



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:45 AM UTC

PDB ID : 7KQ7 / pdb_00007kq7
Title : Crystal structure of IL21R in complex with an antibody Fab fragment
Authors : Mosyak, L.; Svenson, K.
Deposited on : 2020-11-13
Resolution : 2.20 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

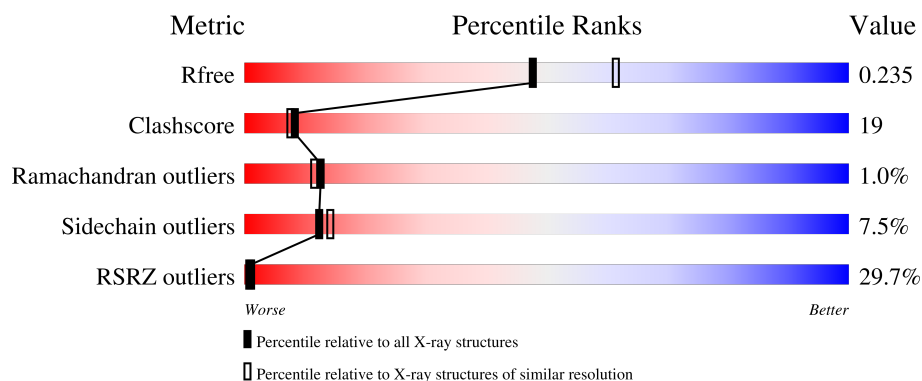
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	H	222	19% 70% 23% 5%
2	L	218	25% 68% 29% •
3	B	214	43% 56% 35% 7% •

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5111 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 Antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	212	Total	C	N	O	S	0	0	0
			1615	1027	273	309	6			

- Molecule 2 is a protein called Antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	217	Total	C	N	O	S	0	0	0
			1663	1035	286	336	6			

- Molecule 3 is a protein called Interleukin-21 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	208	Total	C	N	O	S	0	0	0
			1684	1068	278	327	11			

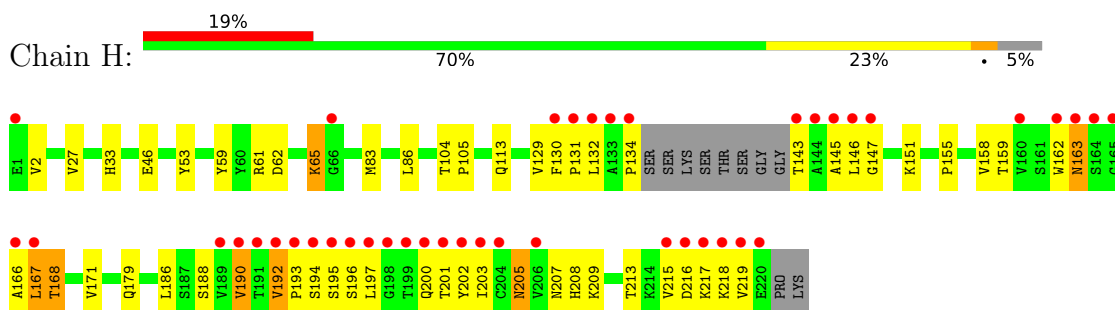
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	73	Total	O	0	0
			73	73		
4	L	65	Total	O	0	0
			65	65		
4	B	11	Total	O	0	0
			11	11		

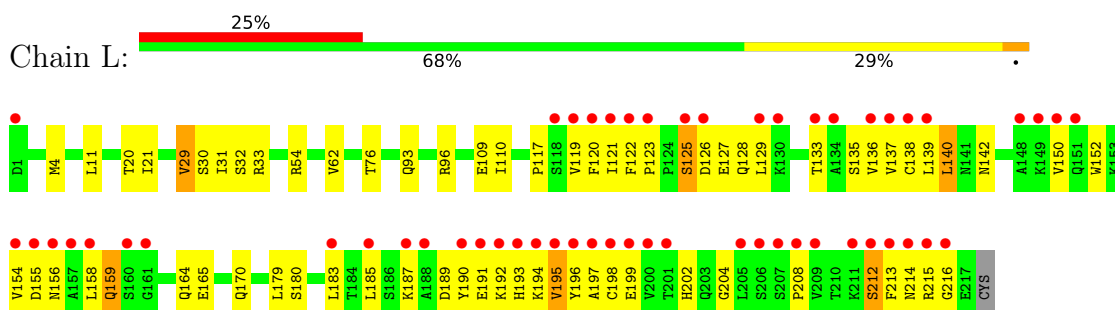
3 Residue-property plots [i](#)

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.

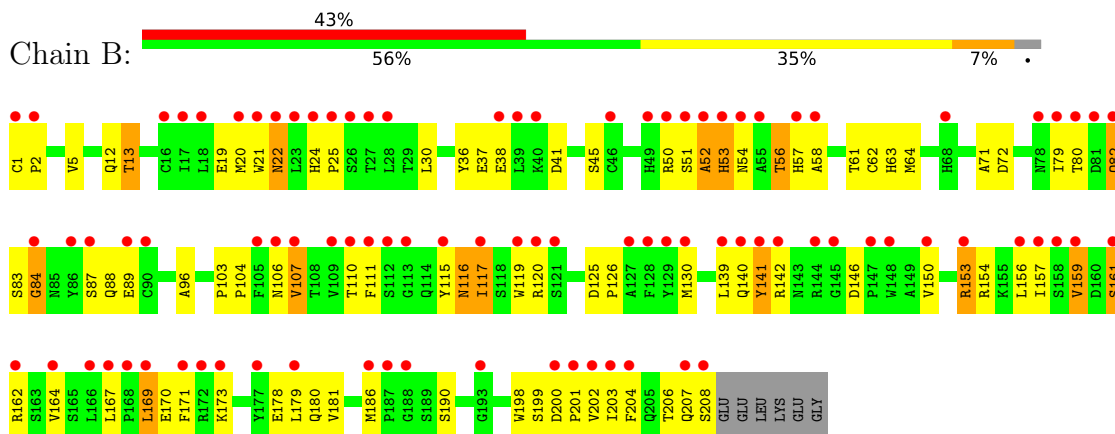
- Molecule 1: Antibody heavy chain



- Molecule 2: Antibody light chain



- Molecule 3: Interleukin-21 receptor



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	155.48Å 246.50Å 55.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.22 – 2.20 42.22 – 2.20	Depositor EDS
% Data completeness (in resolution range)	87.4 (42.22-2.20) 87.5 (42.22-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.6.1 _357	Depositor
R, R_{free}	0.215 , 0.240 0.209 , 0.235	Depositor DCC
R_{free} test set	2497 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.805	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5111	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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](#)

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	H	0.60	0/1656	0.84	0/2261
2	L	0.57	0/1699	0.88	3/2305 (0.1%)
3	B	0.42	0/1734	0.84	4/2364 (0.2%)
All	All	0.53	0/5089	0.85	7/6930 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	62	VAL	N-CA-C	5.96	113.75	108.63
2	L	142	ASN	N-CA-C	5.78	119.21	111.24
3	B	186	MET	CA-C-N	5.71	124.90	118.97
3	B	186	MET	C-N-CA	5.71	124.90	118.97
2	L	137	VAL	N-CA-C	5.40	115.63	107.75
3	B	173	LYS	N-CA-C	5.33	117.16	110.24
3	B	53	HIS	N-CA-C	5.17	116.79	108.32

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	H	1615	0	1585	67	0
2	L	1663	0	1613	58	0
3	B	1684	0	1578	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	11	0	0	1	0
4	H	73	0	0	1	1
4	L	65	0	0	0	3
All	All	5111	0	4776	187	4

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 19.

All (187) 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:B:120:ARG:HG2	3:B:162:ARG:HH21	1.21	1.02
3:B:20:MET:HE1	3:B:53:HIS:HB2	1.41	1.01
2:L:31:ILE:HD11	2:L:96:ARG:CZ	1.94	0.98
1:H:129:VAL:C	1:H:217:LYS:HZ1	1.73	0.96
3:B:22:ASN:HD21	3:B:24:HIS:CG	1.85	0.94
1:H:129:VAL:HG12	1:H:217:LYS:HZ2	1.34	0.92
1:H:217:LYS:HG2	1:H:218:LYS:H	1.39	0.87
2:L:110:ILE:H	2:L:170:GLN:HE22	1.20	0.85
3:B:79:ILE:HG22	3:B:88:GLN:HB3	1.60	0.82
3:B:142:ARG:HD2	3:B:178:GLU:OE2	1.79	0.82
1:H:196:SER:HB3	1:H:200:GLN:HG3	1.60	0.81
2:L:189:ASP:HA	2:L:192:LYS:HG2	1.62	0.80
1:H:162:TRP:HB2	1:H:167:LEU:HD11	1.64	0.79
2:L:119:VAL:O	2:L:120:PHE:HD1	1.68	0.77
1:H:217:LYS:HG2	1:H:218:LYS:N	1.94	0.77
3:B:22:ASN:ND2	3:B:24:HIS:H	1.81	0.77
1:H:163:ASN:HB2	1:H:166:ALA:CB	2.14	0.76
3:B:120:ARG:HG2	3:B:162:ARG:NH2	1.99	0.76
1:H:33:HIS:HD2	1:H:53:TYR:H	1.34	0.76
1:H:201:THR:HA	1:H:218:LYS:NZ	1.99	0.76
1:H:129:VAL:HG12	1:H:217:LYS:NZ	2.01	0.75
3:B:19:GLU:HG2	3:B:57:HIS:CE1	2.22	0.74
3:B:125:ASP:OD1	3:B:126:PRO:HD2	1.86	0.74
3:B:25:PRO:HA	3:B:50:ARG:HH11	1.52	0.74
1:H:134:PRO:HD3	1:H:146:LEU:HB3	1.68	0.73
3:B:20:MET:CE	3:B:53:HIS:HB2	2.17	0.72
2:L:31:ILE:HD11	2:L:96:ARG:NE	2.05	0.72
1:H:162:TRP:HB2	1:H:167:LEU:CD1	2.19	0.72
1:H:179:GLN:HG2	2:L:164:GLN:HE22	1.53	0.71
1:H:113:GLN:HB2	4:H:339:HOH:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:196:SER:HB3	1:H:200:GLN:CG	2.21	0.70
1:H:163:ASN:HB2	1:H:166:ALA:HB2	1.74	0.68
1:H:33:HIS:CD2	1:H:53:TYR:H	2.12	0.67
3:B:167:LEU:HD11	3:B:170:GLU:HG2	1.77	0.67
2:L:128:GLN:HE22	2:L:135:SER:HB2	1.60	0.67
1:H:162:TRP:CB	1:H:167:LEU:HD11	2.26	0.66
3:B:119:TRP:O	3:B:162:ARG:HG2	1.98	0.63
1:H:163:ASN:HB2	1:H:166:ALA:HB3	1.79	0.62
1:H:155:PRO:O	1:H:208:HIS:HE1	1.82	0.62
1:H:194:SER:HB2	1:H:197:LEU:HD23	1.79	0.62
2:L:197:ALA:HA	2:L:212:SER:HB3	1.82	0.61
1:H:203:ILE:HA	1:H:217:LYS:O	2.00	0.61
1:H:171:VAL:HG22	1:H:190:VAL:CG1	2.31	0.61
2:L:154:VAL:HG12	2:L:155:ASP:OD1	2.00	0.61
2:L:54:ARG:NH2	3:B:72:ASP:OD1	2.34	0.60
2:L:156:ASN:ND2	2:L:195:VAL:HG11	2.16	0.60
2:L:119:VAL:O	2:L:120:PHE:CD1	2.53	0.60
1:H:129:VAL:C	1:H:217:LYS:NZ	2.56	0.60
3:B:139:LEU:HD23	3:B:181:VAL:HG22	1.84	0.60
2:L:11:LEU:C	2:L:11:LEU:HD12	2.27	0.60
3:B:159:VAL:HG12	3:B:161:SER:OG	2.00	0.60
1:H:207:ASN:ND2	1:H:209:LYS:HE3	2.17	0.59
3:B:22:ASN:HD21	3:B:24:HIS:CD2	2.19	0.59
3:B:22:ASN:ND2	3:B:24:HIS:CD2	2.71	0.59
2:L:30:SER:O	2:L:31:ILE:HD13	2.03	0.59
1:H:167:LEU:O	1:H:168:THR:HG23	2.03	0.59
3:B:140:GLN:HB2	3:B:198:TRP:CH2	2.38	0.59
2:L:136:VAL:HG12	2:L:183:LEU:HB3	1.86	0.58
3:B:22:ASN:ND2	3:B:24:HIS:CG	2.66	0.58
1:H:2:VAL:HG22	1:H:27:VAL:HG11	1.85	0.58
2:L:136:VAL:CG1	2:L:183:LEU:HB3	2.33	0.58
2:L:138:CYS:HB2	2:L:152:TRP:CZ2	2.39	0.57
3:B:13:THR:HG23	4:B:303:HOH:O	2.04	0.57
1:H:201:THR:HA	1:H:218:LYS:HZ1	1.68	0.57
3:B:1:CYS:HB2	3:B:2:PRO:CD	2.34	0.57
2:L:20:THR:HG23	2:L:76:THR:CG2	2.34	0.57
2:L:119:VAL:C	2:L:120:PHE:CD1	2.83	0.56
2:L:190:TYR:O	2:L:215:ARG:HD3	2.04	0.56
1:H:83:MET:HE2	1:H:86:LEU:HD21	1.88	0.56
1:H:202:TYR:H	1:H:218:LYS:NZ	2.03	0.56
2:L:152:TRP:O	2:L:159:GLN:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:32:SER:OG	2:L:33:ARG:N	2.35	0.55
3:B:13:THR:HG22	3:B:63:HIS:CE1	2.42	0.55
3:B:107:VAL:HG12	3:B:117:ILE:HD11	1.89	0.55
3:B:20:MET:HE2	3:B:58:ALA:N	2.23	0.54
3:B:141:TYR:CE1	3:B:153:ARG:HB3	2.43	0.54
2:L:128:GLN:HE22	2:L:135:SER:CB	2.21	0.54
1:H:179:GLN:HG2	2:L:164:GLN:NE2	2.22	0.54
1:H:186:LEU:C	1:H:186:LEU:HD12	2.32	0.54
1:H:171:VAL:HG22	1:H:190:VAL:HG13	1.90	0.54
3:B:169:LEU:HD22	3:B:169:LEU:C	2.33	0.54
2:L:158:LEU:O	2:L:159:GLN:NE2	2.41	0.53
3:B:71:ALA:HB1	3:B:96:ALA:HB2	1.91	0.52
2:L:129:LEU:HD11	2:L:190:TYR:CE2	2.45	0.52
3:B:20:MET:HE2	3:B:57:HIS:C	2.34	0.52
2:L:122:PHE:O	2:L:136:VAL:HG23	2.09	0.52
1:H:131:PRO:HD2	2:L:125:SER:OG	2.10	0.52
2:L:152:TRP:CZ3	2:L:198:CYS:HB3	2.45	0.52
3:B:37:GLU:O	3:B:41:ASP:HB3	2.11	0.51
3:B:21:TRP:O	3:B:22:ASN:HB3	2.10	0.51
2:L:119:VAL:C	2:L:120:PHE:HD1	2.18	0.51
2:L:187:LYS:O	2:L:191:GLU:HG2	2.12	0.50
3:B:180:GLN:HG2	3:B:199:SER:O	2.12	0.50
3:B:167:LEU:CD1	3:B:170:GLU:HG2	2.40	0.50
1:H:145:ALA:HB2	2:L:120:PHE:CE2	2.46	0.50
3:B:178:GLU:HA	3:B:202:VAL:O	2.11	0.50
1:H:146:LEU:HD21	1:H:202:TYR:CD2	2.46	0.49
3:B:79:ILE:CG2	3:B:88:GLN:HB3	2.36	0.49
3:B:140:GLN:HB2	3:B:198:TRP:CZ3	2.47	0.49
3:B:19:GLU:HG2	3:B:57:HIS:HE1	1.72	0.49
3:B:110:THR:HG22	3:B:116:ASN:HB3	1.94	0.49
1:H:104:THR:N	1:H:105:PRO:CD	2.75	0.49
2:L:129:LEU:HD11	2:L:190:TYR:HE2	1.78	0.49
1:H:194:SER:HB2	1:H:197:LEU:CD2	2.43	0.49
2:L:150:VAL:HA	2:L:199:GLU:O	2.13	0.49
1:H:194:SER:CB	1:H:197:LEU:HD23	2.42	0.49
1:H:201:THR:HA	1:H:218:LYS:HZ3	1.73	0.49
2:L:154:VAL:O	2:L:155:ASP:C	2.56	0.49
1:H:132:LEU:HB3	2:L:122:PHE:CD1	2.48	0.49
3:B:54:ASN:HB2	3:B:57:HIS:H	1.77	0.49
3:B:141:TYR:C	3:B:141:TYR:CD1	2.91	0.49
2:L:154:VAL:H	2:L:159:GLN:HE21	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:62:ASP:OD1	1:H:65:LYS:NZ	2.41	0.48
1:H:215:VAL:HG12	1:H:216:ASP:N	2.29	0.48
3:B:169:LEU:HD13	3:B:170:GLU:N	2.29	0.48
1:H:146:LEU:HB2	1:H:219:VAL:HG11	1.96	0.47
1:H:196:SER:O	1:H:200:GLN:HB2	2.14	0.47
3:B:140:GLN:HG3	3:B:154:ARG:HG2	1.96	0.47
1:H:46:GLU:OE1	1:H:61:ARG:HD3	2.14	0.47
3:B:179:LEU:HD12	3:B:179:LEU:C	2.39	0.47
3:B:12:GLN:HA	3:B:64:MET:O	2.13	0.47
3:B:30:LEU:C	3:B:30:LEU:HD23	2.40	0.47
3:B:51:SER:O	3:B:52:ALA:HB2	2.15	0.47
3:B:146:ASP:HB3	3:B:150:VAL:HG21	1.96	0.47
3:B:156:LEU:C	3:B:156:LEU:HD23	2.40	0.46
3:B:159:VAL:CG1	3:B:161:SER:OG	2.64	0.46
2:L:192:LYS:O	2:L:193:HIS:CD2	2.68	0.46
3:B:54:ASN:HB3	3:B:56:THR:H	1.80	0.46
2:L:20:THR:HG23	2:L:76:THR:HG23	1.98	0.46
1:H:146:LEU:HD12	1:H:146:LEU:O	2.16	0.45
1:H:205:ASN:HD22	1:H:205:ASN:N	2.14	0.45
2:L:126:ASP:OD1	2:L:127:GLU:N	2.44	0.45
2:L:193:HIS:O	2:L:215:ARG:NH2	2.45	0.45
3:B:141:TYR:C	3:B:141:TYR:HD1	2.24	0.45
3:B:141:TYR:HD1	3:B:141:TYR:O	2.00	0.45
1:H:194:SER:O	1:H:195:SER:C	2.59	0.45
1:H:167:LEU:O	1:H:168:THR:CG2	2.65	0.45
2:L:154:VAL:HB	2:L:159:GLN:NE2	2.31	0.45
3:B:61:THR:CG2	3:B:62:CYS:N	2.80	0.45
3:B:156:LEU:HD23	3:B:157:ILE:N	2.32	0.44
1:H:145:ALA:CB	2:L:120:PHE:CD2	3.00	0.44
1:H:205:ASN:HD22	1:H:205:ASN:H	1.66	0.44
2:L:179:LEU:HD23	2:L:180:SER:N	2.32	0.44
1:H:145:ALA:HB3	2:L:120:PHE:CD2	2.53	0.44
1:H:192:VAL:HG12	1:H:193:PRO:HD2	1.99	0.44
2:L:194:LYS:O	2:L:214:ASN:CG	2.61	0.44
1:H:130:PHE:C	1:H:217:LYS:HZ3	2.26	0.44
1:H:201:THR:CA	1:H:218:LYS:HZ3	2.30	0.44
3:B:21:TRP:CE3	3:B:22:ASN:HB3	2.52	0.44
3:B:106:ASN:ND2	3:B:120:ARG:NH1	2.66	0.44
3:B:156:LEU:C	3:B:157:ILE:HD12	2.42	0.44
3:B:207:GLN:HG2	3:B:208:SER:N	2.33	0.43
1:H:147:GLY:HA2	1:H:162:TRP:HH2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:117:PRO:HD3	2:L:202:HIS:CD2	2.53	0.43
3:B:83:SER:O	3:B:84:GLY:C	2.61	0.43
3:B:157:ILE:N	3:B:157:ILE:HD12	2.34	0.43
3:B:171:PHE:HB3	3:B:206:THR:HG21	2.01	0.43
1:H:194:SER:CA	1:H:197:LEU:HD23	2.49	0.43
2:L:29:VAL:O	2:L:29:VAL:CG1	2.67	0.43
3:B:80:THR:C	3:B:82:GLN:H	2.27	0.43
2:L:189:ASP:HA	2:L:192:LYS:CG	2.43	0.42
3:B:200:ASP:HA	3:B:201:PRO:HD3	1.85	0.42
2:L:196:TYR:HB2	2:L:213:PHE:CE2	2.54	0.42
3:B:20:MET:HE1	3:B:53:HIS:CB	2.29	0.42
2:L:110:ILE:N	2:L:170:GLN:HE22	2.01	0.42
3:B:169:LEU:HD22	3:B:169:LEU:O	2.20	0.42
3:B:171:PHE:CE1	3:B:204:PHE:HZ	2.38	0.42
3:B:103:PRO:HA	3:B:104:PRO:HD3	1.95	0.42
1:H:147:GLY:HA3	1:H:188:SER:O	2.20	0.41
1:H:203:ILE:HB	1:H:216:ASP:OD1	2.21	0.41
2:L:126:ASP:CG	2:L:127:GLU:H	2.28	0.41
1:H:130:PHE:N	1:H:217:LYS:NZ	2.69	0.41
3:B:153:ARG:HA	3:B:153:ARG:HD2	1.54	0.41
1:H:202:TYR:N	1:H:218:LYS:HZ3	2.18	0.41
1:H:59:TYR:CZ	3:B:36:TYR:CD2	3.09	0.41
1:H:215:VAL:CG1	1:H:216:ASP:N	2.83	0.41
2:L:139:LEU:C	2:L:140:LEU:HD12	2.45	0.41
3:B:111:PHE:HE1	3:B:115:TYR:CZ	2.39	0.41
1:H:163:ASN:OD1	1:H:163:ASN:N	2.54	0.40
2:L:165:GLU:OE1	2:L:179:LEU:HD11	2.21	0.40
2:L:202:HIS:CD2	2:L:204:GLY:H	2.40	0.40
1:H:202:TYR:H	1:H:218:LYS:HZ2	1.69	0.40
2:L:4:MET:HE2	2:L:4:MET:HB2	1.80	0.40
2:L:190:TYR:CZ	2:L:215:ARG:HG2	2.57	0.40
2:L:122:PHE:HA	2:L:123:PRO:HD3	1.90	0.40
3:B:141:TYR:CD1	3:B:141:TYR:O	2.75	0.40
1:H:151:LYS:HE2	1:H:151:LYS:HB3	1.89	0.40

All (4) 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)
4:H:357:HOH:O	4:H:373:HOH:O[6_545]	1.85	0.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:357:HOH:O	4:L:363:HOH:O[3_655]	1.98	0.22
4:L:346:HOH:O	4:L:357:HOH:O[3_655]	2.03	0.17
4:L:336:HOH:O	4:L:336:HOH:O[3_655]	2.13	0.07

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	H	208/222 (94%)	197 (95%)	10 (5%)	1 (0%)	24	27
2	L	215/218 (99%)	203 (94%)	10 (5%)	2 (1%)	14	14
3	B	206/214 (96%)	185 (90%)	18 (9%)	3 (2%)	8	6
All	All	629/654 (96%)	585 (93%)	38 (6%)	6 (1%)	12	11

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	168	THR
2	L	216	GLY
3	B	82	GLN
3	B	52	ALA
3	B	84	GLY
2	L	208	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	H	177/185 (96%)	167 (94%)	10 (6%)	19	24
2	L	190/191 (100%)	178 (94%)	12 (6%)	16	19
3	B	190/195 (97%)	170 (90%)	20 (10%)	6	6
All	All	557/571 (98%)	515 (92%)	42 (8%)	12	14

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	65	LYS
1	H	143	THR
1	H	158	VAL
1	H	159	THR
1	H	163	ASN
1	H	167	LEU
1	H	190	VAL
1	H	192	VAL
1	H	205	ASN
1	H	213	THR
2	L	21	ILE
2	L	29	VAL
2	L	93	GLN
2	L	109	GLU
2	L	121	ILE
2	L	125	SER
2	L	133	THR
2	L	140	LEU
2	L	159	GLN
2	L	185	LEU
2	L	195	VAL
2	L	212	SER
3	B	5	VAL
3	B	13	THR
3	B	22	ASN
3	B	38	GLU
3	B	45	SER
3	B	56	THR
3	B	87	SER
3	B	89	GLU
3	B	107	VAL
3	B	116	ASN
3	B	117	ILE
3	B	130	MET

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Mol	Chain	Res	Type
3	B	141	TYR
3	B	153	ARG
3	B	159	VAL
3	B	161	SER
3	B	164	VAL
3	B	169	LEU
3	B	190	SER
3	B	203	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	33	HIS
1	H	39	GLN
1	H	84	ASN
1	H	205	ASN
1	H	208	HIS
2	L	42	GLN
2	L	93	GLN
2	L	128	GLN
2	L	141	ASN
2	L	156	ASN
2	L	159	GLN
2	L	162	ASN
2	L	164	GLN
2	L	170	GLN
2	L	202	HIS
2	L	203	GLN
3	B	22	ASN
3	B	49	HIS
3	B	57	HIS
3	B	63	HIS
3	B	106	ASN
3	B	116	ASN
3	B	140	GLN

5.3.3 RNA ⓘ

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	H	212/222 (95%)	0.68	42 (19%) 3 2	24, 44, 109, 132	0
2	L	217/218 (99%)	0.99	55 (25%) 1 1	28, 48, 108, 117	0
3	B	208/214 (97%)	1.85	92 (44%) 0 0	34, 90, 135, 141	0
All	All	637/654 (97%)	1.17	189 (29%) 1 1	24, 62, 124, 141	0

All (189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	196	TYR	6.5
2	L	158	LEU	6.1
2	L	213	PHE	6.0
3	B	23	LEU	5.9
3	B	167	LEU	5.3
3	B	21	TRP	5.1
1	H	197	LEU	5.1
1	H	203	ILE	4.9
1	H	193	PRO	4.9
1	H	202	TYR	4.8
3	B	90	CYS	4.6
3	B	203	ILE	4.5
3	B	121	SER	4.3
3	B	27	THR	4.3
2	L	185	LEU	4.2
3	B	86	TYR	4.2
2	L	194	LYS	4.2
1	H	192	VAL	4.2
2	L	155	ASP	4.2
3	B	1	CYS	4.1
3	B	25	PRO	4.1
3	B	159	VAL	4.1
2	L	198	CYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	H	144	ALA	4.0
2	L	157	ALA	4.0
3	B	128	PHE	4.0
1	H	145	ALA	3.9
2	L	188	ALA	3.9
2	L	208	PRO	3.9
1	H	217	LYS	3.9
2	L	214	ASN	3.9
2	L	120	PHE	3.8
1	H	66	GLY	3.8
3	B	46	CYS	3.8
3	B	52	ALA	3.7
2	L	161	GLY	3.7
1	H	143	THR	3.7
2	L	123	PRO	3.7
2	L	195	VAL	3.7
1	H	216	ASP	3.7
1	H	219	VAL	3.7
3	B	58	ALA	3.6
2	L	209	VAL	3.6
1	H	134	PRO	3.6
3	B	141	TYR	3.6
2	L	160	SER	3.6
2	L	129	LEU	3.6
1	H	196	SER	3.5
3	B	115	TYR	3.5
3	B	39	LEU	3.5
2	L	126	ASP	3.5
3	B	24	HIS	3.5
2	L	136	VAL	3.5
3	B	68	HIS	3.5
1	H	146	LEU	3.5
3	B	144	ARG	3.4
3	B	157	ILE	3.4
3	B	179	LEU	3.4
2	L	148	ALA	3.4
1	H	220	GLU	3.4
3	B	127	ALA	3.4
1	H	167	LEU	3.3
3	B	79	ILE	3.3
2	L	133	THR	3.3
2	L	118	SER	3.3

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Mol	Chain	Res	Type	RSRZ
3	B	129	TYR	3.3
2	L	201	THR	3.3
1	H	133	ALA	3.2
2	L	200	VAL	3.3
3	B	156	LEU	3.2
3	B	202	VAL	3.2
1	H	199	THR	3.2
3	B	105	PHE	3.2
3	B	54	ASN	3.2
2	L	183	LEU	3.1
3	B	171	PHE	3.1
2	L	216	GLY	3.1
2	L	138	CYS	3.1
2	L	149	LYS	3.1
2	L	207	SER	3.1
1	H	198	GLY	3.1
2	L	197	ALA	3.1
3	B	168	PRO	3.1
3	B	55	ALA	3.0
1	H	162	TRP	3.0
3	B	169	LEU	3.0
3	B	120	ARG	3.0
1	H	195	SER	3.0
3	B	161	SER	3.0
3	B	113	GLY	3.0
3	B	201	PRO	3.0
2	L	139	LEU	3.0
3	B	80	THR	3.0
2	L	199	GLU	3.0
3	B	111	PHE	2.9
1	H	191	THR	2.9
1	H	1	GLU	2.9
2	L	212	SER	2.9
3	B	166	LEU	2.9
2	L	119	VAL	2.9
3	B	164	VAL	2.9
1	H	165	GLY	2.9
3	B	78	ASN	2.9
3	B	158	SER	2.9
3	B	40	LYS	2.9
2	L	121	ILE	2.9
3	B	26	SER	2.8

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Mol	Chain	Res	Type	RSRZ
3	B	28	LEU	2.8
2	L	154	VAL	2.8
3	B	109	VAL	2.8
2	L	206	SER	2.8
2	L	1	ASP	2.8
2	L	134	ALA	2.8
3	B	193	GLY	2.7
1	H	190	VAL	2.7
2	L	187	LYS	2.7
3	B	130	MET	2.7
3	B	162	ARG	2.7
3	B	112	SER	2.7
3	B	208	SER	2.7
3	B	177	TYR	2.7
3	B	81	ASP	2.7
3	B	150	VAL	2.7
3	B	89	GLU	2.6
1	H	194	SER	2.6
2	L	193	HIS	2.6
3	B	204	PHE	2.6
3	B	142	ARG	2.6
1	H	147	GLY	2.6
3	B	107	VAL	2.6
2	L	125	SER	2.6
1	H	204	CYS	2.6
3	B	148	TRP	2.6
3	B	200	ASP	2.6
1	H	218	LYS	2.6
3	B	173	LYS	2.6
3	B	139	LEU	2.5
3	B	147	PRO	2.4
1	H	164	SER	2.4
3	B	17	ILE	2.4
1	H	166	ALA	2.4
3	B	87	SER	2.4
1	H	132	LEU	2.4
2	L	122	PHE	2.4
2	L	150	VAL	2.4
2	L	156	ASN	2.3
3	B	106	ASN	2.3
1	H	131	PRO	2.3
3	B	2	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
3	B	117	ILE	2.3
3	B	84	GLY	2.3
1	H	201	THR	2.3
1	H	130	PHE	2.3
1	H	206	VAL	2.3
3	B	38	GLU	2.3
1	H	160	VAL	2.3
3	B	110	THR	2.3
2	L	211	LYS	2.3
1	H	215	VAL	2.3
1	H	200	GLN	2.2
2	L	191	GLU	2.2
2	L	137	VAL	2.2
3	B	16	CYS	2.2
3	B	153	ARG	2.2
3	B	186	MET	2.2
3	B	49	HIS	2.2
3	B	207	GLN	2.2
3	B	22	ASN	2.2
3	B	82	GLN	2.2
3	B	172	ARG	2.1
1	H	163	ASN	2.1
3	B	119	TRP	2.1
2	L	215	ARG	2.1
3	B	51	SER	2.1
3	B	20	MET	2.1
2	L	205	LEU	2.1
3	B	18	LEU	2.1
2	L	190	TYR	2.1
2	L	151	GLN	2.1
3	B	57	HIS	2.1
3	B	188	GLY	2.1
2	L	130	LYS	2.1
3	B	145	GLY	2.1
3	B	50	ARG	2.1
3	B	53	HIS	2.0
3	B	187	PRO	2.0
1	H	189	VAL	2.0
3	B	140	GLN	2.0
2	L	192	LYS	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.