



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:20 PM UTC

PDB ID : 7U5B / pdb_00007u5b
Title : Structure of Human KLK5 bound to anti-KLK5 Fab
Authors : Yin, J.; Sudhamsu, J.
Deposited on : 2022-03-02
Resolution : 2.37 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

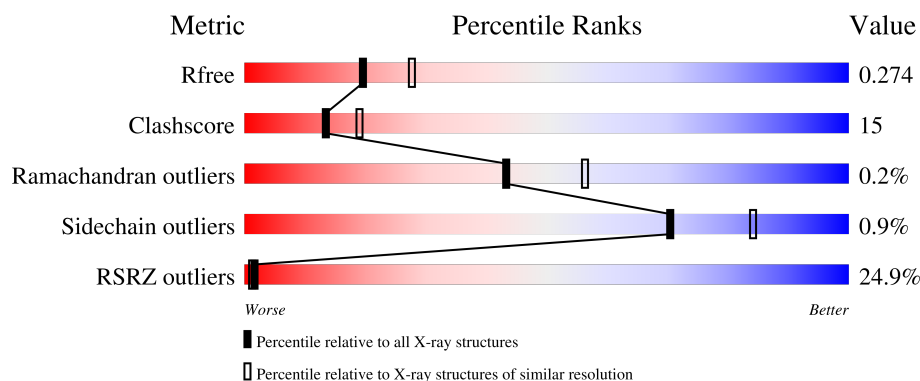
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	224	13% 74% 21% • •
1	H	224	14% 79% 18% •
2	B	217	28% 70% 29% •
2	L	217	21% 75% 23% •
3	I	227	33% 46% 20% 34%

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Mol	Chain	Length	Quality of chain
3	J	227	

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
4	SO4	A	301	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9140 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 anti-KLK5 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	2	0
			1604	1015	264	318	7			
1	H	218	Total	C	N	O	S	0	3	0
			1638	1034	272	326	6			

- Molecule 2 is a protein called anti-KLK5 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	1	0
			1628	1018	271	334	5			
2	L	216	Total	C	N	O	S	0	1	0
			1641	1025	272	339	5			

- Molecule 3 is a protein called Kallikrein-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	163	Total	C	N	O	S	0	0	0
			1271	797	237	225	12			
3	I	149	Total	C	N	O	S	0	0	0
			1161	729	216	206	10			

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		

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

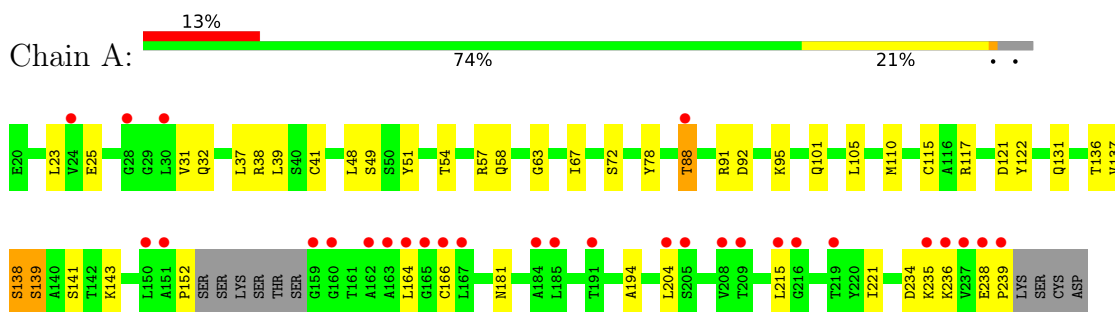
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	22	Total	O	0	0
			22	22		
5	B	29	Total	O	0	0
			29	29		
5	H	20	Total	O	0	0
			20	20		
5	J	5	Total	O	0	0
			5	5		
5	L	40	Total	O	0	0
			40	40		
5	I	6	Total	O	0	0
			6	6		

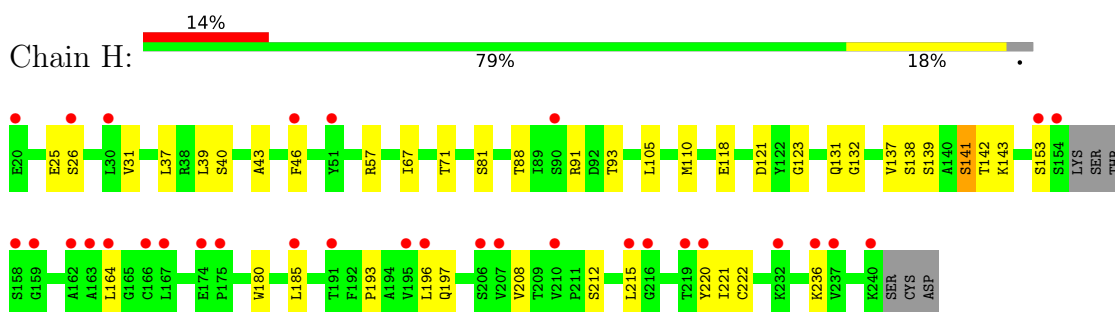
3 Residue-property plots

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.

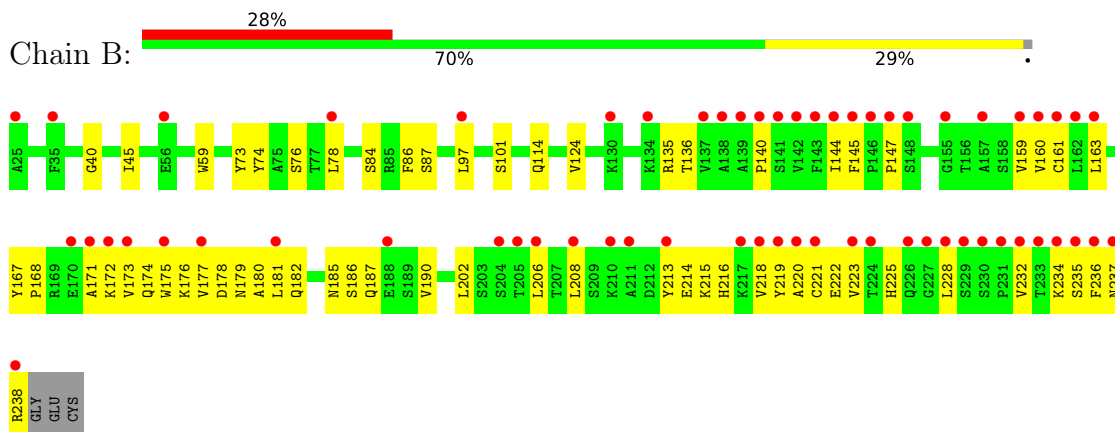
• Molecule 1: anti-KLK5 Fab Heavy Chain



• Molecule 1: anti-KLK5 Fab Heavy Chain

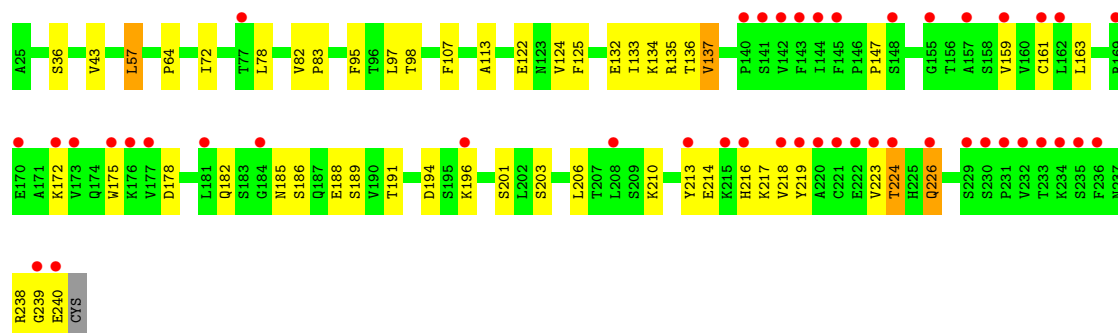


• Molecule 2: anti-KLK5 Fab Light Chain



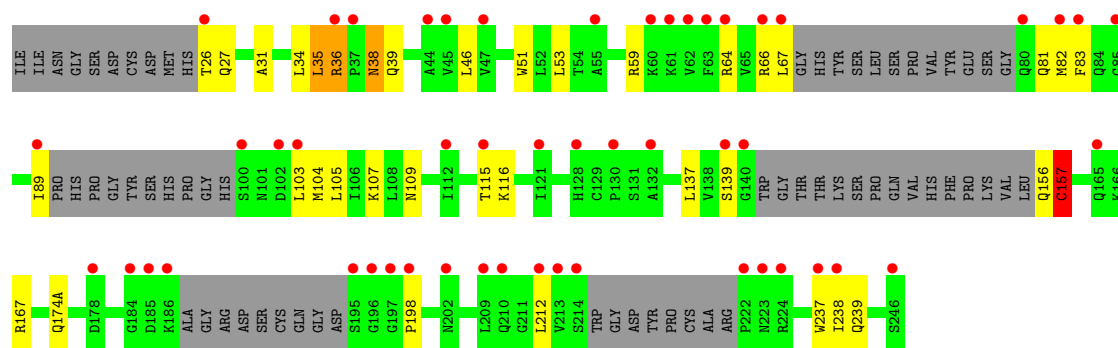
• Molecule 2: anti-KLK5 Fab Light Chain

Chain L: 



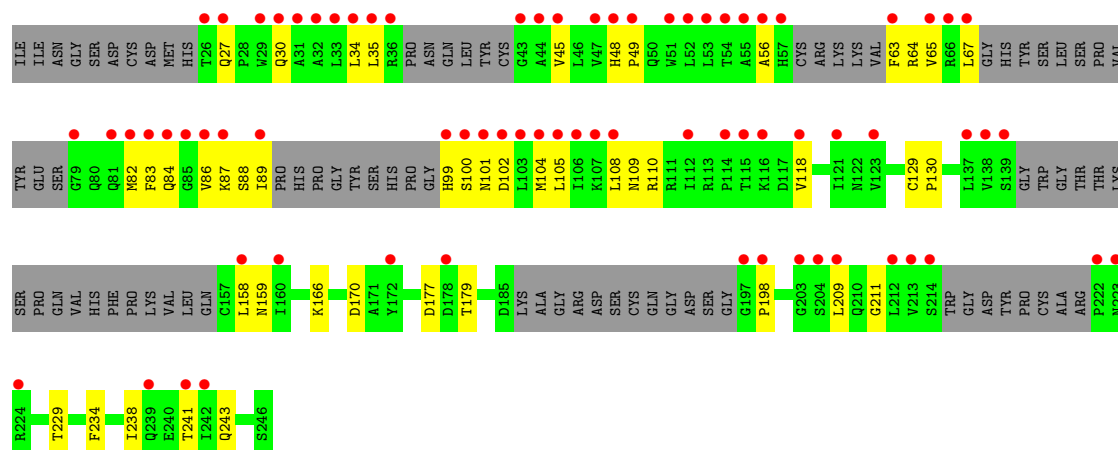
• Molecule 3: Kallikrein-5

Chain J: 



• Molecule 3: Kallikrein-5

Chain I: 



4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	83.69Å 283.62Å 295.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.88 – 2.37 52.88 – 2.37	Depositor EDS
% Data completeness (in resolution range)	99.0 (52.88-2.37) 99.1 (52.88-2.37)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.12-2829_final	Depositor
R, R_{free}	0.222 , 0.270 0.229 , 0.274	Depositor DCC
R_{free} test set	3507 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	56.7	Xtriage
Anisotropy	0.602	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.004 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9140	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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	0.77	8/1650 (0.5%)	0.70	0/2251
1	H	0.67	6/1687 (0.4%)	0.68	0/2299
2	B	0.62	1/1665 (0.1%)	0.82	1/2258 (0.0%)
2	L	0.65	3/1678 (0.2%)	0.76	1/2275 (0.0%)
3	I	0.40	0/1178	0.72	0/1585
3	J	0.51	0/1291	0.75	2/1738 (0.1%)
All	All	0.63	18/9149 (0.2%)	0.74	4/12406 (0.0%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	166	CYS	C-O	-7.94	1.15	1.23
2	B	76	SER	C-O	-7.93	1.14	1.24
1	A	141	SER	C-O	-7.32	1.15	1.23
1	A	122	TYR	C-O	-6.95	1.14	1.23
1	H	141	SER	CA-C	-6.89	1.43	1.52
1	A	121	ASP	C-O	-6.63	1.15	1.24
1	A	138	SER	C-O	-6.43	1.15	1.23
1	H	141	SER	C-O	-6.10	1.16	1.23
2	L	137	VAL	C-O	-5.86	1.18	1.24
1	H	123	GLY	C-O	-5.82	1.16	1.24
1	H	139	SER	C-O	-5.75	1.16	1.24
1	H	121	ASP	C-O	-5.46	1.17	1.24
2	L	135	ARG	C-O	-5.46	1.17	1.23
1	H	138	SER	C-O	-5.32	1.17	1.23
1	A	141	SER	CA-C	-5.09	1.46	1.52
2	L	134	LYS	C-O	-5.09	1.17	1.23
1	A	139	SER	C-O	-5.04	1.17	1.23
1	A	138	SER	CA-C	-5.04	1.46	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	76	SER	N-CA-C	5.43	122.46	113.50
3	J	157	CYS	N-CA-C	5.42	117.56	108.73
3	J	38	ASN	N-CA-C	-5.26	104.31	111.56
2	L	224	THR	CB-CA-C	-5.14	100.83	109.72

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	1604	0	1555	43	0
1	H	1638	0	1594	42	0
2	B	1628	0	1577	62	0
2	L	1641	0	1584	41	0
3	I	1161	0	1172	41	0
3	J	1271	0	1293	39	0
4	A	15	0	0	2	0
4	B	10	0	0	1	0
4	H	15	0	0	1	0
4	I	10	0	0	0	0
4	J	10	0	0	0	0
4	L	15	0	0	0	0
5	A	22	0	0	1	0
5	B	29	0	0	0	0
5	H	20	0	0	0	0
5	I	6	0	0	2	0
5	J	5	0	0	0	0
5	L	40	0	0	0	0
All	All	9140	0	8775	261	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 15.

All (261) 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:H:221:ILE:CD1	1:H:236:LYS:HG2	1.53	1.37
2:B:223:VAL:HG12	2:B:232:VAL:O	1.44	1.18
1:H:221:ILE:HD11	1:H:236:LYS:HG2	1.16	1.12
3:I:109:ASN:O	3:I:110:ARG:HG3	1.48	1.10
3:J:36:ARG:HH21	3:J:36:ARG:HB3	1.17	1.05
3:I:34:LEU:HB2	3:I:64:ARG:O	1.59	1.01
2:L:163:LEU:HD21	2:L:223:VAL:HG21	1.44	1.00
1:H:221:ILE:CD1	1:H:236:LYS:CG	2.45	0.95
3:I:109:ASN:O	3:I:110:ARG:CG	2.15	0.93
2:B:177:VAL:HG22	2:B:182:GLN:NE2	1.85	0.91
1:A:236:LYS:HG2	1:A:238:GLU:OE1	1.71	0.91
1:H:221:ILE:HD12	1:H:236:LYS:HG2	1.54	0.89
1:A:88:THR:HG21	1:H:88:THR:HG21	1.52	0.89
1:H:25:GLU:H	1:H:131:GLN:HE22	1.22	0.87
3:J:36:ARG:HH21	3:J:36:ARG:CB	1.87	0.86
2:B:182:GLN:HB3	2:B:185:ASN:HD21	1.39	0.85
3:I:109:ASN:C	3:I:110:ARG:HG3	2.05	0.82
3:I:99:HIS:CE1	3:I:101:ASN:HB3	2.18	0.78
3:J:115:THR:HG22	3:J:116:LYS:H	1.48	0.76
1:H:221:ILE:HD11	1:H:236:LYS:CG	2.08	0.75
2:B:214:GLU:HA	2:B:238:ARG:HH12	1.51	0.74
2:L:178:ASP:HA	2:L:218:VAL:HG12	1.69	0.74
2:L:172:LYS:HB3	2:L:224:THR:OG1	1.88	0.74
2:B:84:SER:N	4:B:302:SO4:O3	2.24	0.71
1:H:25:GLU:N	1:H:131:GLN:HE22	1.89	0.71
2:B:173:VAL:HA	2:B:222:GLU:O	1.91	0.70
1:H:142:THR:O	1:H:143:LYS:NZ	2.21	0.70
2:B:140:PRO:HD3	2:B:225:HIS:CD2	2.27	0.70
1:H:212:SER:HA	1:H:215:LEU:CD2	2.20	0.70
3:I:34:LEU:CB	3:I:64:ARG:O	2.39	0.70
3:J:36:ARG:HB3	3:J:36:ARG:NH2	2.01	0.70
1:A:38:ARG:HG3	1:A:101:GLN:HG2	1.72	0.69
2:B:182:GLN:HB3	2:B:185:ASN:ND2	2.08	0.69
2:B:187:GLN:OE1	2:B:187:GLN:HA	1.92	0.68
2:L:194:ASP:OD2	2:L:196:LYS:HG2	1.93	0.68
3:J:89:ILE:HG13	3:J:104:MET:HG3	1.75	0.68
3:I:234:PHE:O	3:I:238:ILE:HG13	1.92	0.67
3:J:156:GLN:O	3:J:156:GLN:HG3	1.93	0.67
2:B:147:PRO:HD3	2:B:159:VAL:HG22	1.77	0.67
3:J:46:LEU:HD13	3:J:67:LEU:HD11	1.77	0.67
2:B:206:LEU:HD22	2:B:208:LEU:HD21	1.76	0.66
3:I:99:HIS:CE1	3:I:234:PHE:HE1	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:36:ARG:HG2	3:J:64:ARG:NH1	2.10	0.66
2:B:177:VAL:H	2:B:182:GLN:HE22	1.44	0.66
3:I:177:ASP:OD2	3:I:179:THR:HG23	1.95	0.65
3:J:59:ARG:CZ	3:J:89:ILE:O	2.45	0.65
2:B:218:VAL:HA	2:B:237:ASN:OD1	1.97	0.65
2:L:191:THR:HG22	2:L:201:SER:H	1.62	0.65
1:H:31:VAL:HG21	1:H:105:LEU:HD12	1.76	0.64
1:H:221:ILE:HD12	1:H:236:LYS:CG	2.19	0.64
1:A:152:PRO:HG3	1:A:164:LEU:CD2	2.27	0.64
3:I:56:ALA:HB2	3:I:102:ASP:HA	1.78	0.64
2:L:137:VAL:HG21	2:L:226:GLN:OE1	1.97	0.64
3:J:81:GLN:OE1	3:J:83:PHE:HZ	1.80	0.63
1:H:141:SER:HB2	1:H:143:LYS:HZ1	1.64	0.63
2:L:216:HIS:C	2:L:217:LYS:HZ2	2.07	0.63
2:B:176:LYS:HG2	2:B:179:ASN:C	2.24	0.62
1:H:212:SER:HA	1:H:215:LEU:HD21	1.79	0.62
2:B:175:TRP:CZ3	2:B:221:CYS:HB3	2.35	0.62
1:A:110[B]:MET:HE2	1:A:137:VAL:H	1.65	0.61
2:B:176:LYS:NZ	2:B:181:LEU:HB2	2.15	0.61
1:H:25:GLU:H	1:H:131:GLN:NE2	1.95	0.61
3:I:35:LEU:HD23	3:I:35:LEU:H	1.65	0.61
2:L:159:VAL:CG2	2:L:206:LEU:HB3	2.29	0.61
1:A:152:PRO:HD3	1:A:164:LEU:CD2	2.30	0.61
2:B:214:GLU:O	2:B:238:ARG:NH2	2.34	0.60
1:A:37:LEU:HD13	1:A:39:LEU:HG	1.82	0.60
1:A:23:LEU:HD23	1:A:41:CYS:SG	2.42	0.60
2:L:175:TRP:CD1	2:L:186:SER:HG	2.19	0.60
2:L:214:GLU:HA	2:L:238:ARG:NH1	2.17	0.59
3:I:64:ARG:HD3	3:I:82:MET:HG3	1.83	0.59
2:B:176:LYS:HG2	2:B:179:ASN:HA	1.83	0.59
2:L:147:PRO:HD3	2:L:159:VAL:HG12	1.85	0.59
2:B:214:GLU:HA	2:B:238:ARG:HH22	1.67	0.59
2:L:214:GLU:O	2:L:238:ARG:NH1	2.35	0.59
3:I:89:ILE:HD11	3:I:104:MET:HA	1.85	0.58
1:H:25:GLU:HB2	1:H:131:GLN:NE2	2.19	0.58
3:J:53:LEU:HG	3:J:212:LEU:HD11	1.85	0.58
2:B:163:LEU:HD22	2:B:202:LEU:HD22	1.85	0.57
3:J:53:LEU:HD11	3:J:103:LEU:HD22	1.86	0.57
2:B:175:TRP:CE3	2:B:206:LEU:HD12	2.39	0.57
3:I:45:VAL:HG11	3:I:198:PRO:HB3	1.86	0.57
2:B:178:ASP:HA	2:B:218:VAL:HB	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:91:ARG:HD3	1:H:93:THR:HG23	1.87	0.57
3:I:48:HIS:CG	3:I:49:PRO:HD2	2.40	0.57
2:B:214:GLU:HA	2:B:238:ARG:NH1	2.20	0.57
2:B:73:TYR:C	2:B:73:TYR:CD2	2.83	0.57
2:B:145:PHE:HB2	2:B:160:VAL:CG1	2.35	0.56
2:B:175:TRP:CG	2:B:206:LEU:HG	2.40	0.56
2:B:176:LYS:HZ2	2:B:181:LEU:HB2	1.70	0.56
3:J:36:ARG:HH21	3:J:36:ARG:CG	2.19	0.56
1:A:152:PRO:HD3	1:A:164:LEU:HD22	1.87	0.56
2:L:161:CYS:HB2	2:L:175:TRP:CZ2	2.41	0.56
1:H:37:LEU:HD13	1:H:39:LEU:HG	1.89	0.55
1:A:236:LYS:NZ	1:A:238:GLU:OE1	2.29	0.55
2:L:72:ILE:HG12	2:L:78:LEU:HD23	1.89	0.55
2:L:191:THR:CG2	2:L:201:SER:H	2.18	0.55
1:A:38:ARG:NH2	4:A:301:SO4:O3	2.32	0.54
2:B:175:TRP:HB3	2:B:206:LEU:HD11	1.89	0.54
3:I:99:HIS:CE1	3:I:234:PHE:CE1	2.93	0.54
2:L:239:GLY:O	2:L:240:GLU:HG3	2.08	0.54
3:I:105:LEU:HD11	3:I:238:ILE:HG23	1.89	0.54
1:A:194:ALA:HA	1:A:204:LEU:HB3	1.90	0.54
2:L:182:GLN:CG	2:L:185:ASN:HD21	2.21	0.54
1:A:152:PRO:CG	1:A:164:LEU:CD2	2.86	0.54
3:I:64:ARG:HE	3:I:84:GLN:HE21	1.55	0.53
2:L:210:LYS:O	2:L:214:GLU:HG2	2.09	0.53
1:H:141:SER:HB2	1:H:143:LYS:NZ	2.23	0.52
2:L:113:ALA:HB1	2:L:124:VAL:HG12	1.91	0.52
1:H:185:LEU:HD21	1:H:208:VAL:HG21	1.90	0.52
2:B:59:TRP:CE2	2:B:97:LEU:HB2	2.45	0.52
2:B:214:GLU:CA	2:B:238:ARG:HH22	2.22	0.52
2:B:144:ILE:HG12	2:B:236:PHE:CD2	2.45	0.52
2:L:57:LEU:HD22	2:L:95:PHE:CG	2.45	0.52
3:I:129:CYS:SG	3:I:130:PRO:HD2	2.50	0.52
1:A:221:ILE:HD11	1:A:234:ASP:HB3	1.92	0.51
1:H:110:MET:HB2	1:H:137:VAL:HG22	1.93	0.51
3:J:115:THR:HG22	3:J:116:LYS:N	2.21	0.51
3:J:31:ALA:HB2	3:J:67:LEU:HD23	1.92	0.51
2:L:163:LEU:CD2	2:L:223:VAL:HG21	2.30	0.51
3:I:56:ALA:CB	3:I:102:ASP:HA	2.40	0.51
1:H:212:SER:HA	1:H:215:LEU:HD23	1.91	0.50
1:H:131:GLN:HG2	1:H:132:GLY:O	2.10	0.50
2:B:176:LYS:HG2	2:B:179:ASN:CA	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:225:HIS:H	2:B:228:LEU:HD21	1.77	0.50
2:B:144:ILE:HG12	2:B:236:PHE:CE2	2.47	0.50
3:I:83:PHE:HE2	3:I:110:ARG:N	2.10	0.50
1:A:95:LYS:NZ	4:A:301:SO4:O2	2.41	0.50
2:L:172:LYS:CB	2:L:224:THR:OG1	2.58	0.49
1:A:110[A]:MET:HE2	1:A:136:THR:CG2	2.42	0.49
1:A:181:ASN:HA	1:A:221:ILE:HG23	1.95	0.49
3:I:86:VAL:HG11	3:I:109:ASN:HA	1.94	0.49
1:H:57:ARG:HB3	1:H:67:ILE:HD11	1.94	0.49
1:H:81:SER:HB2	2:L:122:GLU:CD	2.37	0.49
1:A:49:SER:HA	1:A:72:SER:O	2.13	0.49
3:I:238:ILE:O	3:I:241:THR:HG22	2.13	0.49
3:J:103:LEU:HD11	3:J:237:TRP:CZ3	2.47	0.48
3:I:67:LEU:HD22	3:I:118:VAL:HG22	1.94	0.48
3:I:158:LEU:HD12	3:I:159:ASN:N	2.27	0.48
1:A:78:TYR:CE1	3:J:174(A):GLN:HG3	2.48	0.48
3:I:63:PHE:O	5:I:401:HOH:O	2.20	0.48
3:I:170:ASP:HB2	5:I:403:HOH:O	2.13	0.48
2:B:180:ALA:O	2:B:182:GLN:NE2	2.46	0.48
1:H:81:SER:HB2	2:L:122:GLU:OE2	2.14	0.48
1:A:51:TYR:CZ	1:A:117:ARG:NH1	2.82	0.47
1:H:31:VAL:O	1:H:137:VAL:HA	2.14	0.47
3:J:34:LEU:HD23	3:J:38:ASN:HA	1.96	0.47
2:B:114:GLN:O	2:B:124:VAL:HG22	2.14	0.47
2:B:220:ALA:HA	2:B:235:SER:OG	2.13	0.47
3:J:89:ILE:HG21	3:J:237:TRP:CH2	2.49	0.47
1:H:196:LEU:HD13	1:H:197:GLN:O	2.14	0.47
1:A:51:TYR:HB3	1:A:117:ARG:HG3	1.95	0.47
1:A:57:ARG:HB3	1:A:67:ILE:HD11	1.97	0.47
2:B:135:ARG:NH2	2:B:136:THR:CG2	2.77	0.47
3:J:26:THR:HB	3:J:27:GLN:H	1.44	0.47
3:J:66:ARG:HG2	3:J:82:MET:SD	2.54	0.47
2:L:107:PHE:HB2	2:L:133:ILE:HD12	1.95	0.47
3:I:158:LEU:HD12	3:I:159:ASN:H	1.79	0.47
2:B:74:TYR:OH	3:J:167:ARG:NH1	2.47	0.47
2:L:113:ALA:HB2	2:L:125:PHE:CD2	2.49	0.47
1:A:32:GLN:HA	1:A:138:SER:O	2.14	0.46
1:A:91:ARG:HB3	5:A:402:HOH:O	2.14	0.46
1:A:31:VAL:O	1:A:137:VAL:HA	2.15	0.46
3:J:31:ALA:HB2	3:J:67:LEU:CD2	2.44	0.46
3:I:99:HIS:CD2	3:I:100:SER:H	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:PRO:HD3	1:A:164:LEU:HD23	1.96	0.46
3:J:103:LEU:HD12	3:J:103:LEU:C	2.40	0.46
2:B:78:LEU:HD11	2:B:86:PHE:O	2.15	0.46
3:J:89:ILE:HG12	3:J:104:MET:HA	1.96	0.46
2:B:87:SER:O	2:B:97:LEU:HD12	2.16	0.46
2:B:214:GLU:C	2:B:238:ARG:HH22	2.23	0.46
2:B:175:TRP:CH2	2:B:221:CYS:HB3	2.51	0.46
3:J:59:ARG:NH2	3:J:89:ILE:O	2.48	0.46
2:L:224:THR:OG1	2:L:224:THR:O	2.28	0.46
3:I:83:PHE:CE2	3:I:109:ASN:HB2	2.51	0.46
2:L:188:GLU:HA	2:L:203:SER:O	2.16	0.46
1:A:110[A]:MET:HE2	1:A:136:THR:HG23	1.96	0.46
3:I:105:LEU:HD12	3:I:241:THR:HG21	1.98	0.45
3:I:65:VAL:HG11	3:I:108:LEU:HD21	1.98	0.45
2:B:225:HIS:O	2:B:228:LEU:HG	2.17	0.45
3:I:211:GLY:HA2	3:I:229:THR:O	2.17	0.45
1:H:164:LEU:HD21	1:H:220:TYR:CD2	2.51	0.45
3:J:238:ILE:HD12	3:J:239:GLN:N	2.31	0.45
3:J:36:ARG:NH2	3:J:36:ARG:CG	2.77	0.45
1:A:143:LYS:HB3	1:A:143:LYS:HE2	1.77	0.45
1:H:193:PRO:HG2	2:L:189:SER:OG	2.17	0.45
2:B:213:TYR:HA	2:B:219:TYR:OH	2.16	0.45
1:A:37:LEU:C	1:A:37:LEU:HD12	2.42	0.44
3:J:103:LEU:CD1	3:J:237:TRP:CZ3	3.00	0.44
3:I:45:VAL:HG21	3:I:209:LEU:HD21	1.99	0.44
2:B:161:CYS:HB2	2:B:175:TRP:CH2	2.53	0.44
1:H:141:SER:CB	1:H:143:LYS:NZ	2.81	0.44
3:J:35:LEU:HB3	3:J:39:GLN:HB2	1.99	0.44
2:L:175:TRP:HD1	2:L:186:SER:HG	1.64	0.44
2:L:213:TYR:CZ	2:L:238:ARG:HG3	2.52	0.44
2:L:36:SER:HA	2:L:132:GLU:O	2.17	0.44
2:B:172:LYS:HD3	2:B:173:VAL:H	1.82	0.44
2:L:239:GLY:C	2:L:240:GLU:HG3	2.42	0.44
3:I:89:ILE:H	3:I:89:ILE:HG13	1.62	0.44
2:L:57:LEU:HD22	2:L:95:PHE:CD2	2.52	0.44
1:A:221:ILE:HD12	1:A:235:LYS:O	2.18	0.44
2:B:145:PHE:HB2	2:B:160:VAL:HG13	2.00	0.43
1:H:91:ARG:HD2	4:H:302:SO4:O4	2.18	0.43
3:J:35:LEU:CB	3:J:39:GLN:HB2	2.48	0.43
1:A:152:PRO:CD	1:A:164:LEU:CD2	2.95	0.43
2:B:174:GLN:O	2:B:222:GLU:HB3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:LYS:HG2	2:B:180:ALA:N	2.32	0.43
2:B:215:LYS:HB3	2:B:215:LYS:HE2	1.74	0.43
3:J:81:GLN:OE1	3:J:83:PHE:CZ	2.66	0.43
2:L:159:VAL:HG22	2:L:206:LEU:HB3	1.99	0.43
1:A:48:LEU:HD13	1:A:91:ARG:HG3	2.00	0.43
2:B:234:LYS:C	2:B:235:SER:HG	2.25	0.43
1:H:141:SER:CB	1:H:143:LYS:HZ1	2.32	0.43
1:A:58:GLN:HG3	1:A:63:GLY:O	2.19	0.43
1:H:153:SER:O	1:H:153:SER:OG	2.34	0.43
3:J:89:ILE:HG12	3:J:105:LEU:H	1.84	0.43
1:H:26:SER:HB3	1:H:40:SER:HB2	2.00	0.43
2:L:43:VAL:O	2:L:98:THR:HA	2.19	0.42
2:B:145:PHE:HB2	2:B:160:VAL:HG12	2.01	0.42
1:A:92:ASP:CG	1:A:95:LYS:HG3	2.45	0.42
3:J:139:SER:O	3:J:198:PRO:HD2	2.19	0.42
1:A:221:ILE:HD12	1:A:235:LYS:C	2.45	0.42
3:J:83:PHE:HB3	3:J:109:ASN:OD1	2.19	0.42
1:A:236:LYS:HZ2	1:A:238:GLU:CD	2.21	0.42
2:B:167:TYR:CD1	2:B:168:PRO:HA	2.54	0.42
2:L:107:PHE:HB2	2:L:133:ILE:CD1	2.50	0.42
2:B:190:VAL:HB	2:B:202:LEU:HD12	2.02	0.42
2:B:214:GLU:HA	2:B:238:ARG:NH2	2.31	0.42
3:J:137:LEU:HD11	3:J:157:CYS:HB2	2.02	0.42
3:I:83:PHE:HB3	3:I:108:LEU:HD22	2.01	0.42
1:A:152:PRO:HG3	1:A:164:LEU:HD21	1.99	0.42
1:H:25:GLU:HA	1:H:40:SER:O	2.19	0.42
1:A:54:THR:O	1:A:115:CYS:HA	2.20	0.41
1:H:110:MET:HE2	1:H:137:VAL:H	1.85	0.41
2:B:45:ILE:HD11	2:B:97:LEU:HD23	2.02	0.41
2:L:97:LEU:C	2:L:97:LEU:HD23	2.46	0.41
1:H:71:THR:O	1:H:91:ARG:NH2	2.53	0.41
1:H:180:TRP:CH2	1:H:222:CYS:HB3	2.55	0.41
2:B:178:ASP:CG	2:B:216:HIS:HB3	2.46	0.41
1:H:118:GLU:OE1	3:I:166:LYS:NZ	2.48	0.41
1:A:194:ALA:HB2	1:A:204:LEU:HD23	2.03	0.41
1:A:25:GLU:H	1:A:131:GLN:HE22	1.69	0.41
2:B:40:GLY:HA2	2:B:101:SER:OG	2.21	0.41
3:J:81:GLN:HB2	3:J:83:PHE:CZ	2.55	0.41
1:A:105:LEU:HD23	1:A:105:LEU:HA	1.87	0.41
2:B:176:LYS:HG3	2:B:180:ALA:C	2.45	0.41
3:J:59:ARG:CA	3:J:104:MET:HE1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:191:THR:HG22	2:L:201:SER:O	2.21	0.41
2:B:135:ARG:NH2	2:B:136:THR:HG22	2.36	0.41
3:J:51:TRP:CH2	3:J:107:LYS:HB2	2.56	0.41
3:I:27:GLN:HB3	3:I:30:GLN:HB2	2.03	0.40
3:I:109:ASN:O	3:I:110:ARG:HG2	2.14	0.40
2:B:213:TYR:O	2:B:238:ARG:NH1	2.54	0.40
2:L:82:VAL:HA	2:L:83:PRO:HD3	1.97	0.40
1:A:152:PRO:HB3	1:A:164:LEU:HD23	2.02	0.40
1:A:215:LEU:HG	1:A:239:PRO:CG	2.51	0.40
1:H:37:LEU:HD12	1:H:37:LEU:O	2.22	0.40
2:L:213:TYR:HA	2:L:219:TYR:OH	2.22	0.40
3:I:87:LYS:HE2	3:I:88:SER:O	2.21	0.40
3:I:243:GLN:HE21	3:I:243:GLN:HB2	1.67	0.40
1:H:43:ALA:HB1	1:H:46:PHE:CZ	2.56	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	212/224 (95%)	206 (97%)	6 (3%)	0	100	100
1	H	217/224 (97%)	210 (97%)	7 (3%)	0	100	100
2	B	213/217 (98%)	198 (93%)	14 (7%)	1 (0%)	24	34
2	L	215/217 (99%)	204 (95%)	10 (5%)	1 (0%)	24	34
3	I	133/227 (59%)	126 (95%)	7 (5%)	0	100	100
3	J	151/227 (66%)	140 (93%)	11 (7%)	0	100	100
All	All	1141/1336 (85%)	1084 (95%)	55 (5%)	2 (0%)	43	56

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	171	ALA
2	L	64	PRO

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	177/185 (96%)	175 (99%)	2 (1%)	65	81
1	H	182/185 (98%)	182 (100%)	0	100	100
2	B	185/186 (100%)	184 (100%)	1 (0%)	81	90
2	L	186/186 (100%)	183 (98%)	3 (2%)	55	74
3	I	131/197 (66%)	131 (100%)	0	100	100
3	J	144/197 (73%)	141 (98%)	3 (2%)	47	67
All	All	1005/1136 (88%)	996 (99%)	9 (1%)	70	84

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	THR
1	A	139	SER
2	B	186	SER
3	J	35	LEU
3	J	36	ARG
3	J	157	CYS
2	L	57	LEU
2	L	136	THR
2	L	226	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	GLN
2	B	179	ASN
2	B	182	GLN

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Mol	Chain	Res	Type
1	H	131	GLN
3	J	39	GLN
3	J	81	GLN
3	J	156	GLN
3	J	174(A)	GLN
3	J	243	GLN
2	L	103	GLN
3	I	99	HIS
3	I	101	ASN
3	I	243	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

15 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	$\# Z > 2$
4	SO4	L	302	-	4,4,4	0.23	0	6,6,6	0.13	0
4	SO4	A	303	-	4,4,4	0.29	0	6,6,6	0.37	0
4	SO4	J	301	-	4,4,4	0.27	0	6,6,6	0.18	0
4	SO4	L	303	-	4,4,4	0.25	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	J	302	-	4,4,4	0.24	0	6,6,6	0.15	0
4	SO4	I	302	-	4,4,4	0.26	0	6,6,6	0.08	0
4	SO4	I	301	-	4,4,4	0.29	0	6,6,6	0.30	0
4	SO4	B	301	-	4,4,4	0.23	0	6,6,6	0.30	0
4	SO4	A	301	-	4,4,4	0.31	0	6,6,6	0.16	0
4	SO4	H	301	-	4,4,4	0.29	0	6,6,6	0.22	0
4	SO4	A	302	-	4,4,4	0.43	0	6,6,6	0.08	0
4	SO4	H	302	-	4,4,4	0.32	0	6,6,6	0.42	0
4	SO4	L	301	-	4,4,4	0.22	0	6,6,6	0.22	0
4	SO4	H	303	-	4,4,4	0.26	0	6,6,6	0.08	0
4	SO4	B	302	-	4,4,4	0.55	0	6,6,6	1.46	1 (16%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	302	SO4	O4-S-O2	2.92	124.83	109.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	301	SO4	2	0
4	H	302	SO4	1	0
4	B	302	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	214/224 (95%)	0.93	29 (13%) 7 6	37, 67, 105, 121	2 (0%)
1	H	218/224 (97%)	0.99	32 (14%) 6 5	31, 65, 100, 115	3 (1%)
2	B	214/217 (98%)	1.32	61 (28%) 1 1	35, 69, 119, 130	1 (0%)
2	L	216/217 (99%)	1.11	45 (20%) 2 2	37, 66, 112, 124	1 (0%)
3	I	149/227 (65%)	2.22	74 (49%) 0 0	53, 101, 128, 140	0
3	J	163/227 (71%)	1.65	51 (31%) 1 1	49, 81, 110, 123	0
All	All	1174/1336 (87%)	1.31	292 (24%) 2 1	31, 70, 117, 140	7 (0%)

All (292) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	236	PHE	7.3
3	I	43	GLY	7.0
3	I	33	LEU	6.9
2	L	232	VAL	6.3
3	I	197	GLY	6.2
3	I	32	ALA	5.7
3	I	31	ALA	5.7
3	J	214	SER	5.6
3	I	103	LEU	5.6
2	B	231	PRO	5.3
3	I	35	LEU	5.2
3	I	212	LEU	5.0
2	B	232	VAL	5.0
2	L	231	PRO	5.0
3	I	44	ALA	5.0
3	J	196	GLY	4.9
2	L	223	VAL	4.9
3	J	212	LEU	4.7
3	I	198	PRO	4.6

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Mol	Chain	Res	Type	RSRZ
3	J	197	GLY	4.6
3	I	66	ARG	4.6
3	I	222	PRO	4.5
2	L	221	CYS	4.5
2	B	159	VAL	4.5
3	J	222	PRO	4.5
2	B	221	CYS	4.5
2	L	236	PHE	4.5
3	I	36	ARG	4.4
3	I	83	PHE	4.4
3	I	34	LEU	4.4
3	J	223	ASN	4.4
2	B	219	TYR	4.3
3	I	63	PHE	4.3
3	J	83	PHE	4.2
1	A	159	GLY	4.2
1	H	236	LYS	4.2
3	I	213	VAL	4.1
3	J	67	LEU	4.1
1	A	204	LEU	4.0
2	B	217	LYS	4.0
2	B	160	VAL	4.0
2	B	223	VAL	3.9
3	I	65	VAL	3.9
3	I	105	LEU	3.9
3	I	139	SER	3.9
3	I	29	TRP	3.9
3	I	112	ILE	3.9
2	L	240	GLU	3.9
2	L	230	SER	3.8
3	I	89	ILE	3.8
3	I	85	GLY	3.8
1	H	240	LYS	3.8
2	B	238	ARG	3.7
3	J	62	VAL	3.7
3	J	26	THR	3.7
2	L	224	THR	3.6
2	B	175	TRP	3.6
3	I	54	THR	3.6
2	L	173	VAL	3.6
3	I	48	HIS	3.6
3	J	102	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	25	ALA	3.6
3	I	55	ALA	3.6
3	J	121	ILE	3.5
1	H	164	LEU	3.5
2	L	219	TYR	3.5
2	L	144	ILE	3.5
3	I	108	LEU	3.5
3	I	137	LEU	3.5
2	L	233	THR	3.5
2	B	233	THR	3.4
3	I	45	VAL	3.4
1	H	153	SER	3.4
3	I	67	LEU	3.4
3	J	198	PRO	3.4
3	I	99	HIS	3.4
2	L	175	TRP	3.3
2	L	170	GLU	3.3
2	B	218	VAL	3.3
3	J	47	VAL	3.3
3	J	246	SER	3.3
1	H	216	GLY	3.2
2	L	181	LEU	3.2
2	B	146	PRO	3.2
2	L	229	SER	3.2
1	A	167	LEU	3.2
2	B	145	PHE	3.2
3	J	85	GLY	3.2
2	B	206	LEU	3.2
2	L	161	CYS	3.2
3	I	79	GLY	3.2
3	J	80	GLN	3.2
2	B	144	ILE	3.2
3	I	100	SER	3.1
1	A	237	VAL	3.1
2	B	147	PRO	3.1
1	A	215	LEU	3.1
2	L	208	LEU	3.1
3	J	60	LYS	3.1
3	J	195	SER	3.1
1	H	166	CYS	3.1
2	B	143	PHE	3.0
3	I	203	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
2	L	222	GLU	3.0
1	A	216	GLY	3.0
2	B	161	CYS	3.0
2	B	172	LYS	3.0
3	J	224	ARG	3.0
2	B	220	ALA	3.0
2	B	173	VAL	3.0
2	L	159	VAL	3.0
3	I	56	ALA	2.9
1	H	215	LEU	2.9
3	J	209	LEU	2.9
3	I	57	HIS	2.9
3	J	112	ILE	2.9
2	L	77	THR	2.9
2	B	230	SER	2.9
3	J	82	MET	2.9
2	B	157	ALA	2.9
2	B	162	LEU	2.9
2	B	228	LEU	2.9
3	J	115	THR	2.9
2	B	210	LYS	2.8
3	J	44	ALA	2.8
1	A	164	LEU	2.8
2	B	171	ALA	2.8
1	A	24	VAL	2.8
3	I	26	THR	2.8
3	I	241	THR	2.8
2	B	227	GLY	2.8
2	B	235	SER	2.8
3	I	209	LEU	2.8
3	J	61	LYS	2.8
1	A	166	CYS	2.8
2	B	170	GLU	2.8
1	A	185	LEU	2.8
3	J	100	SER	2.7
2	B	213	TYR	2.7
2	L	157	ALA	2.7
3	I	30	GLN	2.7
3	J	140	GLY	2.7
1	H	220	TYR	2.7
2	B	177	VAL	2.7
3	I	102	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	236	LYS	2.7
2	L	141	SER	2.7
2	B	139	ALA	2.7
3	J	128	HIS	2.7
3	J	63	PHE	2.7
2	B	205	THR	2.7
1	H	158	SER	2.7
1	H	167	LEU	2.7
1	H	163	ALA	2.6
2	B	211	ALA	2.6
2	L	220	ALA	2.6
2	B	237	ASN	2.6
2	L	218	VAL	2.6
3	J	213	VAL	2.6
2	L	155	GLY	2.6
2	L	162	LEU	2.6
3	I	223	ASN	2.6
2	L	148	SER	2.6
3	I	104	MET	2.6
3	I	106	ILE	2.6
1	A	150	LEU	2.6
1	H	185	LEU	2.6
3	I	51	TRP	2.6
3	J	178	ASP	2.6
1	H	51	TYR	2.6
1	H	175	PRO	2.6
2	L	177	VAL	2.6
1	A	151	ALA	2.6
1	A	160	GLY	2.6
2	B	140	PRO	2.6
2	B	229	SER	2.6
2	B	226	GLN	2.5
3	I	82	MET	2.5
3	J	37	PRO	2.5
1	H	26	SER	2.5
1	A	235	LYS	2.5
2	L	184	GLY	2.5
3	J	184	GLY	2.5
3	I	84	GLN	2.5
3	I	204	SER	2.5
3	I	178	ASP	2.5
1	A	88	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	191	THR	2.5
2	B	148	SER	2.5
2	L	145	PHE	2.5
3	I	242	ILE	2.5
1	H	30	LEU	2.5
1	H	159	GLY	2.5
1	H	195	VAL	2.4
2	L	142	VAL	2.4
3	I	121	ILE	2.4
2	L	234	LYS	2.4
2	L	226	GLN	2.4
3	I	115	THR	2.4
2	B	138	ALA	2.4
3	I	49	PRO	2.4
2	B	141	SER	2.4
3	J	139	SER	2.4
3	I	123	VAL	2.4
3	I	160	ILE	2.4
3	I	53	LEU	2.4
3	J	64	ARG	2.4
3	J	66	ARG	2.4
2	L	140	PRO	2.4
1	H	191	THR	2.4
3	I	214	SER	2.4
3	J	45	VAL	2.4
3	J	36	ARG	2.4
1	A	165	GLY	2.3
2	L	235	SER	2.3
3	I	86	VAL	2.3
3	I	138	VAL	2.3
1	H	174	GLU	2.3
3	I	101	ASN	2.3
2	L	172	LYS	2.3
1	A	162	ALA	2.3
1	A	205	SER	2.3
2	L	176	LYS	2.3
2	B	163	LEU	2.3
1	A	28	GLY	2.3
3	I	172	TYR	2.3
1	H	232	LYS	2.3
2	L	196	LYS	2.3
2	B	78	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
3	I	52	LEU	2.2
1	H	219	THR	2.2
2	B	224	THR	2.2
2	L	216	HIS	2.2
1	H	154	SER	2.2
3	J	186	LYS	2.2
1	A	30	LEU	2.2
1	H	196	LEU	2.2
1	A	239	PRO	2.2
3	J	130	PRO	2.2
2	B	134	LYS	2.2
3	I	27	GLN	2.2
3	I	87	LYS	2.2
3	J	237	TRP	2.2
2	L	143	PHE	2.2
2	L	239	GLY	2.2
3	I	239	GLN	2.2
1	H	162	ALA	2.2
3	J	55	ALA	2.2
3	J	89	ILE	2.2
3	I	224	ARG	2.2
2	B	142	VAL	2.2
2	B	35	PHE	2.2
2	B	208	LEU	2.1
2	B	137	VAL	2.1
3	I	47	VAL	2.1
1	H	46	PHE	2.1
2	B	234	LYS	2.1
1	H	20	GLU	2.1
1	A	208	VAL	2.1
1	H	210	VAL	2.1
1	A	209	THR	2.1
1	A	184	ALA	2.1
2	B	204	SER	2.1
1	A	238	GLU	2.1
2	L	213	TYR	2.1
3	J	185	ASP	2.1
3	J	202	ASN	2.1
1	H	207	VAL	2.1
3	I	114	PRO	2.1
2	B	155	GLY	2.1
1	A	219	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	90	SER	2.1
3	I	116	LYS	2.1
2	B	188	GLU	2.1
2	B	97	LEU	2.1
2	B	181	LEU	2.1
3	J	103	LEU	2.1
3	J	238	ILE	2.1
3	I	81	GLN	2.1
3	I	118	VAL	2.1
2	L	215	LYS	2.0
1	A	163	ALA	2.0
3	J	132	ALA	2.0
3	J	165	GLN	2.0
3	I	158	LEU	2.0
1	H	237	VAL	2.0
2	L	169	ARG	2.0
1	H	206	SER	2.0
2	B	56	GLU	2.0
3	J	210	GLN	2.0
2	B	130	LYS	2.0
3	I	107	LYS	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 ⓘ

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
4	SO4	L	303	5/5	0.33	0.15	130,132,137,142	0
4	SO4	A	303	5/5	0.64	0.13	68,98,113,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	H	303	5/5	0.64	0.10	111,127,145,149	0
4	SO4	A	302	5/5	0.64	0.14	100,106,116,118	0
4	SO4	J	302	5/5	0.69	0.13	116,117,127,128	0
4	SO4	B	302	5/5	0.72	0.17	92,99,100,115	0
4	SO4	I	301	5/5	0.73	0.15	74,81,105,105	0
4	SO4	A	301	5/5	0.75	0.12	93,112,129,132	0
4	SO4	H	301	5/5	0.76	0.14	105,107,108,122	0
4	SO4	I	302	5/5	0.76	0.11	114,118,127,135	0
4	SO4	H	302	5/5	0.81	0.14	83,86,88,105	0
4	SO4	L	302	5/5	0.85	0.12	95,96,101,101	0
4	SO4	J	301	5/5	0.85	0.13	74,87,103,107	0
4	SO4	B	301	5/5	0.86	0.11	84,86,92,112	0
4	SO4	L	301	5/5	0.88	0.10	87,91,96,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.