



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 31, 2021 – 06:02 PM EDT

PDB ID : 7KQ7  
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](mailto: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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.18  
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) : 2.18

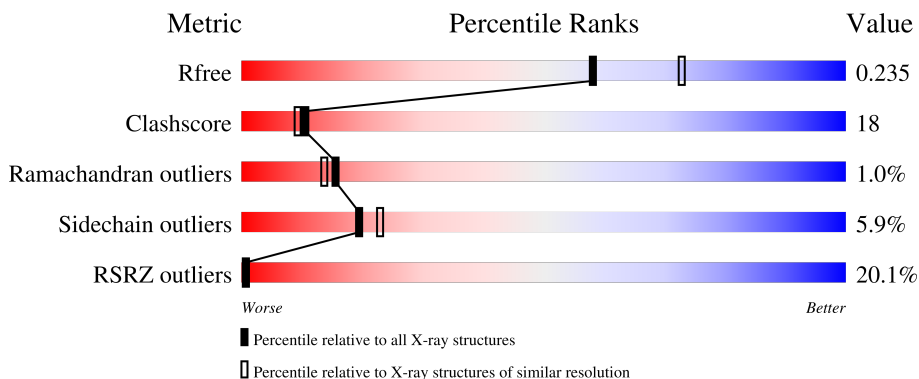
# 1 Overall quality at a glance

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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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  $\geq 3$ , 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	 10% 70% 23% • 5%
2	L	218	 14% 72% 25% •
3	B	214	 35% 59% 32% 6% •

## 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
			Total	C	N	O	S			
1	H	212	1615	1027	273	309	6	0	0	0

- Molecule 2 is a protein called Antibody light chain.

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

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

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

- Molecule 4 is water.

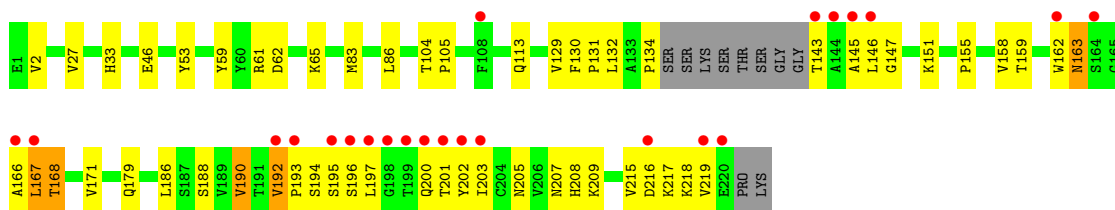
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	73	Total 73	O 73	0	0
4	L	65	Total 65	O 65	0	0
4	B	11	Total 11	O 11	0	0

### 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.

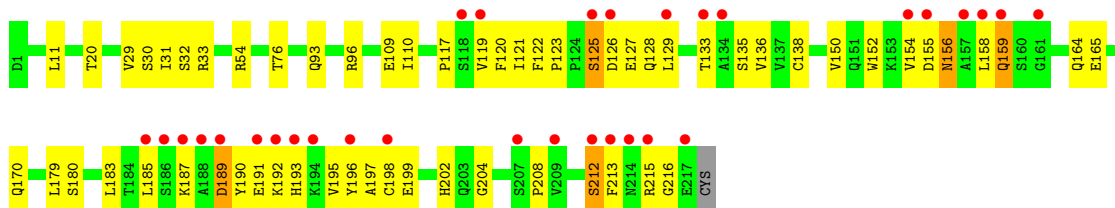
- Molecule 1: Antibody heavy chain

Chain H: 



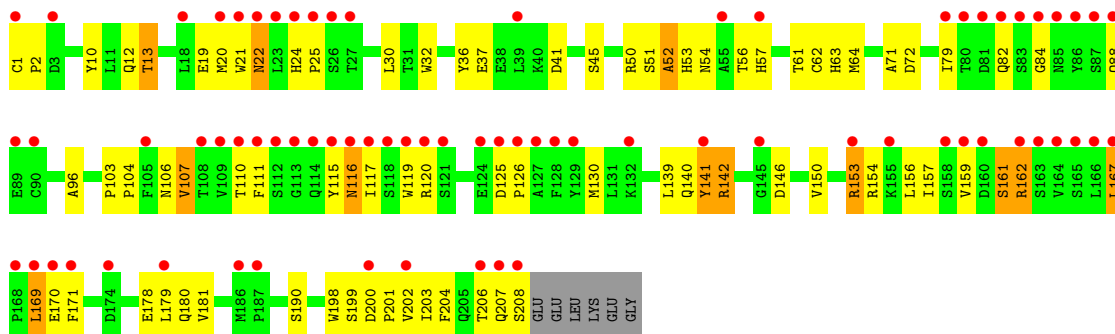
- Molecule 2: Antibody light chain

Chain L: 



- Molecule 3: Interleukin-21 receptor

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 2.20Å)	Xtrriage
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 (5.28%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.7	Xtrriage
Anisotropy	0.805	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 52.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5111	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.52	0/1656	0.62	0/2261
2	L	0.47	0/1699	0.64	0/2305
3	B	0.36	0/1734	0.54	0/2364
All	All	0.46	0/5089	0.60	0/6930

There are no bond length outliers.

There are no bond angle outliers.

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	69	0
2	L	1663	0	1613	53	0
3	B	1684	0	1578	67	0
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	180	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 18.

All (180) 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:129:VAL:HG12	1:H:217:LYS:HZ1	1.24	1.02
3:B:120:ARG:HG2	3:B:162:ARG:HH21	1.21	1.02
2:L:31:ILE:HD11	2:L:96:ARG:CZ	1.94	0.98
3:B:22:ASN:HD21	3:B:24:HIS:CG	1.85	0.94
3:B:20:MET:HE1	3:B:53:HIS:HB2	1.56	0.88
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
1:H:129:VAL:C	1:H:217:LYS:HZ3	1.83	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
3:B:19:GLU:HG2	3:B:57:HIS:CE1	2.22	0.74
3:B:20:MET:CE	3:B:53:HIS:HB2	2.17	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:129:VAL:CG1	1:H:217:LYS:HZ1	1.99	0.73
1:H:134:PRO:HD3	1:H:146:LEU:HB3	1.68	0.73
2:L:31:ILE:HD11	2:L:96:ARG:NE	2.05	0.72
1:H:129:VAL:HG12	1:H:217:LYS:NZ	2.01	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
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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:B:139:LEU:HD23	3:B:181:VAL:HG22	1.84	0.60
3:B:159:VAL:HG12	3:B:161:SER:OG	2.00	0.60
2:L:32:SER:OG	2:L:33:ARG:N	2.35	0.59
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:190:TYR:O	2:L:215:ARG:HD3	2.04	0.56
1:H:129:VAL:C	1:H:217:LYS:NZ	2.56	0.56
1:H:202:TYR:H	1:H:218:LYS:NZ	2.03	0.56
2:L:11:LEU:C	2:L:11:LEU:HD12	2.27	0.55
2:L:152:TRP:O	2:L:159:GLN:HB2	2.06	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: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:171:VAL:HG22	1:H:190:VAL:HG13	1.90	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
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

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:119:VAL:C	2:L:120:PHE:CD1	2.83	0.51
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
1:H:130:PHE:N	1:H:217:LYS:HZ3	2.08	0.50
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
3:B:32:TRP:HE1	3:B:64:MET:HE1	1.76	0.49
1:H:186:LEU:C	1:H:186:LEU:HD12	2.32	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
3:B:169:LEU:HD22	3:B:169:LEU:C	2.33	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
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
2:L:154:VAL:H	2:L:159:GLN:HE21	1.60	0.48
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:32:TRP:NE1	3:B:64:MET:HE1	2.27	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:12:GLN:HA	3:B:64:MET:O	2.13	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: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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	3:B:141:TYR:HD1	2.00	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:154:VAL:O	2:L:155:ASP:C	2.56	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:141:TYR:C	3:B:141:TYR:CD1	2.91	0.44
3:B:106:ASN:ND2	3:B:120:ARG:NH1	2.66	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
2:L:117:PRO:HD3	2:L:202:HIS:CD2	2.53	0.43
1:H:83:MET:HE2	1:H:86:LEU:HD21	1.99	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:CG1	2:L:29:VAL:O	2.67	0.43
3:B:179:LEU:HD12	3:B:179:LEU:C	2.39	0.42
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
3:B:30:LEU:C	3:B:30:LEU:HD23	2.40	0.42
2:L:196:TYR:HB2	2:L:213:PHE:CE2	2.54	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
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
3:B:156:LEU:HD23	3:B:156:LEU:C	2.40	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:194:SER:O	1:H:195:SER:C	2.59	0.41
1:H:215:VAL:CG1	1:H:216:ASP:N	2.83	0.41
3:B:111:PHE:HE1	3:B:115:TYR:CZ	2.39	0.41
1:H:130:PHE:CA	1:H:217:LYS:HZ3	2.34	0.40
1:H:163:ASN:N	1:H:163:ASN:OD1	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
3:B:141:TYR:HD1	3:B:141:TYR:C	2.24	0.40
1:H:202:TYR:H	1:H:218:LYS:HZ2	1.69	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:O	3:B:141:TYR:CD1	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
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%)	29	31
2	L	215/218 (99%)	203 (94%)	10 (5%)	2 (1%)	17	16

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	206/214 (96%)	185 (90%)	18 (9%)	3 (2%)	10	8
All	All	629/654 (96%)	585 (93%)	38 (6%)	6 (1%)	15	14

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%)	170 (96%)	7 (4%)	31	40
2	L	190/191 (100%)	180 (95%)	10 (5%)	22	27
3	B	190/195 (97%)	174 (92%)	16 (8%)	11	11
All	All	557/571 (98%)	524 (94%)	33 (6%)	19	23

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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
2	L	93	GLN
2	L	109	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	L	121	ILE
2	L	125	SER
2	L	133	THR
2	L	156	ASN
2	L	159	GLN
2	L	185	LEU
2	L	189	ASP
2	L	212	SER
3	B	10	TYR
3	B	13	THR
3	B	22	ASN
3	B	45	SER
3	B	107	VAL
3	B	116	ASN
3	B	130	MET
3	B	141	TYR
3	B	142	ARG
3	B	153	ARG
3	B	161	SER
3	B	162	ARG
3	B	167	LEU
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 (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	33	HIS
1	H	77	ASN
1	H	82	GLN
1	H	179	GLN
1	H	205	ASN
1	H	208	HIS
2	L	93	GLN
2	L	128	GLN
2	L	156	ASN
2	L	159	GLN
2	L	164	GLN
2	L	170	GLN
2	L	202	HIS
2	L	203	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	B	22	ASN
3	B	49	HIS
3	B	57	HIS
3	B	106	ASN
3	B	116	ASN
3	B	140	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](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	H	212/222 (95%)	0.70	23 (10%) 5 5	24, 44, 109, 132	0
2	L	217/218 (99%)	0.83	31 (14%) 2 2	28, 48, 108, 117	0
3	B	208/214 (97%)	1.81	74 (35%) 0 0	34, 90, 135, 141	0
All	All	637/654 (97%)	1.11	128 (20%) 1 1	24, 62, 124, 141	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	86	TYR	12.9
3	B	23	LEU	10.1
2	L	158	LEU	9.8
3	B	25	PRO	9.3
3	B	24	HIS	7.7
3	B	85	ASN	7.6
3	B	111	PHE	7.5
3	B	1	CYS	7.3
3	B	158	SER	7.1
3	B	115	TYR	7.1
3	B	81	ASP	7.1
3	B	21	TRP	6.7
1	H	201	THR	6.4
1	H	196	SER	6.4
2	L	155	ASP	6.3
3	B	20	MET	5.9
3	B	171	PHE	5.9
1	H	166	ALA	5.8
3	B	208	SER	5.8
3	B	164	VAL	5.7
3	B	207	GLN	5.7
3	B	167	LEU	5.4
1	H	167	LEU	5.3

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	L	154	VAL	5.3
3	B	22	ASN	5.3
2	L	213	PHE	5.2
3	B	112	SER	5.1
3	B	166	LEU	5.1
3	B	159	VAL	5.1
1	H	195	SER	5.1
3	B	80	THR	5.0
3	B	187	PRO	4.9
1	H	193	PRO	4.9
3	B	27	THR	4.7
3	B	82	GLN	4.7
2	L	196	TYR	4.7
3	B	79	ILE	4.5
1	H	197	LEU	4.4
3	B	169	LEU	4.4
3	B	170	GLU	4.4
3	B	84	GLY	4.4
3	B	141	TYR	4.4
2	L	191	GLU	4.3
3	B	168	PRO	4.2
1	H	144	ALA	4.2
3	B	127	ALA	4.2
3	B	120	ARG	4.2
2	L	126	ASP	4.2
1	H	145	ALA	4.2
3	B	109	VAL	4.1
3	B	179	LEU	4.0
3	B	117	ILE	4.0
3	B	128	PHE	3.9
3	B	108	THR	3.8
3	B	110	THR	3.8
1	H	199	THR	3.7
3	B	124	GLU	3.5
3	B	55	ALA	3.5
2	L	129	LEU	3.5
2	L	207	SER	3.5
3	B	145	GLY	3.5
3	B	83	SER	3.4
3	B	88	GLN	3.4
3	B	186	MET	3.4
2	L	209	VAL	3.3

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	L	212	SER	3.3
3	B	26	SER	3.3
2	L	188	ALA	3.3
2	L	125	SER	3.3
3	B	153	ARG	3.3
1	H	146	LEU	3.2
1	H	216	ASP	3.2
3	B	114	GLN	3.2
1	H	200	GLN	3.2
1	H	220	GLU	3.2
2	L	198	CYS	3.1
3	B	165	SER	3.0
2	L	161	GLY	3.0
1	H	219	VAL	3.0
3	B	162	ARG	3.0
3	B	160	ASP	3.0
1	H	202	TYR	2.9
1	H	164	SER	2.9
3	B	125	ASP	2.8
2	L	134	ALA	2.8
3	B	113	GLY	2.8
3	B	90	CYS	2.8
3	B	116	ASN	2.7
2	L	186	SER	2.7
2	L	119	VAL	2.7
3	B	202	VAL	2.7
2	L	157	ALA	2.7
3	B	174	ASP	2.6
3	B	118	SER	2.6
1	H	203	ILE	2.6
2	L	192	LYS	2.6
3	B	129	TYR	2.6
3	B	18	LEU	2.6
3	B	126	PRO	2.5
3	B	87	SER	2.5
3	B	132	LYS	2.5
2	L	194	LYS	2.4
3	B	57	HIS	2.4
3	B	155	LYS	2.4
3	B	206	THR	2.4
2	L	217	GLU	2.4
3	B	105	PHE	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	H	198	GLY	2.3
2	L	193	HIS	2.2
3	B	121	SER	2.2
2	L	214	ASN	2.2
2	L	189	ASP	2.2
2	L	159	GLN	2.2
2	L	187	LYS	2.2
3	B	119	TRP	2.2
3	B	3	ASP	2.2
3	B	89	GLU	2.1
2	L	215	ARG	2.1
2	L	133	THR	2.1
1	H	192	VAL	2.1
3	B	39	LEU	2.1
1	H	143	THR	2.1
1	H	162	TRP	2.1
3	B	163	SER	2.1
1	H	108	PHE	2.0
3	B	200	ASP	2.0
2	L	185	LEU	2.0
2	L	118	SER	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.