:HB2	1:C:209:LEU:HB3	2.01	0.41
1:C:89:SER:HB2	1:C:301:CYS:O	2.21	0.41
1:C:106:GLY:O	1:C:110:ARG:HG3	2.20	0.41
1:A:29:TYR:CE2	1:A:31:ALA:HB3	2.55	0.41
1:B:128:PHE:CE2	1:B:214:GLN:HG2	2.56	0.41
1:E:122:MET:HB3	1:E:122:MET:HE3	1.95	0.41
1:A:141:LYS:HD3	1:D:147:ASP:CG	2.40	0.41
1:C:207:ILE:HD11	1:C:282:MET:CE	2.49	0.41
1:B:123:ASP:O	1:B:124:GLU:CG	2.69	0.41
1:E:58:GLN:O	1:E:61:VAL:HG22	2.21	0.41
1:B:317:LEU:HD23	1:B:317:LEU:HA	1.87	0.41
1:D:119:ILE:CD1	1:D:130:ILE:HD11	2.51	0.41
1:E:223:LEU:HD23	1:E:223:LEU:HA	1.73	0.41
1:E:321:ARG:NH1	3:E:510:HOH:O	2.53	0.41
1:B:10:LYS:HE3	1:B:12:MET:HE1	2.02	0.41
1:K:147:ASP:OD2	1:K:150:LYS:HE3	2.20	0.41
1:A:20:GLU:O	1:A:21:SER:CB	2.69	0.41
1:A:219:THR:OG1	1:A:221:GLN:HG2	2.21	0.41
1:D:69:ILE:O	1:D:73:VAL:HG23	2.20	0.41
1:K:135:PHE:HA	1:K:145:LEU:HG	2.03	0.41
1:B:302:CYS:HB3	1:B:312:THR:HB	2.03	0.40
1:C:278:ARG:HE	1:C:278:ARG:HB3	1.70	0.40
1:A:108:ILE:HB	1:A:109:PRO:HD3	2.02	0.40
1:A:173:VAL:HG21	1:A:179:VAL:HG22	2.03	0.40
1:D:73:VAL:HG21	1:D:227:LEU:HB2	2.03	0.40
1:B:10:LYS:HE3	1:B:12:MET:CE	2.51	0.40
1:C:17:PRO:HB3	1:C:54:SER:HB3	2.03	0.40
1:E:129:HIS:ND1	3:E:506:HOH:O	2.37	0.40
1:E:62:TYR:CD1	1:E:66:ALA:HB3	2.57	0.40
1:K:58:GLN:O	1:K:61:VAL:HG22	2.22	0.40
1:B:143:ARG:HD2	1:B:151:THR:O	2.22	0.40
1:C:126:LEU:HD12	1:C:126:LEU:HA	1.97	0.40
1:K:252:LYS:HE3	1:K:252:LYS:HB3	1.85	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	305/325 (94%)	286 (94%)	12 (4%)	7 (2%)	8	28
1	B	302/325 (93%)	283 (94%)	16 (5%)	3 (1%)	19	52
1	C	300/325 (92%)	279 (93%)	14 (5%)	7 (2%)	8	28
1	D	304/325 (94%)	291 (96%)	9 (3%)	4 (1%)	15	44
1	E	295/325 (91%)	280 (95%)	12 (4%)	3 (1%)	19	52
1	K	299/325 (92%)	281 (94%)	15 (5%)	3 (1%)	19	52
All	All	1805/1950 (93%)	1700 (94%)	78 (4%)	27 (2%)	13	40

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	8	ASN
1	A	21	SER
1	B	124	GLU
1	C	18	LEU
1	C	20	GLU
1	C	30	ILE
1	C	123	ASP
1	E	28	LYS
1	K	123	ASP
1	A	7	SER
1	B	122	MET
1	D	18	LEU
1	D	123	ASP
1	E	198	ASN
1	E	245	GLY
1	C	124	GLU
1	D	30	ILE
1	A	18	LEU
1	A	100	HIS

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Mol	Chain	Res	Type
1	C	7	SER
1	D	124	GLU
1	K	124	GLU
1	B	123	ASP
1	C	27	ASP
1	A	30	ILE
1	K	104	GLY

5.3.2 Protein sidechains [i](#)

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	251/286 (88%)	245 (98%)	6 (2%)	57	85
1	B	229/286 (80%)	219 (96%)	10 (4%)	35	69
1	C	243/286 (85%)	241 (99%)	2 (1%)	86	96
1	D	246/286 (86%)	244 (99%)	2 (1%)	86	96
1	E	225/286 (79%)	220 (98%)	5 (2%)	60	87
1	K	238/286 (83%)	237 (100%)	1 (0%)	93	98
All	All	1432/1716 (83%)	1406 (98%)	26 (2%)	66	89

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	19	ASN
1	A	34	GLN
1	A	114	ASP
1	A	314	SER
1	A	321	ARG
1	B	50	ARG
1	B	60	GLN
1	B	67	LYS
1	B	99	LEU
1	B	113	GLN

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Mol	Chain	Res	Type
1	B	134	TYR
1	B	143	ARG
1	B	170	GLU
1	B	308	ASN
1	B	311	GLU
1	C	217	THR
1	C	256	LYS
1	D	134	TYR
1	D	278	ARG
1	E	60	GLN
1	E	122	MET
1	E	188	SER
1	E	256	LYS
1	E	323	LYS
1	K	53	GLN

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

Mol	Chain	Res	Type
1	A	308	ASN
1	B	320	GLN
1	C	320	GLN
1	E	156	HIS
1	K	189	ASN
1	K	308	ASN
1	K	320	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 carbohydrates in this entry.

5.6 Ligand geometry

12 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	0.20	0	6,6,6	0.24	0
2	SO4	A	402	-	4,4,4	0.18	0	6,6,6	0.48	0
2	SO4	B	401	-	4,4,4	0.04	0	6,6,6	0.30	0
2	SO4	C	401	-	4,4,4	0.14	0	6,6,6	0.38	0
2	SO4	C	402	-	4,4,4	0.28	0	6,6,6	0.11	0
2	SO4	D	401	-	4,4,4	0.05	0	6,6,6	0.47	0
2	SO4	D	402	-	4,4,4	0.38	0	6,6,6	0.19	0
2	SO4	D	403	-	4,4,4	0.45	0	6,6,6	0.18	0
2	SO4	D	404	-	4,4,4	0.15	0	6,6,6	0.32	0
2	SO4	E	401	-	4,4,4	0.23	0	6,6,6	0.53	0
2	SO4	K	401	-	4,4,4	0.15	0	6,6,6	0.26	0
2	SO4	K	402	-	4,4,4	0.30	0	6,6,6	0.29	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	401	-	-	0/0/0/0	0/0/0/0
2	SO4	A	402	-	-	0/0/0/0	0/0/0/0
2	SO4	B	401	-	-	0/0/0/0	0/0/0/0
2	SO4	C	401	-	-	0/0/0/0	0/0/0/0
2	SO4	C	402	-	-	0/0/0/0	0/0/0/0
2	SO4	D	401	-	-	0/0/0/0	0/0/0/0
2	SO4	D	402	-	-	0/0/0/0	0/0/0/0
2	SO4	D	403	-	-	0/0/0/0	0/0/0/0
2	SO4	D	404	-	-	0/0/0/0	0/0/0/0
2	SO4	E	401	-	-	0/0/0/0	0/0/0/0
2	SO4	K	401	-	-	0/0/0/0	0/0/0/0
2	SO4	K	402	-	-	0/0/0/0	0/0/0/0

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.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	SO4	1	0
2	C	402	SO4	1	0
2	D	404	SO4	1	0
2	K	401	SO4	1	0
2	K	402	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	313/325 (96%)	0.13	9 (2%) 55 50	26, 44, 82, 105	0
1	B	308/325 (94%)	0.36	14 (4%) 37 31	36, 59, 93, 133	0
1	C	308/325 (94%)	0.17	4 (1%) 79 78	33, 50, 86, 105	0
1	D	311/325 (95%)	0.13	7 (2%) 64 60	29, 46, 72, 95	0
1	E	305/325 (93%)	0.32	9 (2%) 54 48	36, 58, 88, 109	0
1	K	307/325 (94%)	0.36	11 (3%) 46 40	35, 59, 85, 110	0
All	All	1852/1950 (94%)	0.25	54 (2%) 55 50	26, 53, 85, 133	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	246	ALA	4.8
1	K	247	VAL	4.2
1	B	195	THR	3.6
1	E	244	GLU	3.5
1	K	193	ALA	3.3
1	C	41	ILE	3.3
1	B	97	GLY	3.3
1	E	198	ASN	3.2
1	K	248	LEU	3.1
1	E	202	SER	3.0
1	A	37	ASP	3.0
1	E	197	MET	3.0
1	B	40	VAL	2.9
1	E	89	SER	2.8
1	K	246	ALA	2.8
1	K	140	ASP	2.8
1	K	199	GLU	2.8
1	K	308	ASN	2.8
1	D	325	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	244	GLU	2.7
1	B	308	ASN	2.7
1	B	147	ASP	2.7
1	A	307	TYR	2.7
1	A	43	SER	2.7
1	K	56	THR	2.6
1	B	184	ASP	2.6
1	K	192	VAL	2.6
1	K	40	VAL	2.5
1	B	20	GLU	2.4
1	B	194	VAL	2.4
1	K	99	LEU	2.4
1	D	88	SER	2.4
1	D	244	GLU	2.4
1	B	50	ARG	2.4
1	C	39	VAL	2.4
1	A	42	ALA	2.4
1	E	42	ALA	2.4
1	B	193	ALA	2.3
1	A	29	TYR	2.3
1	D	249	ASP	2.2
1	C	194	VAL	2.2
1	E	147	ASP	2.2
1	D	6	GLU	2.2
1	A	236	GLU	2.2
1	A	41	ILE	2.2
1	A	308	ASN	2.2
1	E	15	PHE	2.1
1	D	43	SER	2.1
1	D	85	GLY	2.1
1	B	201	SER	2.1
1	E	47	ALA	2.1
1	C	40	VAL	2.0
1	A	45	PRO	2.0
1	B	202	SER	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 [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	C	402	5/5	0.93	0.26	2.36	59,61,64,68	0
2	SO4	D	402	5/5	0.87	0.26	1.29	72,72,76,80	0
2	SO4	D	404	5/5	0.91	0.22	0.36	58,67,70,70	0
2	SO4	A	402	5/5	0.92	0.18	-0.66	54,58,63,72	0
2	SO4	D	401	5/5	0.95	0.14	-0.80	48,56,62,67	0
2	SO4	E	401	5/5	0.91	0.17	-1.13	66,73,75,79	0
2	SO4	K	402	5/5	0.93	0.16	-1.92	71,72,73,74	0
2	SO4	D	403	5/5	0.95	0.13	-1.93	66,66,68,68	0
2	SO4	K	401	5/5	0.89	0.14	-2.14	60,67,74,75	0
2	SO4	C	401	5/5	0.94	0.13	-2.25	58,63,69,74	0
2	SO4	B	401	5/5	0.96	0.12	-2.53	63,70,72,77	0
2	SO4	A	401	5/5	0.97	0.10	-3.07	52,56,59,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.