



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:37 PM UTC

PDB ID : 7UR2 / pdb_00007ur2
Title : Crystal structure of the Sec14 domain of the RhoGEF Kalirin
Authors : Li, Y.; Doukov, T.I.; Hao, B.
Deposited on : 2022-04-21
Resolution : 1.89 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

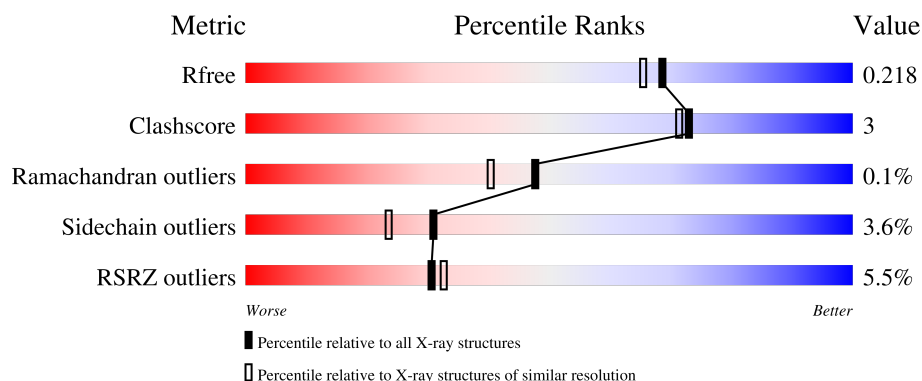
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	195	 6% 73% 9% 12%
1	B	195	 4% 79% 9% 11%
1	C	195	 5% 78% 8% 12%
1	D	195	 5% 79% 6% 14%
1	E	195	 3% 74% 7% 17%

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Mol	Chain	Length	Quality of chain
1	F	195	4% 80% 8% 12%
1	G	195	5% 72% 8% • 17%
1	H	195	7% 74% 8% • 16%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12143 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 Isoform 7 of Kalirin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	160	Total	C	N	O	S	0	1	0
			1280	822	218	236	4			
1	B	174	Total	C	N	O	S	0	1	0
			1401	898	240	259	4			
1	C	171	Total	C	N	O	S	0	4	0
			1394	896	240	254	4			
1	D	167	Total	C	N	O	S	0	2	0
			1351	868	231	248	4			
1	E	162	Total	C	N	O	S	0	1	0
			1296	830	222	240	4			
1	F	171	Total	C	N	O	S	0	1	0
			1379	887	236	252	4			
1	G	162	Total	C	N	O	S	0	1	0
			1293	829	221	239	4			
1	H	163	Total	C	N	O	S	0	1	0
			1302	837	222	239	4			

There are 32 discrepancies between the modelled and reference sequences:

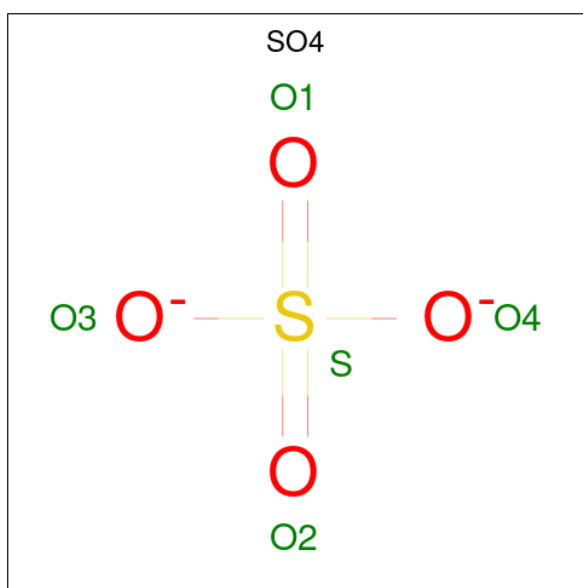
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A2CG49
A	-1	GLY	-	expression tag	UNP A2CG49
A	0	GLY	-	expression tag	UNP A2CG49
A	1	ARG	-	expression tag	UNP A2CG49
B	-2	GLY	-	expression tag	UNP A2CG49
B	-1	GLY	-	expression tag	UNP A2CG49
B	0	GLY	-	expression tag	UNP A2CG49
B	1	ARG	-	expression tag	UNP A2CG49
C	-2	GLY	-	expression tag	UNP A2CG49
C	-1	GLY	-	expression tag	UNP A2CG49
C	0	GLY	-	expression tag	UNP A2CG49
C	1	ARG	-	expression tag	UNP A2CG49
D	-2	GLY	-	expression tag	UNP A2CG49

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP A2CG49
D	0	GLY	-	expression tag	UNP A2CG49
D	1	ARG	-	expression tag	UNP A2CG49
E	-2	GLY	-	expression tag	UNP A2CG49
E	-1	GLY	-	expression tag	UNP A2CG49
E	0	GLY	-	expression tag	UNP A2CG49
E	1	ARG	-	expression tag	UNP A2CG49
F	-2	GLY	-	expression tag	UNP A2CG49
F	-1	GLY	-	expression tag	UNP A2CG49
F	0	GLY	-	expression tag	UNP A2CG49
F	1	ARG	-	expression tag	UNP A2CG49
G	-2	GLY	-	expression tag	UNP A2CG49
G	-1	GLY	-	expression tag	UNP A2CG49
G	0	GLY	-	expression tag	UNP A2CG49
G	1	ARG	-	expression tag	UNP A2CG49
H	-2	GLY	-	expression tag	UNP A2CG49
H	-1	GLY	-	expression tag	UNP A2CG49
H	0	GLY	-	expression tag	UNP A2CG49
H	1	ARG	-	expression tag	UNP A2CG49

- 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	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		

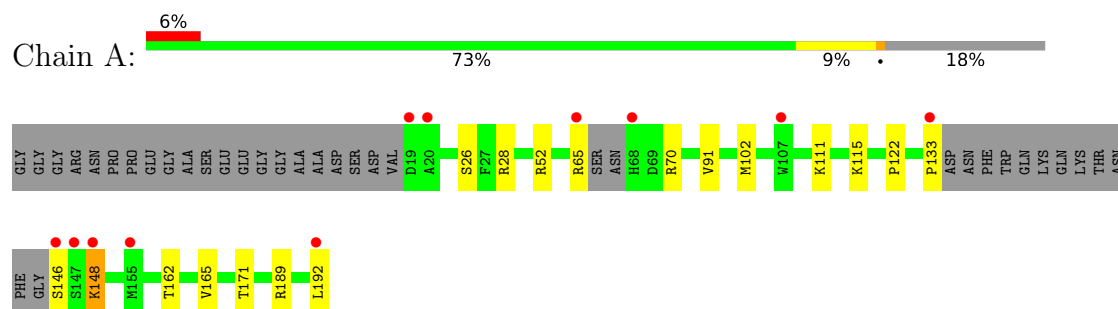
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	183	Total	O	0	0
			183	183		
3	B	203	Total	O	0	0
			203	203		
3	C	172	Total	O	0	0
			172	172		
3	D	141	Total	O	0	0
			141	141		
3	E	201	Total	O	0	0
			201	201		
3	F	172	Total	O	0	0
			172	172		
3	G	187	Total	O	0	0
			187	187		
3	H	153	Total	O	0	0
			153	153		

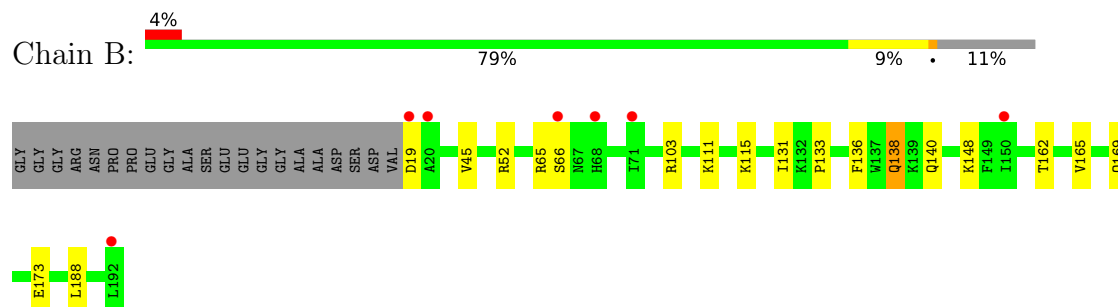
3 Residue-property plots [i](#)

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.

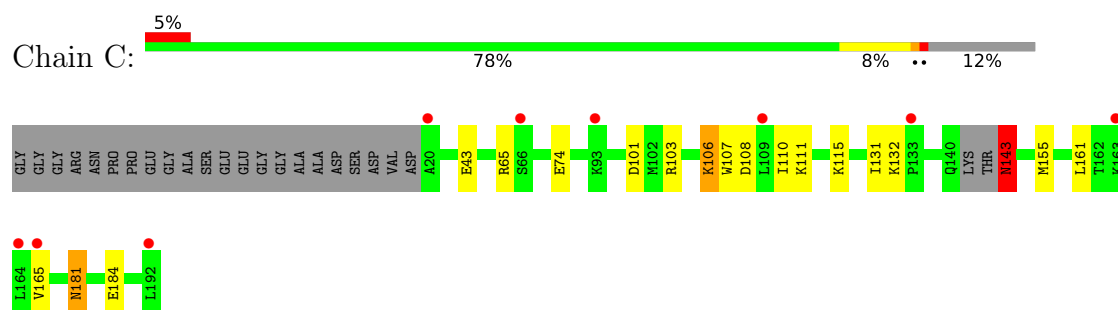
• Molecule 1: Isoform 7 of Kalirin



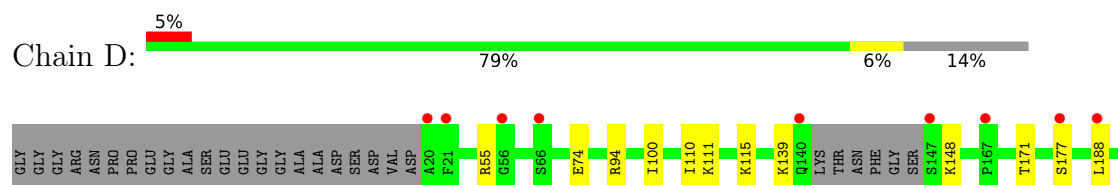
• Molecule 1: Isoform 7 of Kalirin



• Molecule 1: Isoform 7 of Kalirin

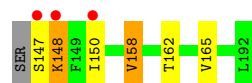
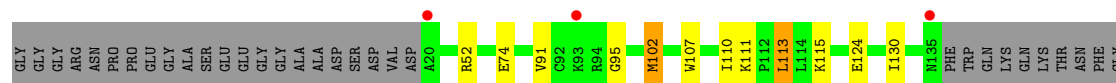
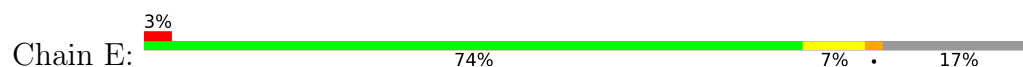


• Molecule 1: Isoform 7 of Kalirin

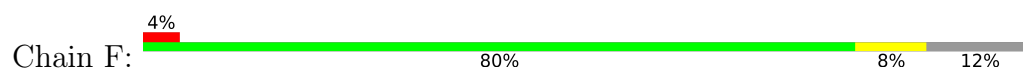




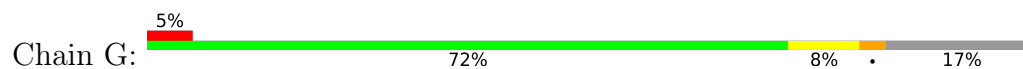
● Molecule 1: Isoform 7 of Kalirin



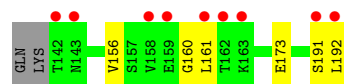
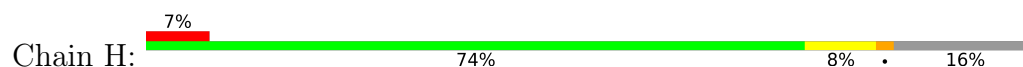
● Molecule 1: Isoform 7 of Kalirin



● Molecule 1: Isoform 7 of Kalirin



● Molecule 1: Isoform 7 of Kalirin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	72.16Å 82.42Å 83.27Å 81.09° 71.79° 79.88°	Depositor
Resolution (Å)	61.01 – 1.89 61.01 – 1.89	Depositor EDS
% Data completeness (in resolution range)	95.9 (61.01-1.89) 95.9 (61.01-1.89)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 1.88Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.195 , 0.218 0.192 , 0.218	Depositor DCC
R_{free} test set	6768 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12143	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.72% 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	0.84	0/1307	1.04	2/1760 (0.1%)
1	B	0.80	0/1434	1.05	2/1934 (0.1%)
1	C	0.81	0/1435	1.04	1/1932 (0.1%)
1	D	0.80	0/1385	1.08	4/1867 (0.2%)
1	E	0.86	1/1324 (0.1%)	1.06	1/1785 (0.1%)
1	F	0.78	0/1411	1.08	2/1901 (0.1%)
1	G	0.81	0/1321	1.12	7/1781 (0.4%)
1	H	0.80	0/1330	1.12	2/1791 (0.1%)
All	All	0.81	1/10947 (0.0%)	1.07	21/14751 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	102	MET	SD-CE	-10.63	1.52	1.79

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	171	THR	CA-C-N	6.98	129.94	120.38
1	G	171	THR	C-N-CA	6.98	129.94	120.38
1	G	119	GLU	CB-CG-CD	6.77	124.11	112.60
1	D	171	THR	CA-C-N	6.72	130.90	120.82
1	D	171	THR	C-N-CA	6.72	130.90	120.82
1	B	131	ILE	CA-C-N	6.05	129.88	120.68
1	B	131	ILE	C-N-CA	6.05	129.88	120.68
1	A	171	THR	CA-C-N	6.04	128.66	120.38
1	A	171	THR	C-N-CA	6.04	128.66	120.38
1	C	143	ASN	CA-CB-CG	6.03	118.63	112.60
1	D	139	LYS	CA-C-N	5.55	131.69	121.70
1	D	139	LYS	C-N-CA	5.55	131.69	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	191	SER	CA-C-N	5.48	131.56	121.70
1	G	191	SER	C-N-CA	5.48	131.56	121.70
1	H	131	ILE	CA-C-N	5.47	128.25	120.49
1	H	131	ILE	C-N-CA	5.47	128.25	120.49
1	F	171	THR	CA-C-N	5.29	128.75	120.82
1	F	171	THR	C-N-CA	5.29	128.75	120.82
1	G	156	VAL	N-CA-CB	-5.17	102.26	111.92
1	G	172	GLU	CB-CG-CD	5.09	121.26	112.60
1	E	158	VAL	N-CA-CB	5.01	117.35	110.54

There are no chirality outliers.

There are no planarity outliers.

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	1280	0	1305	9	0
1	B	1401	0	1414	7	0
1	C	1394	0	1420	9	0
1	D	1351	0	1371	4	0
1	E	1296	0	1318	13	0
1	F	1379	0	1398	6	0
1	G	1293	0	1314	14	0
1	H	1302	0	1326	18	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	D	5	0	0	0	0
2	E	10	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
3	A	183	0	0	0	0
3	B	203	0	0	0	0
3	C	172	0	0	0	0
3	D	141	0	0	0	0
3	E	201	0	0	1	0
3	F	172	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	187	0	0	0	0
3	H	153	0	0	1	0
All	All	12143	0	10866	69	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 3.

All (69) 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:G:42:LYS:NZ	1:H:192:LEU:HB2	1.93	0.81
1:G:52:ARG:H	1:G:169:GLN:HE21	1.30	0.77
1:B:52:ARG:H	1:B:169:GLN:HE21	1.32	0.77
1:E:102:MET:HE1	1:E:107:TRP:HE3	1.50	0.76
1:E:124:GLU:HG2	3:E:399:HOH:O	1.93	0.68
1:B:103:ARG:HG2	1:B:133:PRO:HA	1.77	0.67
1:G:42:LYS:HZ3	1:H:192:LEU:HB2	1.59	0.66
1:A:26:SER:OG	1:A:28:ARG:HG3	1.96	0.66
1:D:188:LEU:HD11	1:F:190:LEU:HB3	1.80	0.62
1:C:101:ASP:OD1	1:C:103:ARG:HD3	2.02	0.60
1:G:42:LYS:CE	1:H:192:LEU:HD22	2.33	0.59
1:G:42:LYS:HE2	1:H:192:LEU:HD22	1.85	0.58
1:H:53:ASP:HB3	1:H:55:ARG:H	1.69	0.58
1:G:42:LYS:HE3	1:H:192:LEU:CD2	2.35	0.57
1:G:42:LYS:CE	1:H:192:LEU:HB2	2.33	0.57
1:H:65:ARG:O	1:H:68:HIS:HB2	2.04	0.57
1:G:38:LEU:HD21	1:H:191:SER:O	2.04	0.57
1:G:77:ARG:O	1:G:81:THR:HG23	2.04	0.57
1:C:106:LYS:HD3	1:C:108:ASP:H	1.71	0.56
1:H:37:VAL:HG23	1:H:41:LEU:HD22	1.86	0.56
1:A:102:MET:HE3	1:A:133:PRO:HD3	1.89	0.54
1:A:70:ARG:HH11	1:A:70:ARG:HG3	1.73	0.53
1:C:43:GLU:HB3	1:C:65[A]:ARG:HH22	1.73	0.53
1:E:102:MET:HE1	1:E:107:TRP:CE3	2.37	0.52
1:A:28:ARG:HG2	1:A:122:PRO:HB3	1.92	0.52
1:A:111:LYS:HE2	1:A:115:LYS:HE3	1.91	0.52
1:B:111:LYS:HE2	1:B:115:LYS:HE3	1.91	0.52
1:E:52:ARG:NH1	1:E:91:VAL:HG21	2.25	0.51
1:F:119:GLU:HG3	3:F:351:HOH:O	2.09	0.51
1:C:43:GLU:HB3	1:C:65[A]:ARG:NH2	2.27	0.50
1:H:111:LYS:HE2	1:H:115:LYS:HE3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:111:LYS:HE2	1:E:115:LYS:HE3	1.93	0.49
1:G:77:ARG:O	1:G:81:THR:CG2	2.59	0.49
1:D:111:LYS:HE2	1:D:115:LYS:HE3	1.94	0.49
1:C:111:LYS:HE2	1:C:115:LYS:HE2	1.94	0.49
1:C:132:LYS:HD3	1:C:155:MET:HG2	1.94	0.48
1:E:102:MET:HE2	1:E:110:ILE:HG13	1.96	0.48
1:E:110:ILE:O	1:E:113:LEU:HB2	2.13	0.48
1:F:111:LYS:HE2	1:F:115:LYS:HE2	1.95	0.48
1:B:136:PHE:HZ	1:F:92[A]:CYS:SG	2.37	0.47
1:F:130:ILE:HD11	1:F:153:THR:HG23	1.96	0.47
1:G:132:LYS:HD3	1:G:155:MET:HG2	1.97	0.47
1:G:42:LYS:NZ	1:H:192:LEU:CB	2.72	0.46
1:A:148:LYS:HE2	1:A:148:LYS:HB2	1.47	0.46
1:E:162:THR:HA	1:E:165:VAL:O	2.16	0.46
1:E:102:MET:HE2	1:E:110:ILE:CG1	2.46	0.46
1:A:52:ARG:NH1	1:A:91:VAL:HG21	2.30	0.45
1:A:162:THR:HA	1:A:165:VAL:O	2.16	0.45
1:D:55:ARG:NH2	1:D:94:ARG:O	2.50	0.45
1:E:148:LYS:HB3	1:E:148:LYS:HE2	1.65	0.45
1:B:162:THR:HA	1:B:165:VAL:O	2.16	0.45
1:E:102:MET:HE3	1:E:130:ILE:HG21	1.98	0.44
1:H:156:VAL:HG22	1:H:160:GLY:HA3	2.00	0.44
1:A:189:ARG:HA	1:A:192:LEU:HD13	2.00	0.43
1:G:42:LYS:HE3	1:H:192:LEU:HD23	2.01	0.43
1:C:107:TRP:HE1	1:C:143:ASN:ND2	2.17	0.43
1:C:181:ASN:ND2	1:C:184:GLU:H	2.17	0.43
1:E:102:MET:HG3	1:E:110:ILE:HG13	2.00	0.42
1:G:191:SER:O	1:G:192:LEU:HB2	2.19	0.42
1:H:23:ARG:HD2	3:H:223:HOH:O	2.18	0.42
1:D:100:ILE:HG21	1:D:110:ILE:HG23	2.00	0.42
1:H:131:ILE:HD11	1:H:161:LEU:HD13	2.02	0.42
1:C:131:ILE:HD11	1:C:161:LEU:HD13	2.01	0.42
1:H:53:ASP:HB2	1:H:57:GLY:H	1.85	0.42
1:E:95:GLY:HA2	1:E:124:GLU:HG3	2.01	0.42
1:B:138:GLN:HB2	1:B:140:GLN:HG2	2.03	0.41
1:H:192:LEU:N	1:H:192:LEU:CD1	2.84	0.41
1:F:162:THR:HA	1:F:165:VAL:O	2.21	0.40
1:B:45:VAL:HA	1:B:65:ARG:HD3	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	155/195 (80%)	153 (99%)	2 (1%)	0	100	100
1	B	173/195 (89%)	172 (99%)	1 (1%)	0	100	100
1	C	171/195 (88%)	170 (99%)	1 (1%)	0	100	100
1	D	165/195 (85%)	162 (98%)	3 (2%)	0	100	100
1	E	159/195 (82%)	158 (99%)	1 (1%)	0	100	100
1	F	168/195 (86%)	167 (99%)	1 (1%)	0	100	100
1	G	159/195 (82%)	156 (98%)	2 (1%)	1 (1%)	21	13
1	H	158/195 (81%)	155 (98%)	3 (2%)	0	100	100
All	All	1308/1560 (84%)	1293 (99%)	14 (1%)	1 (0%)	48	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	148	LYS

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	143/167 (86%)	140 (98%)	3 (2%)	47	44
1	B	156/167 (93%)	150 (96%)	6 (4%)	29	21
1	C	156/167 (93%)	150 (96%)	6 (4%)	29	21
1	D	151/167 (90%)	148 (98%)	3 (2%)	48	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	145/167 (87%)	139 (96%)	6 (4%)	27	19
1	F	153/167 (92%)	148 (97%)	5 (3%)	33	26
1	G	144/167 (86%)	134 (93%)	10 (7%)	14	7
1	H	145/167 (87%)	141 (97%)	4 (3%)	38	32
All	All	1193/1336 (89%)	1150 (96%)	43 (4%)	31	23

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ARG
1	A	146	SER
1	A	148	LYS
1	B	19	ASP
1	B	66	SER
1	B	138	GLN
1	B	148	LYS
1	B	173	GLU
1	B	188	LEU
1	C	74	GLU
1	C	106	LYS
1	C	110	ILE
1	C	143	ASN
1	C	165	VAL
1	C	181	ASN
1	D	74	GLU
1	D	148	LYS
1	D	177	SER
1	E	74	GLU
1	E	113	LEU
1	E	147	SER
1	E	148	LYS
1	E	150	ILE
1	E	158	VAL
1	F	68	HIS
1	F	97	THR
1	F	158	VAL
1	F	161	LEU
1	F	188	LEU
1	G	43	GLU
1	G	81	THR
1	G	103	ARG

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Mol	Chain	Res	Type
1	G	119	GLU
1	G	147	SER
1	G	148	LYS
1	G	156	VAL
1	G	161	LEU
1	G	173	GLU
1	G	188	LEU
1	H	23	ARG
1	H	41	LEU
1	H	78	LYS
1	H	173	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	126	HIS
1	B	126	HIS
1	B	169	GLN
1	C	143	ASN
1	C	181	ASN
1	E	126	HIS
1	G	169	GLN
1	H	29	ASN
1	H	126	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 [i](#)

7 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	F	201	-	4,4,4	0.28	0	6,6,6	0.14	0
2	SO4	B	201	-	4,4,4	0.22	0	6,6,6	0.24	0
2	SO4	E	201	-	4,4,4	0.41	0	6,6,6	0.39	0
2	SO4	E	202	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	D	201	-	4,4,4	0.19	0	6,6,6	0.10	0
2	SO4	G	201	-	4,4,4	0.28	0	6,6,6	0.11	0
2	SO4	A	201	-	4,4,4	0.26	0	6,6,6	0.13	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.

No monomer is involved in short contacts.

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	160/195 (82%)	0.35	11 (6%)	23	24	23, 41, 72, 83	1 (0%)
1	B	174/195 (89%)	0.27	7 (4%)	42	45	27, 42, 66, 83	1 (0%)
1	C	171/195 (87%)	0.38	9 (5%)	32	34	23, 43, 68, 120	4 (2%)
1	D	167/195 (85%)	0.60	10 (5%)	27	29	32, 48, 76, 85	2 (1%)
1	E	162/195 (83%)	0.11	6 (3%)	45	48	24, 37, 65, 102	1 (0%)
1	F	171/195 (87%)	0.34	7 (4%)	41	44	32, 45, 70, 83	1 (0%)
1	G	162/195 (83%)	0.39	9 (5%)	30	32	24, 45, 82, 102	1 (0%)
1	H	163/195 (83%)	0.46	14 (8%)	16	17	27, 46, 74, 88	1 (0%)
All	All	1330/1560 (85%)	0.36	73 (5%)	30	32	23, 43, 72, 120	12 (0%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	192	LEU	5.5
1	E	20	ALA	5.1
1	A	146	SER	5.1
1	A	20	ALA	5.1
1	G	192	LEU	4.6
1	A	65	ARG	4.5
1	G	146	SER	4.1
1	B	20	ALA	4.0
1	D	20	ALA	4.0
1	E	150	ILE	3.9
1	H	68	HIS	3.9
1	B	19	ASP	3.9
1	D	192	LEU	3.8
1	F	192	LEU	3.8
1	A	68	HIS	3.7
1	E	135	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	H	142	THR	3.7
1	A	147	SER	3.5
1	H	159	GLU	3.4
1	C	164	LEU	3.3
1	B	150	ILE	3.2
1	H	133	PRO	3.2
1	A	19	ASP	3.2
1	F	20	ALA	3.2
1	E	147	SER	3.0
1	B	192	LEU	2.9
1	F	150	ILE	2.9
1	G	68	HIS	2.8
1	A	192	LEU	2.8
1	H	191	SER	2.8
1	C	20	ALA	2.7
1	A	148	LYS	2.7
1	D	21	PHE	2.7
1	C	165	VAL	2.7
1	D	56	GLY	2.7
1	G	28	ARG	2.7
1	C	93[A]	LYS	2.6
1	D	66	SER	2.6
1	G	20	ALA	2.6
1	E	148	LYS	2.6
1	G	66	SER	2.6
1	G	188	LEU	2.4
1	F	134	ASP	2.4
1	H	143	ASN	2.4
1	D	147	SER	2.4
1	B	66	SER	2.4
1	C	66	SER	2.4
1	C	163	LYS	2.4
1	H	163	LYS	2.4
1	C	133	PRO	2.3
1	C	192	LEU	2.3
1	D	188	LEU	2.3
1	A	155	MET	2.3
1	H	20	ALA	2.3
1	D	177	SER	2.3
1	F	104	GLY	2.2
1	G	71	ILE	2.2
1	H	158	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	68	HIS	2.2
1	A	107	TRP	2.2
1	D	140	GLN	2.2
1	H	162	THR	2.2
1	H	104	GLY	2.1
1	E	93	LYS	2.1
1	H	161	LEU	2.1
1	A	133	PRO	2.0
1	D	167	PRO	2.0
1	F	158	VAL	2.0
1	C	109	LEU	2.0
1	F	191	SER	2.0
1	B	71	ILE	2.0
1	G	67	ASN	2.0
1	H	28	ARG	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	E	202	5/5	0.40	0.24	257,259,260,261	0
2	SO4	A	201	5/5	0.52	0.23	208,209,209,211	0
2	SO4	D	201	5/5	0.61	0.17	138,140,140,142	0
2	SO4	G	201	5/5	0.71	0.13	114,116,120,120	0
2	SO4	F	201	5/5	0.84	0.13	100,100,103,103	0
2	SO4	B	201	5/5	0.90	0.09	89,89,91,92	0
2	SO4	E	201	5/5	0.97	0.06	41,44,46,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.