



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 04:14 PM EDT

PDB ID : 7U5B
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

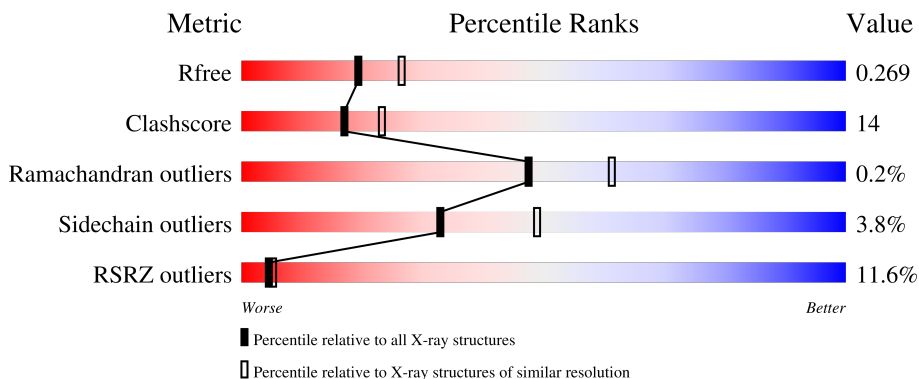
1 Overall quality at a glance

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.



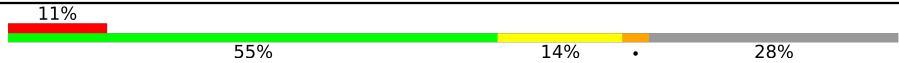
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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	 4% 75% 20%
1	H	224	 5% 80% 17%
2	B	217	 10% 67% 31%
2	L	217	 5% 76% 23%
3	I	227	 25% 44% 21% 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
			Total	C	N	O	S			
1	A	214	Total 1604	C 1015	N 264	O 318	S 7	0	2	0
1	H	218	Total 1638	C 1034	N 272	O 326	S 6	0	3	0

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

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

- Molecule 3 is a protein called Kallikrein-5.

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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

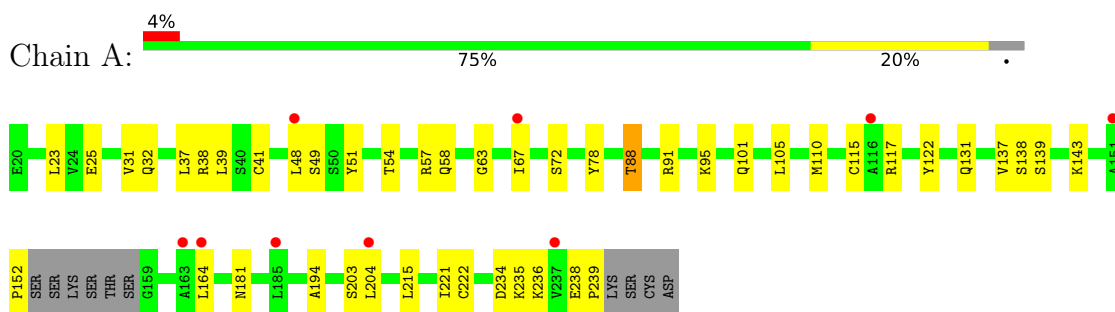
- Molecule 5 is water.

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		

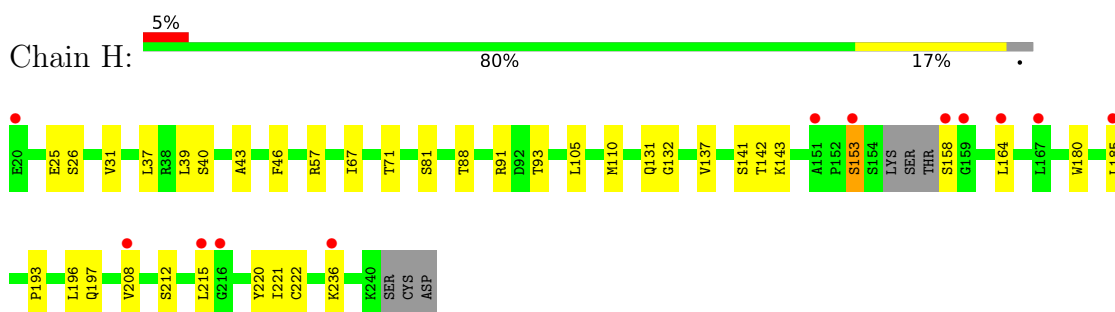
3 Residue-property plots [i](#)

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.

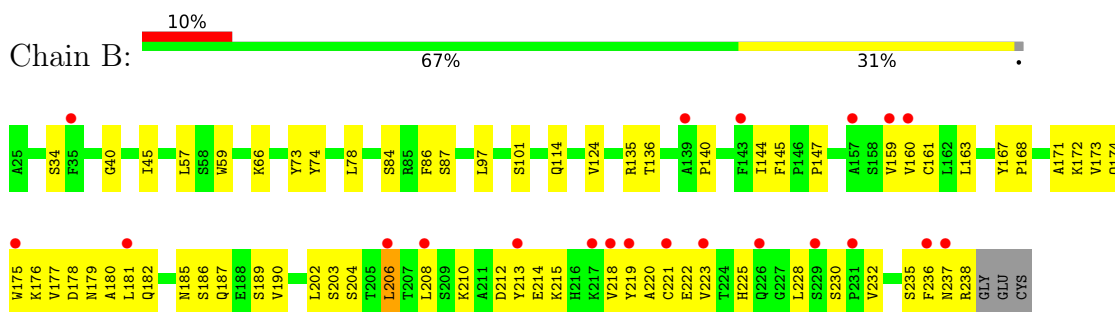
- Molecule 1: anti-KLK5 Fab Heavy Chain



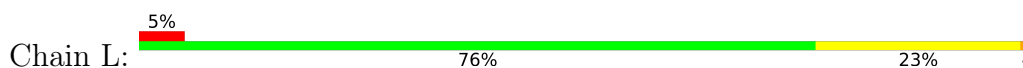
- Molecule 1: anti-KLK5 Fab Heavy Chain

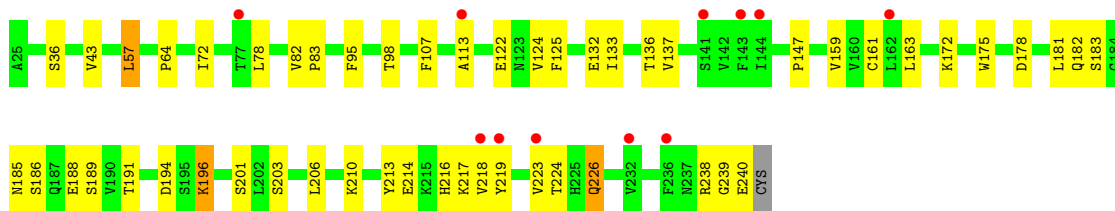


- Molecule 2: anti-KLK5 Fab Light Chain

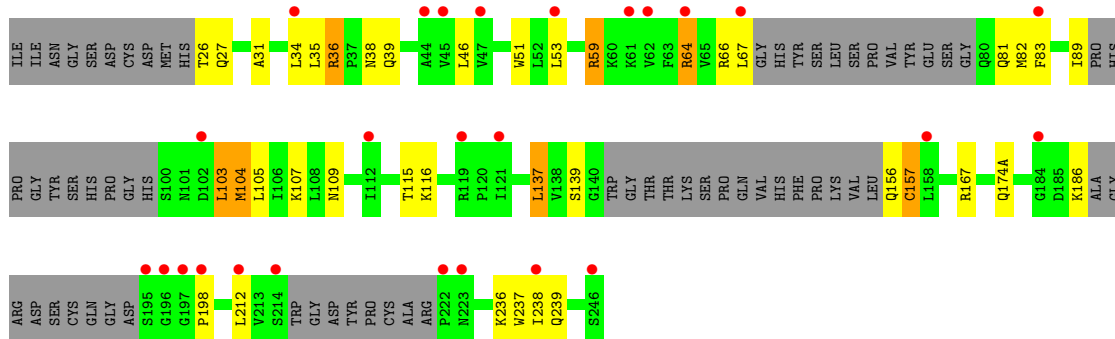


- Molecule 2: anti-KLK5 Fab Light Chain

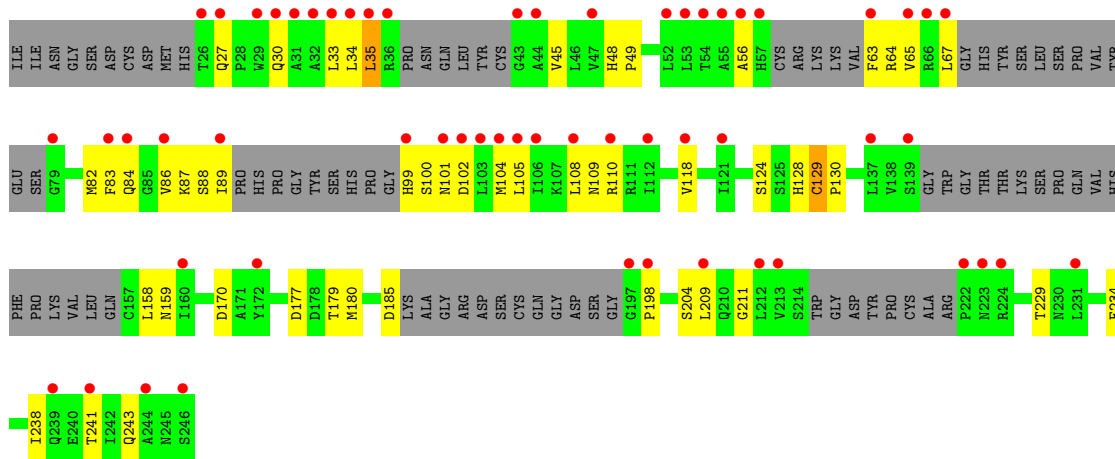




• Molecule 3: Kallikrein-5



• Molecule 3: Kallikrein-5



4 Data and refinement statistics i

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 – 2.37 147.79 – 2.37	Depositor EDS
% Data completeness (in resolution range)	99.0 (52.88-2.37) 99.1 (147.79-2.37)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.37Å)	Xtrriage
Refinement program	PHENIX 1.12-2829_final	Depositor
R, R_{free}	0.222 , 0.270 0.223 , 0.269	Depositor DCC
R_{free} test set	3507 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	56.7	Xtrriage
Anisotropy	0.602	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 57.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.004 for -h,l,k	Xtrriage
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

Xtrriage'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	0.72	3/1650 (0.2%)	0.65	0/2251
1	H	0.62	0/1687	0.66	0/2299
2	B	0.60	0/1665	0.74	0/2258
2	L	0.60	0/1678	0.72	0/2275
3	I	0.44	0/1178	0.66	1/1585 (0.1%)
3	J	0.51	0/1291	0.68	0/1738
All	All	0.60	3/9149 (0.0%)	0.69	1/12406 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	122	TYR	CE1-CZ	-7.13	1.29	1.38
1	A	122	TYR	CD2-CE2	-5.06	1.31	1.39
1	A	122	TYR	CG-CD1	-5.06	1.32	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	128	HIS	C-N-CA	-5.97	106.78	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	38	0
1	H	1638	0	1594	42	0
2	B	1628	0	1577	59	0
2	L	1641	0	1584	38	0
3	I	1161	0	1172	40	0
3	J	1271	0	1293	38	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	249	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 14.

All (249) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:99:HIS:CE1	3:I:101:ASN:HB3	2.18	0.78
3:I:109:ASN:C	3:I:110:ARG:HG3	2.05	0.77
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
1:H:142:THR:O	1:H:143:LYS:NZ	2.21	0.71
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
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
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: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
2:B:176:LYS:NZ	2:B:181:LEU:HB2	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:176:LYS:HG2	2:B:179:ASN:C	2.24	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
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: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:110[B]:MET:HE2	1:A:137:VAL:H	1.69	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:141:SER:HB2	1:H:143:LYS:HZ1	1.71	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:73:TYR:C	2:B:73:TYR:CD2	2.83	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
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: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:A:49:SER:HA	1:A:72:SER:O	2.13	0.49
2:L:216:HIS:C	2:L:217:LYS:HZ2	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:152:PRO:HD3	1:A:164:LEU:HD23	1.96	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:TYR:HA	2:B:219:TYR:OH	2.16	0.45
3:J:103:LEU:CD1	3:J:237:TRP:CZ3	3.00	0.44
1:H:81:SER:HB2	2:L:122:GLU:CD	2.37	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
1:H:158:SER:O	1:H:158:SER:OG	2.34	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
1:H:142:THR:C	1:H:143:LYS:HZ2	2.17	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
2:B:176:LYS:HG2	2:B:180:ALA:N	2.32	0.43
1:A:110[B]:MET:HE2	1:A:110[B]:MET:HB2	1.75	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
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
3:J:139:SER:O	3:J:198:PRO:HD2	2.19	0.42
3:J:83:PHE:HB3	3:J:109:ASN:OD1	2.19	0.42
2:B:167:TYR:CD1	2:B:168:PRO:HA	2.54	0.42
1:H:110:MET:HE2	1:H:137:VAL:H	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:J:103:LEU:HD12	3:J:103:LEU:C	2.40	0.41
2:B:45:ILE:HD11	2:B:97:LEU:HD23	2.02	0.41
2:B:214:GLU:C	2:B:238:ARG:HH22	2.23	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
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: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 [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	29	39
2	L	215/217 (99%)	204 (95%)	10 (5%)	1 (0%)	29	39
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%)	47	61

All (2) Ramachandran outliers are listed below:

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

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	177/185 (96%)	173 (98%)	4 (2%)	50	68
1	H	182/185 (98%)	181 (100%)	1 (0%)	88	95
2	B	185/186 (100%)	174 (94%)	11 (6%)	19	29
2	L	186/186 (100%)	180 (97%)	6 (3%)	39	56
3	I	131/197 (66%)	124 (95%)	7 (5%)	22	34
3	J	144/197 (73%)	135 (94%)	9 (6%)	18	26
All	All	1005/1136 (88%)	967 (96%)	38 (4%)	33	49

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	THR
1	A	139	SER
1	A	203	SER

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Mol	Chain	Res	Type
1	A	222	CYS
2	B	34	SER
2	B	57	LEU
2	B	66	LYS
2	B	186	SER
2	B	189	SER
2	B	203	SER
2	B	204	SER
2	B	206	LEU
2	B	210	LYS
2	B	212	ASP
2	B	230	SER
1	H	153	SER
3	J	36	ARG
3	J	59	ARG
3	J	64	ARG
3	J	103	LEU
3	J	104	MET
3	J	137	LEU
3	J	157	CYS
3	J	186	LYS
3	J	236	LYS
2	L	57	LEU
2	L	136	THR
2	L	181	LEU
2	L	183	SER
2	L	196	LYS
2	L	226	GLN
3	I	33	LEU
3	I	35	LEU
3	I	124	SER
3	I	129	CYS
3	I	180	MET
3	I	185	ASP
3	I	204	SER

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

Mol	Chain	Res	Type
2	B	182	GLN
1	H	131	GLN
3	J	81	GLN

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Mol	Chain	Res	Type
3	J	156	GLN
3	I	84	GLN
3	I	99	HIS
3	I	243	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	H	303	-	4,4,4	0.15	0	6,6,6	0.09	0
4	SO4	A	301	-	4,4,4	0.20	0	6,6,6	0.12	0
4	SO4	H	302	-	4,4,4	0.21	0	6,6,6	0.41	0
4	SO4	J	301	-	4,4,4	0.19	0	6,6,6	0.15	0
4	SO4	I	302	-	4,4,4	0.14	0	6,6,6	0.07	0
4	SO4	A	303	-	4,4,4	0.21	0	6,6,6	0.35	0
4	SO4	A	302	-	4,4,4	0.33	0	6,6,6	0.05	0
4	SO4	L	303	-	4,4,4	0.15	0	6,6,6	0.11	0
4	SO4	B	302	-	4,4,4	0.48	0	6,6,6	1.47	1 (16%)
4	SO4	J	302	-	4,4,4	0.14	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	B	301	-	4,4,4	0.18	0	6,6,6	0.32	0
4	SO4	H	301	-	4,4,4	0.19	0	6,6,6	0.25	0
4	SO4	L	301	-	4,4,4	0.14	0	6,6,6	0.20	0
4	SO4	I	301	-	4,4,4	0.18	0	6,6,6	0.30	0
4	SO4	L	302	-	4,4,4	0.17	0	6,6,6	0.15	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	B	302	SO4	O4-S-O2	2.97	124.83	109.31

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%)	0.73	9 (4%) 36 39	44, 67, 105, 121	0
1	H	218/224 (97%)	0.84	12 (5%) 25 27	44, 65, 100, 115	0
2	B	214/217 (98%)	0.93	21 (9%) 7 8	42, 69, 119, 130	0
2	L	216/217 (99%)	0.79	11 (5%) 28 30	40, 66, 112, 124	0
3	I	149/227 (65%)	2.05	57 (38%) 0 0	53, 101, 128, 140	0
3	J	163/227 (71%)	1.12	26 (15%) 1 2	49, 81, 110, 123	0
All	All	1174/1336 (87%)	1.02	136 (11%) 4 5	40, 70, 117, 140	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	33	LEU	10.8
3	I	43	GLY	10.0
3	I	103	LEU	8.4
3	I	66	ARG	8.4
3	I	197	GLY	8.3
3	I	31	ALA	8.2
3	I	32	ALA	8.0
2	B	236	PHE	7.5
3	I	65	VAL	7.2
3	I	34	LEU	5.7
3	I	83	PHE	5.6
3	I	105	LEU	5.4
3	I	99	HIS	5.2
3	I	55	ALA	5.1
3	J	246	SER	5.0
3	I	139	SER	5.0
2	B	219	TYR	4.7
3	J	212	LEU	4.6
3	I	110	ARG	4.5

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Mol	Chain	Res	Type	RSRZ
1	H	236	LYS	4.4
3	I	101	ASN	4.4
3	I	29	TRP	4.4
1	H	153	SER	4.4
2	L	232	VAL	4.2
3	I	198	PRO	4.2
3	I	79	GLY	4.2
3	I	44	ALA	4.2
3	I	63	PHE	4.1
3	I	137	LEU	4.1
3	I	30	GLN	4.0
3	J	61	LYS	3.9
3	J	62	VAL	3.9
3	I	89	ILE	3.8
3	I	36	ARG	3.8
3	J	223	ASN	3.7
3	I	84	GLN	3.7
3	I	67	LEU	3.7
2	B	223	VAL	3.7
2	B	221	CYS	3.6
3	J	197	GLY	3.6
3	I	102	ASP	3.5
3	I	54	THR	3.5
2	L	219	TYR	3.3
3	J	67	LEU	3.3
3	J	102	ASP	3.3
3	J	158	LEU	3.3
2	L	236	PHE	3.3
3	I	212	LEU	3.2
2	B	231	PRO	3.2
1	H	164	LEU	3.2
3	I	246	SER	3.2
2	L	218	VAL	3.2
3	I	53	LEU	3.2
3	I	56	ALA	3.1
1	H	215	LEU	3.1
3	J	83	PHE	3.1
3	I	112	ILE	3.1
3	J	121	ILE	3.1
3	I	106	ILE	3.0
3	J	195	SER	3.0
3	I	222	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	218	VAL	3.0
3	I	47	VAL	3.0
1	H	158	SER	2.9
3	I	213	VAL	2.9
1	H	167	LEU	2.9
3	I	26	THR	2.9
2	B	160	VAL	2.9
3	J	196	GLY	2.8
3	I	104	MET	2.8
1	H	185	LEU	2.8
3	I	108	LEU	2.8
1	A	204	LEU	2.8
3	J	238	ILE	2.7
3	I	223	ASN	2.7
3	I	224	ARG	2.7
3	I	239	GLN	2.6
2	L	144	ILE	2.6
3	I	244	ALA	2.6
1	H	159	GLY	2.6
2	B	175	TRP	2.6
3	I	86	VAL	2.6
3	I	35	LEU	2.5
1	A	164	LEU	2.5
1	A	163	ALA	2.5
1	H	20	GLU	2.5
2	B	181	LEU	2.5
2	L	141	SER	2.5
2	L	223	VAL	2.4
3	J	47	VAL	2.4
1	H	216	GLY	2.4
3	J	214	SER	2.4
1	A	237	VAL	2.4
2	B	208	LEU	2.4
2	B	226	GLN	2.4
3	J	184	GLY	2.4
3	J	112	ILE	2.4
2	B	139	ALA	2.4
1	H	208	VAL	2.4
3	J	45	VAL	2.3
3	J	222	PRO	2.3
1	A	185	LEU	2.3
3	J	53	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
3	I	172	TYR	2.3
2	B	229	SER	2.3
3	J	34	LEU	2.3
3	I	209	LEU	2.3
3	I	231	LEU	2.3
3	I	118	VAL	2.3
2	L	77	THR	2.2
3	J	64	ARG	2.2
2	B	159	VAL	2.2
3	J	198	PRO	2.2
2	B	217	LYS	2.2
3	I	52	LEU	2.2
2	L	143	PHE	2.2
2	B	213	TYR	2.1
1	A	48	LEU	2.1
2	B	35	PHE	2.1
3	I	27	GLN	2.1
3	I	241	THR	2.1
2	B	237	ASN	2.1
2	B	206	LEU	2.1
2	B	143	PHE	2.1
1	A	116	ALA	2.1
3	I	121	ILE	2.1
3	I	57	HIS	2.1
2	L	113	ALA	2.1
3	J	44	ALA	2.1
1	A	67	ILE	2.0
2	B	157	ALA	2.0
3	I	160	ILE	2.0
1	A	151	ALA	2.0
1	H	151	ALA	2.0
3	J	119	ARG	2.0
2	L	162	LEU	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 monosaccharides 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
4	SO4	B	302	5/5	0.57	0.30	92,99,100,115	0
4	SO4	A	301	5/5	0.76	0.28	93,112,129,132	0
4	SO4	L	303	5/5	0.79	0.14	130,132,137,142	0
4	SO4	A	303	5/5	0.83	0.31	68,98,113,127	0
4	SO4	H	301	5/5	0.85	0.16	105,107,108,122	0
4	SO4	I	301	5/5	0.85	0.17	74,81,105,105	0
4	SO4	A	302	5/5	0.90	0.21	100,106,116,118	0
4	SO4	I	302	5/5	0.90	0.12	114,118,127,135	0
4	SO4	J	302	5/5	0.91	0.15	116,117,127,128	0
4	SO4	H	303	5/5	0.92	0.16	111,127,145,149	0
4	SO4	B	301	5/5	0.94	0.16	84,86,92,112	0
4	SO4	J	301	5/5	0.94	0.18	74,87,103,107	0
4	SO4	L	302	5/5	0.95	0.14	95,96,101,101	0
4	SO4	H	302	5/5	0.96	0.11	83,86,88,105	0
4	SO4	L	301	5/5	0.96	0.16	87,91,96,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.