



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:59 PM UTC

PDB ID : 7REW / pdb_00007rew
Title : Crystal Structure of IL-13 in complex with MMAb3 Fab
Authors : Sudom, A.; Min, X.
Deposited on : 2021-07-13
Resolution : 2.10 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
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

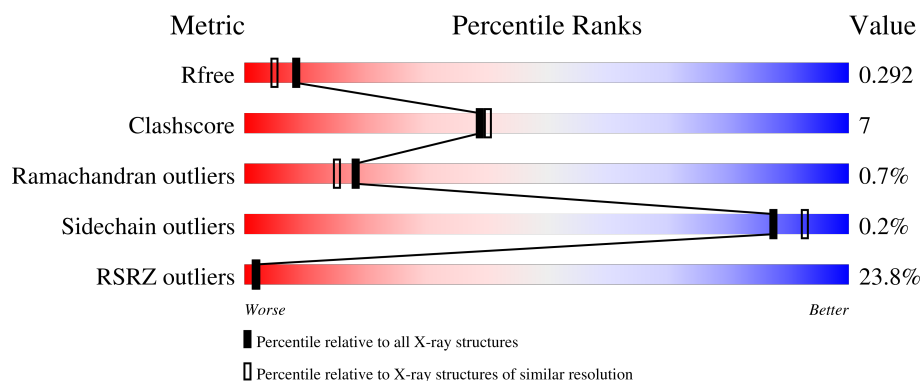
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	227	32% 75% 15% 11%
1	H	227	24% 73% 13% 13%
2	B	212	17% 80% 17% ..
2	L	212	19% 83% 15% .
3	G	112	11% 75% 7% 18%

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Mol	Chain	Length	Quality of chain
3	I	112	21% 70% 12% 17%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7712 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-cyno interleukin 13 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	197	Total	C	N	O	S	0	0	0
			1492	951	245	289	7			
1	A	203	Total	C	N	O	S	0	0	0
			1529	975	250	297	7			

- Molecule 2 is a protein called anti-cyno interleukin 13 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	206	Total	C	N	O	S	0	0	0
			1557	979	256	317	5			
2	B	208	Total	C	N	O	S	0	0	0
			1570	986	258	321	5			

- Molecule 3 is a protein called IL13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	92	Total	C	N	O	S	0	0	0
			716	455	123	132	6			
3	I	93	Total	C	N	O	S	0	0	0
			717	456	124	131	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	2	GLY	-	expression tag	UNP Q0PW92
I	2	GLY	-	expression tag	UNP Q0PW92

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	29	Total	O	0	0
			29	29		

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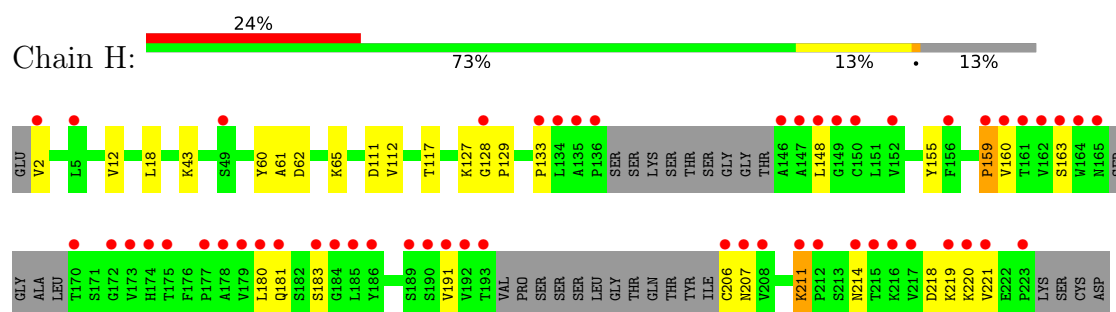
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	38	Total 38	O 38	0	0
4	A	29	Total 29	O 29	0	0
4	B	20	Total 20	O 20	0	0
4	G	10	Total 10	O 10	0	0
4	I	5	Total 5	O 5	0	0

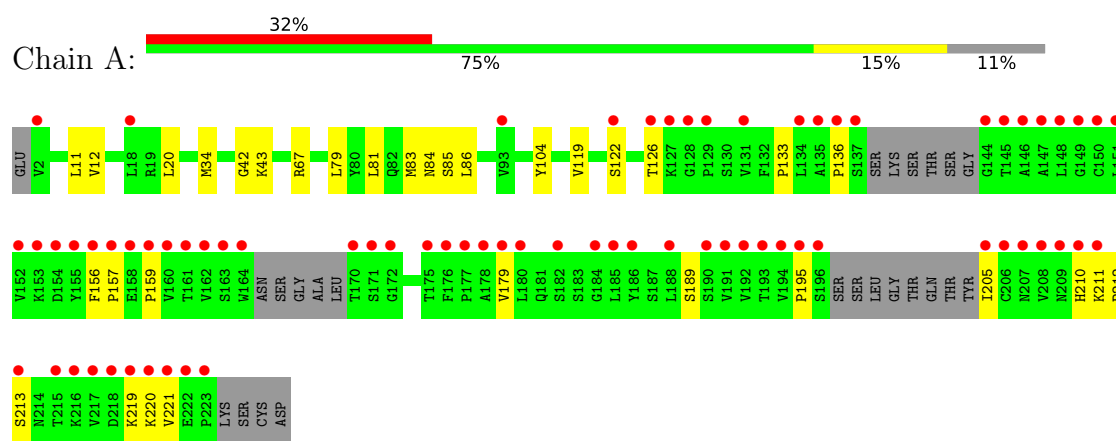
3 Residue-property plots [i](#)

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.

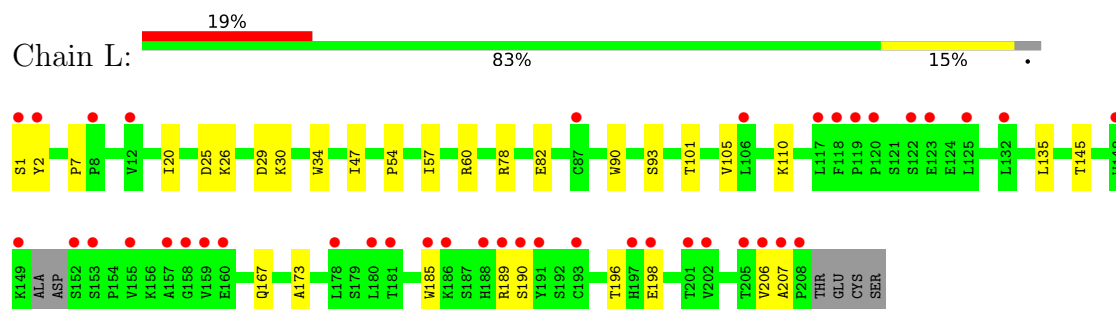
- Molecule 1: anti-cyno interleukin 13 Fab heavy chain



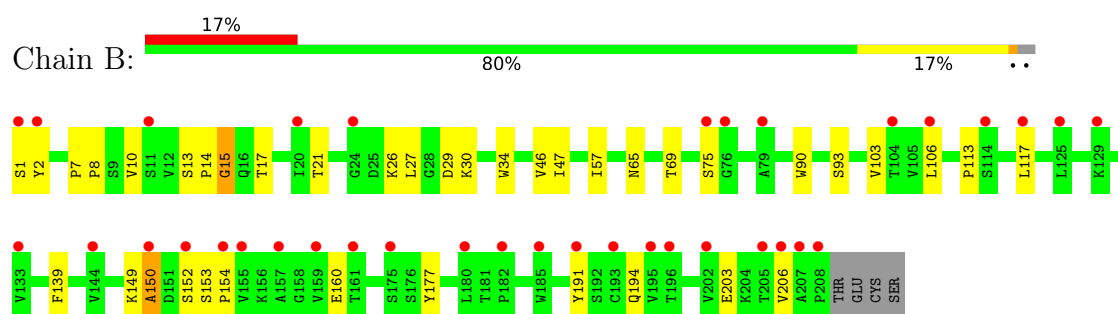
- Molecule 1: anti-cyno interleukin 13 Fab heavy chain



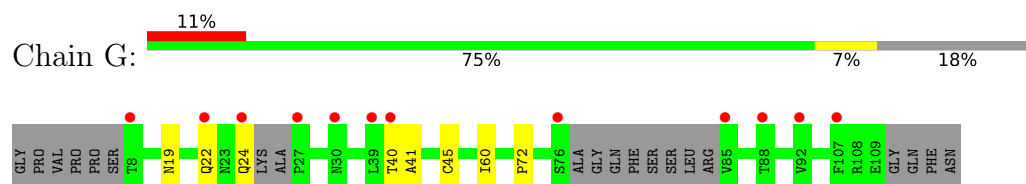
- Molecule 2: anti-cyno interleukin 13 Fab light chain



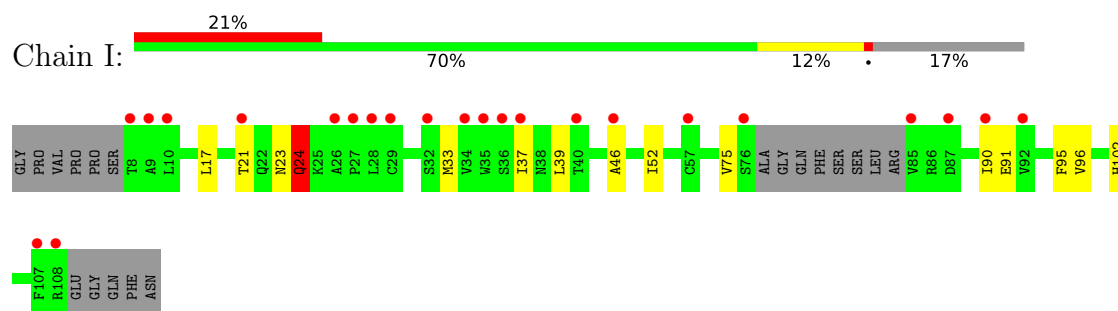
- Molecule 2: anti-cyno interleukin 13 Fab light chain



- Molecule 3: IL13



- Molecule 3: IL13



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.79Å 74.35Å 76.53Å 96.85° 109.89° 112.49°	Depositor
Resolution (Å)	35.96 – 2.10 35.96 – 2.10	Depositor EDS
% Data completeness (in resolution range)	87.9 (35.96-2.10) 87.9 (35.96-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.245 , 0.291 0.246 , 0.292	Depositor DCC
R_{free} test set	2622 reflections (4.26%)	wwPDB-VP
Wilson B-factor (Å ²)	39.0	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 32.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for h,-h-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7712	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.64% 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

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	0.14	0/1568	0.36	0/2136
1	H	0.15	0/1530	0.39	0/2083
2	B	0.11	0/1612	0.43	2/2202 (0.1%)
2	L	0.16	0/1598	0.38	1/2181 (0.0%)
3	G	0.14	0/723	0.37	0/972
3	I	0.22	0/725	0.41	0/978
All	All	0.15	0/7756	0.39	3/10552 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	I	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	152	SER	CA-C-N	8.74	137.54	120.94
2	B	152	SER	C-N-CA	8.74	137.54	120.94
2	L	189	ARG	NE-CZ-NH1	-5.66	115.84	121.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	I	23	ASN	Peptide
3	I	24	GLN	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1529	0	1475	23	0
1	H	1492	0	1434	20	1
2	B	1570	0	1511	24	0
2	L	1557	0	1501	21	0
3	G	716	0	740	7	0
3	I	717	0	741	12	1
4	A	29	0	0	0	0
4	B	20	0	0	0	0
4	G	10	0	0	0	0
4	H	29	0	0	0	0
4	I	5	0	0	0	0
4	L	38	0	0	0	0
All	All	7712	0	7402	102	1

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 7.

All (102) 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)
3:G:22:GLN:NE2	3:G:24:GLN:O	1.90	1.04
1:A:211:LYS:HG3	1:A:212:PRO:HD3	1.64	0.79
1:H:62:ASP:HA	1:H:65:LYS:HD2	1.63	0.78
1:A:179:VAL:HG11	2:B:160:GLU:HB3	1.69	0.74
3:I:37:ILE:HG12	3:I:46:ALA:HB1	1.72	0.69
2:L:1:SER:HA	2:L:30:LYS:HE3	1.75	0.69
1:A:220:LYS:HD2	1:A:221:VAL:H	1.59	0.68
2:L:1:SER:OG	2:L:2:TYR:N	2.32	0.61
1:A:20:LEU:HD12	1:A:81:LEU:HD23	1.83	0.61
3:I:24:GLN:NE2	3:I:24:GLN:HA	2.16	0.60
2:B:117:LEU:HD13	2:B:206:VAL:HG23	1.84	0.60
1:H:60:TYR:HB2	1:H:65:LYS:HG2	1.85	0.59
3:I:24:GLN:HA	3:I:24:GLN:HE21	1.68	0.58
2:L:185:TRP:HH2	2:L:206:VAL:HG12	1.69	0.57
1:H:211:LYS:O	2:B:26:LYS:NZ	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:26:LYS:HD2	2:L:29:ASP:HB2	1.86	0.57
2:B:1:SER:OG	2:B:2:TYR:N	2.38	0.57
1:H:211:LYS:HD3	1:H:214:ASN:HA	1.87	0.56
1:H:211:LYS:HA	1:H:214:ASN:H	1.70	0.56
3:G:22:GLN:O	3:G:22:GLN:HG3	2.05	0.56
2:B:46:VAL:HA	2:B:57:ILE:HD13	1.89	0.55
1:A:210:HIS:CD2	1:A:212:PRO:HD2	2.42	0.55
2:L:185:TRP:CH2	2:L:206:VAL:HG12	2.41	0.54
2:L:7:PRO:O	2:L:101:THR:HG22	2.07	0.54
2:B:34:TRP:HB2	2:B:47:ILE:HB	1.91	0.52
2:L:60:ARG:CZ	2:L:78:ARG:HD3	2.39	0.51
3:I:17:LEU:O	3:I:21:THR:HG23	2.11	0.51
1:H:220:LYS:HG3	1:H:221:VAL:H	1.77	0.49
2:L:20:ILE:HG23	2:L:101:THR:HG21	1.94	0.49
1:A:12:VAL:HG11	1:A:86:LEU:HD13	1.94	0.49
2:B:13:SER:O	2:B:15:GLY:N	2.41	0.49
2:L:26:LYS:HE3	2:L:30:LYS:HE2	1.95	0.49
3:G:40:THR:OG1	3:G:41:ALA:N	2.43	0.49
2:B:113:PRO:HB3	2:B:139:PHE:HB3	1.95	0.49
1:H:127:LYS:NZ	1:H:128:GLY:O	2.45	0.49
2:L:110:LYS:HD2	2:L:198:GLU:HG3	1.96	0.48
3:I:33:MET:SD	3:I:91:GLU:HG2	2.54	0.48
3:I:52:ILE:HD13	3:I:75:VAL:HG23	1.95	0.48
3:I:24:GLN:NE2	3:I:24:GLN:CA	2.77	0.47
3:I:90:ILE:HD11	3:I:95:PHE:HD2	1.77	0.47
2:B:1:SER:HA	2:B:30:LYS:HE3	1.95	0.47
1:H:191:VAL:HG21	2:L:135:LEU:HD13	1.96	0.47
2:B:194:GLN:NE2	2:B:203:GLU:OE2	2.36	0.47
1:A:42:GLY:H	1:A:43:LYS:HE2	1.80	0.47
2:L:82:GLU:HG3	2:L:105:VAL:HG23	1.96	0.47
2:B:150:ALA:HA	2:B:191:TYR:CE1	2.50	0.47
1:A:159:PRO:O	1:A:210:HIS:HD2	1.98	0.46
2:L:90:TRP:CZ2	2:L:93:SER:HA	2.50	0.46
2:L:190:SER:OG	2:L:207:ALA:HB2	2.15	0.46
1:A:67:ARG:CG	1:A:85:SER:HB2	2.46	0.46
2:B:17:THR:HG22	2:B:75:SER:HA	1.97	0.46
2:L:54:PRO:HG2	2:L:57:ILE:HG13	1.98	0.46
1:A:210:HIS:CE1	1:A:213:SER:HG	2.34	0.46
1:A:133:PRO:HD3	1:A:219:LYS:HZ3	1.81	0.45
1:H:12:VAL:HG21	1:H:18:LEU:HG	1.98	0.45
2:B:21:THR:HG23	2:B:69:THR:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:82:GLU:CG	2:L:105:VAL:H	2.29	0.45
1:A:34:MET:HB3	1:A:79:LEU:HD22	1.98	0.45
1:A:67:ARG:HG2	1:A:84:ASN:O	2.17	0.45
1:H:43:LYS:HE3	1:H:43:LYS:HB3	1.87	0.45
3:I:37:ILE:HD12	3:I:37:ILE:HA	1.88	0.44
2:B:10:VAL:O	2:B:103:VAL:HA	2.18	0.44
1:A:83:MET:HE1	1:A:119:VAL:HG21	2.00	0.43
2:B:26:LYS:HB3	2:B:29:ASP:OD1	2.18	0.43
1:H:180:LEU:HD23	1:H:181:GLN:O	2.19	0.43
1:A:189:SER:HB3	2:B:177:TYR:OH	2.18	0.43
2:B:27:LEU:O	2:B:27:LEU:HD13	2.18	0.43
2:L:82:GLU:HG3	2:L:105:VAL:H	1.83	0.43
3:G:45:CYS:SG	3:G:72:PRO:HD2	2.59	0.43
1:A:205:ILE:HA	1:A:220:LYS:HD3	2.00	0.43
1:H:206:CYS:O	1:H:218:ASP:HA	2.19	0.43
2:L:167:GLN:OE1	2:L:173:ALA:HB2	2.18	0.43
2:B:149:LYS:HE2	2:B:154:PRO:HG3	2.01	0.43
3:I:17:LEU:HD22	3:I:96:VAL:HG13	1.99	0.43
1:H:129:PRO:HB3	1:H:155:TYR:HB3	2.01	0.43
2:B:150:ALA:HB3	2:B:153:SER:HB2	1.99	0.43
3:I:39:LEU:HD13	3:I:102:HIS:HB2	2.01	0.43
1:A:122:SER:OG	1:A:156:PHE:HZ	2.02	0.43
1:A:157:PRO:HD2	1:A:212:PRO:HB2	2.01	0.42
1:H:163:SER:HB2	1:H:207:ASN:HB2	2.00	0.42
3:I:37:ILE:HG12	3:I:46:ALA:CB	2.45	0.42
2:B:90:TRP:CZ2	2:B:93:SER:HA	2.55	0.42
1:H:61:ALA:O	1:H:65:LYS:HG3	2.20	0.42
2:L:25:ASP:O	2:L:26:LYS:HG3	2.19	0.42
2:L:34:TRP:HB2	2:L:47:ILE:HB	2.02	0.42
1:H:111:ASP:HB3	1:H:112:VAL:H	1.70	0.42
2:B:14:PRO:HD3	2:B:106:LEU:O	2.19	0.42
1:A:156:PHE:CD1	1:A:157:PRO:HA	2.55	0.41
1:H:148:LEU:HD12	1:H:148:LEU:HA	1.77	0.41
1:H:159:PRO:HB2	1:H:160:VAL:H	1.69	0.41
2:B:7:PRO:HA	2:B:8:PRO:HD3	1.92	0.41
1:H:133:PRO:HD3	1:H:219:LYS:HE2	2.03	0.41
1:H:219:LYS:HZ2	1:H:219:LYS:HG2	1.44	0.41
1:A:11:LEU:HD11	1:A:122:SER:OG	2.21	0.41
1:A:126:THR:HG22	1:A:213:SER:OG	2.20	0.41
3:G:19:ASN:O	3:G:22:GLN:HG2	2.21	0.41
2:B:27:LEU:HD13	2:B:65:ASN:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:60:ILE:H	3:G:60:ILE:HG13	1.75	0.41
2:B:27:LEU:CD1	2:B:65:ASN:OD1	2.69	0.40
2:L:145:THR:OG1	2:L:196:THR:HB	2.22	0.40
1:A:104:TYR:CZ	3:G:72:PRO:HB3	2.56	0.40
1:A:133:PRO:HD3	1:A:219:LYS:NZ	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:183:SER:N	3:I:24:GLN:OE1[1_565]	1.94	0.26

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	195/227 (86%)	176 (90%)	17 (9%)	2 (1%)	12	9
1	H	189/227 (83%)	177 (94%)	10 (5%)	2 (1%)	11	8
2	B	206/212 (97%)	196 (95%)	8 (4%)	2 (1%)	12	9
2	L	202/212 (95%)	195 (96%)	7 (4%)	0	100	100
3	G	86/112 (77%)	80 (93%)	6 (7%)	0	100	100
3	I	89/112 (80%)	84 (94%)	4 (4%)	1 (1%)	11	8
All	All	967/1102 (88%)	908 (94%)	52 (5%)	7 (1%)	18	15

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	150	ALA
3	I	24	GLN
2	B	15	GLY

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Mol	Chain	Res	Type
1	A	195	PRO
1	H	211	LYS
1	H	159	PRO
1	A	136	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	170/190 (90%)	170 (100%)	0	100	100
1	H	165/190 (87%)	163 (99%)	2 (1%)	63	72
2	B	178/182 (98%)	178 (100%)	0	100	100
2	L	177/182 (97%)	177 (100%)	0	100	100
3	G	82/97 (84%)	82 (100%)	0	100	100
3	I	81/97 (84%)	81 (100%)	0	100	100
All	All	853/938 (91%)	851 (100%)	2 (0%)	87	93

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	2	VAL
1	H	117	THR

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

Mol	Chain	Res	Type
1	H	39	GLN
1	H	181	GLN
2	L	37	GLN
1	A	82	GLN
1	A	84	ASN
1	A	98	GLN
1	A	181	GLN

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Mol	Chain	Res	Type
2	B	126	GLN
3	G	68	ASN
3	I	24	GLN
3	I	64	GLN
3	I	73	HIS
3	I	94	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	203/227 (89%)	1.59	72 (35%) 1 1	30, 48, 83, 91	0
1	H	197/227 (86%)	1.32	54 (27%) 1 1	29, 47, 78, 92	0
2	B	208/212 (98%)	1.23	36 (17%) 4 4	33, 52, 70, 75	0
2	L	206/212 (97%)	1.32	41 (19%) 3 3	30, 51, 83, 95	0
3	G	92/112 (82%)	1.07	12 (13%) 7 7	35, 53, 78, 93	0
3	I	93/112 (83%)	1.45	23 (24%) 2 2	34, 56, 87, 92	0
All	All	999/1102 (90%)	1.34	238 (23%) 2 2	29, 51, 80, 95	0

All (238) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	164	TRP	5.6
1	A	160	VAL	5.5
1	H	206	CYS	4.8
1	A	155	TYR	4.7
1	H	148	LEU	4.3
2	L	185	TRP	4.2
1	A	205	ILE	4.2
1	A	221	VAL	4.1
1	A	136	PRO	4.1
1	A	148	LEU	4.0
1	H	136	PRO	4.0
1	A	154	ASP	4.0
2	L	181	THR	3.9
1	H	221	VAL	3.9
2	L	206	VAL	3.9
1	H	217	VAL	3.8
1	A	217	VAL	3.8
1	A	206	CYS	3.8
1	A	220	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
2	L	1	SER	3.8
2	L	202	VAL	3.8
1	A	170	THR	3.8
1	A	157	PRO	3.8
1	A	178	ALA	3.8
1	H	146	ALA	3.7
2	B	182	PRO	3.6
3	I	28	LEU	3.6
1	A	191	VAL	3.6
1	A	161	THR	3.6
1	A	177	PRO	3.6
2	L	208	PRO	3.6
1	A	208	VAL	3.5
2	L	159	VAL	3.5
1	A	184	GLY	3.5
2	L	120	PRO	3.5
1	H	149	GLY	3.5
1	A	188	LEU	3.5
1	A	147	ALA	3.4
1	A	122	SER	3.4
2	B	1	SER	3.4
1	H	150	CYS	3.4
1	A	186	TYR	3.4
2	L	155	VAL	3.4
2	B	206	VAL	3.4
1	A	153	LYS	3.4
1	A	180	LEU	3.4
1	H	164	TRP	3.3
1	H	211	LYS	3.3
2	L	193	CYS	3.3
1	A	213	SER	3.3
3	G	92	VAL	3.3
3	I	85	VAL	3.3
1	A	216	LYS	3.3
1	H	161	THR	3.2
1	A	159	PRO	3.2
1	H	160	VAL	3.2
1	A	131	VAL	3.2
2	B	155	VAL	3.2
1	H	135	ALA	3.2
3	I	107	PHE	3.2
2	B	75	SER	3.2

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Mol	Chain	Res	Type	RSRZ
3	I	76	SER	3.2
1	A	152	VAL	3.2
1	A	179	VAL	3.2
1	A	210	HIS	3.2
2	L	198	GLU	3.2
2	B	208	PRO	3.2
1	H	220	LYS	3.2
1	H	208	VAL	3.2
1	A	171	SER	3.2
1	A	195	PRO	3.2
2	B	152	SER	3.1
2	L	205	THR	3.1
1	H	173	VAL	3.1
2	L	153	SER	3.1
2	L	190	SER	3.1
2	L	207	ALA	3.1
2	L	180	LEU	3.1
1	A	223	PRO	3.1
2	B	150	ALA	3.1
2	L	186	LYS	3.1
1	H	180	LEU	3.0
1	A	162	VAL	3.0
2	B	202	VAL	3.0
1	A	209	ASN	3.0
2	B	76	GLY	3.0
1	A	158	GLU	3.0
2	L	201	THR	3.0
1	A	135	ALA	2.9
2	L	157	ALA	2.9
2	L	158	GLY	2.9
1	H	162	VAL	2.9
2	L	2	TYR	2.9
2	B	191	TYR	2.9
1	H	152	VAL	2.9
1	A	93	VAL	2.9
3	I	87	ASP	2.9
1	A	129	PRO	2.9
1	A	190	SER	2.9
2	L	152	SER	2.9
1	A	128	GLY	2.9
3	I	27	PRO	2.8
3	I	8	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	175	THR	2.8
1	H	193	THR	2.8
1	H	219	LYS	2.8
1	A	193	THR	2.8
1	H	174	HIS	2.7
1	H	178	ALA	2.7
1	A	146	ALA	2.7
1	H	186	TYR	2.7
3	G	40	THR	2.7
1	H	133	PRO	2.7
1	A	194	VAL	2.7
1	H	190	SER	2.7
1	A	222	GLU	2.7
2	L	178	LEU	2.7
2	L	197	HIS	2.7
3	G	76	SER	2.7
2	B	106	LEU	2.7
1	H	223	PRO	2.7
1	A	144	GLY	2.7
1	H	185	LEU	2.6
1	A	126	THR	2.6
2	L	87	CYS	2.6
3	I	29	CYS	2.6
2	L	106	LEU	2.6
1	H	163	SER	2.6
1	A	2	VAL	2.6
2	B	195	VAL	2.6
1	H	134	LEU	2.6
1	H	212	PRO	2.6
1	A	151	LEU	2.6
3	I	108	ARG	2.6
2	L	132	LEU	2.6
2	L	148	TRP	2.6
2	B	114	SER	2.6
3	G	39	LEU	2.6
1	A	175	THR	2.5
1	A	185	LEU	2.5
1	A	156	PHE	2.5
1	A	150	CYS	2.5
1	A	134	LEU	2.5
3	I	35	TRP	2.5
1	A	211	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	179	VAL	2.5
1	H	170	THR	2.5
3	I	40	THR	2.5
2	L	125	LEU	2.5
2	B	185	TRP	2.5
3	I	10	LEU	2.4
3	G	30	ASN	2.4
3	G	22	GLN	2.4
2	B	193	CYS	2.4
2	L	122	SER	2.4
2	L	191	TYR	2.4
1	H	215	THR	2.4
3	I	21	THR	2.4
1	H	177	PRO	2.4
1	H	216	LYS	2.4
2	L	189	ARG	2.4
3	I	26	ALA	2.4
2	L	188	HIS	2.4
1	A	176	PHE	2.4
3	I	90	ILE	2.4
1	H	49	SER	2.4
1	A	137	SER	2.4
2	B	2	TYR	2.4
2	B	79	ALA	2.4
1	A	192	VAL	2.4
2	B	133	VAL	2.4
1	A	163	SER	2.4
3	G	8	THR	2.4
2	L	119	PRO	2.4
2	L	118	PHE	2.3
3	I	37	ILE	2.3
1	H	128	GLY	2.3
1	H	184	GLY	2.3
1	A	182	SER	2.3
2	B	144	VAL	2.3
2	B	207	ALA	2.3
2	B	24	GLY	2.3
1	H	189	SER	2.3
1	H	181	GLN	2.3
1	H	2	VAL	2.3
3	I	34	VAL	2.3
1	H	159	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
3	G	27	PRO	2.3
1	H	214	ASN	2.3
2	B	117	LEU	2.3
3	G	24	GLN	2.2
1	H	191	VAL	2.2
1	H	192	VAL	2.2
1	A	218	ASP	2.2
1	H	147	ALA	2.2
1	A	18	LEU	2.2
1	H	165	ASN	2.2
1	H	207	ASN	2.2
1	A	145	THR	2.2
1	A	207	ASN	2.2
2	B	196	THR	2.2
3	G	85	VAL	2.2
1	A	172	GLY	2.2
3	I	32	SER	2.2
1	A	215	THR	2.2
3	G	88	THR	2.2
2	L	12	VAL	2.2
2	L	160	GLU	2.2
1	A	196	SER	2.2
2	B	11	SER	2.2
1	A	127	LYS	2.2
2	B	161	THR	2.2
1	H	156	PHE	2.1
2	B	159	VAL	2.1
2	L	8	PRO	2.1
3	I	9	ALA	2.1
1	H	183	SER	2.1
2	B	125	LEU	2.1
2	L	117	LEU	2.1
2	B	175	SER	2.1
2	B	104	THR	2.1
2	B	154	PRO	2.1
1	A	149	GLY	2.1
2	L	149	LYS	2.1
3	I	92	VAL	2.1
2	B	205	THR	2.0
2	B	20	ILE	2.0
2	L	123	GLU	2.0
3	G	107	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
3	I	36	SER	2.0
2	B	157	ALA	2.0
3	I	46	ALA	2.0
1	H	5	LEU	2.0
2	B	180	LEU	2.0
3	I	57	CYS	2.0
1	A	219	LYS	2.0
2	B	129	LYS	2.0
1	H	172	GLY	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.