



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 08:35 am BST

PDB ID : 6K7O
Title : Complex structure of LILRB4 and h128-3 antibody
Authors : Song, H.; Chai, Y.; Xu, X.; Gao, F.G.
Deposited on : 2019-06-08
Resolution : 3.00 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 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	:	2.11
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)	:	2.11

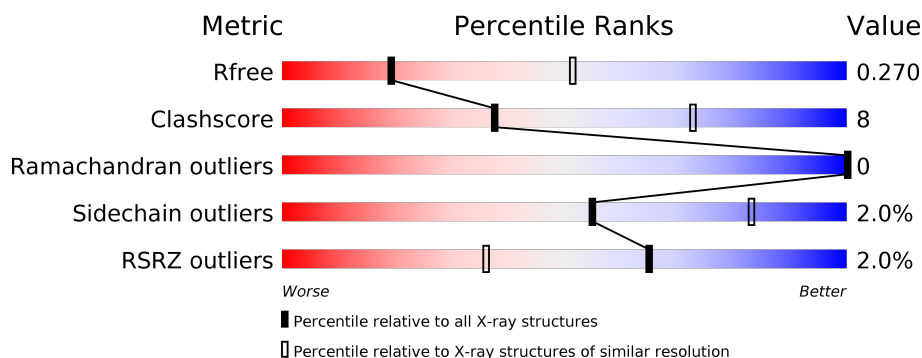
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 on 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	95	
1	P	95	
1	Q	95	
1	R	95	
2	B	228	
2	D	228	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	228	<div><div></div><div>7%</div><div>69%</div><div>29%</div><div>..</div></div>
2	H	228	<div><div></div><div>81%</div><div>18%</div><div>.</div></div>
3	C	218	<div><div></div><div>86%</div><div>12%</div><div>.</div></div>
3	E	218	<div><div></div><div>%</div><div>78%</div><div>21%</div></div>
3	G	218	<div><div></div><div>4%</div><div>82%</div><div>17%</div></div>
3	L	218	<div><div></div><div>86%</div><div>14%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16436 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 Leukocyte immunoglobulin-like receptor subfamily B member 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	94	Total	C	N	O	S	0	0	0
			763	486	130	143	4			
1	P	94	Total	C	N	O	S	0	0	0
			763	486	130	143	4			
1	R	94	Total	C	N	O	S	0	0	0
			763	486	130	143	4			
1	Q	94	Total	C	N	O	S	0	0	0
			763	486	130	143	4			

- Molecule 2 is a protein called h128-3 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	225	Total	C	N	O	S	0	0	0
			1676	1052	281	335	8			
2	D	225	Total	C	N	O	S	0	0	0
			1676	1052	281	335	8			
2	F	225	Total	C	N	O	S	0	0	0
			1676	1052	281	335	8			
2	H	225	Total	C	N	O	S	0	0	0
			1676	1052	281	335	8			

- Molecule 3 is a protein called h128-3 Fab light chain.

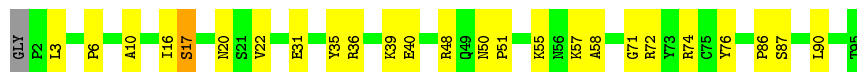
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	218	Total	C	N	O	S	0	0	0
			1670	1042	277	345	6			
3	E	218	Total	C	N	O	S	0	0	0
			1670	1042	277	345	6			
3	G	218	Total	C	N	O	S	0	0	0
			1670	1042	277	345	6			
3	L	218	Total	C	N	O	S	0	0	0
			1670	1042	277	345	6			

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA 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: Leukocyte immunoglobulin-like receptor subfamily B member 4

Chain A: 



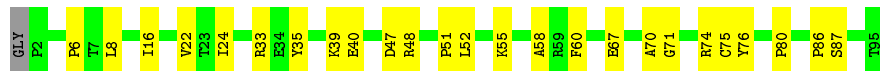
- Molecule 1: Leukocyte immunoglobulin-like receptor subfamily B member 4

Chain P: 



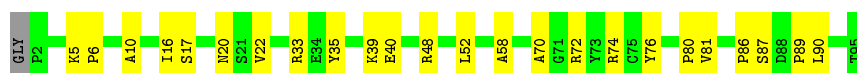
- Molecule 1: Leukocyte immunoglobulin-like receptor subfamily B member 4

Chain R: 




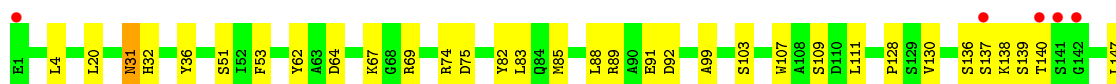
- Molecule 1: Leukocyte immunoglobulin-like receptor subfamily B member 4

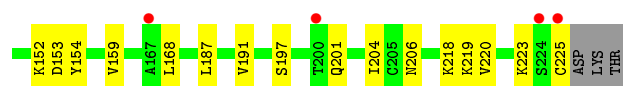
Chain Q: 



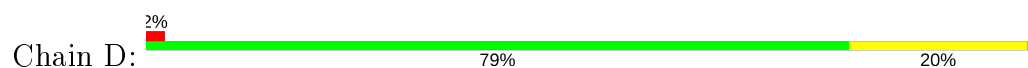
- Molecule 2: h128-3 Fab heavy chain

Chain B: 

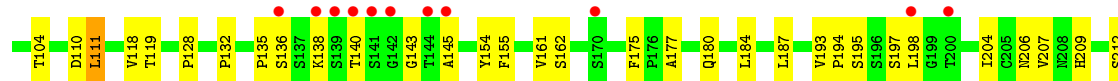




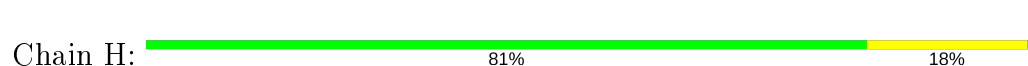
- Molecule 2: h128-3 Fab heavy chain



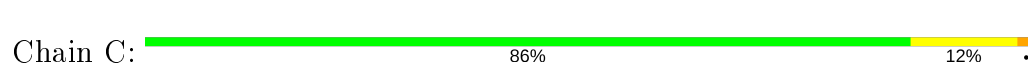
- Molecule 2: h128-3 Fab heavy chain



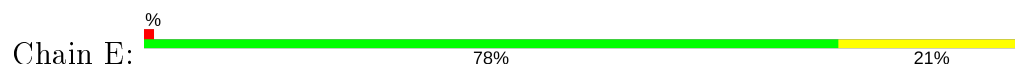
- Molecule 2: h128-3 Fab heavy chain

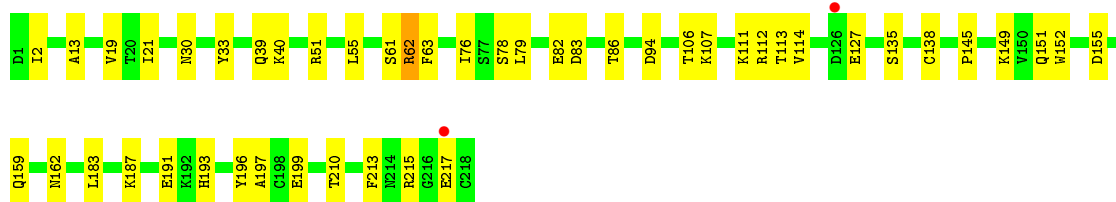


- Molecule 3: h128-3 Fab light chain

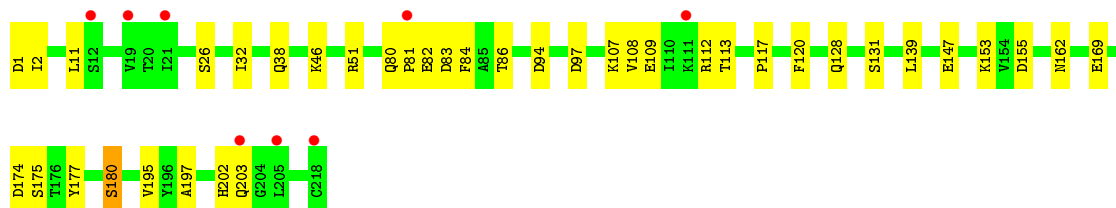
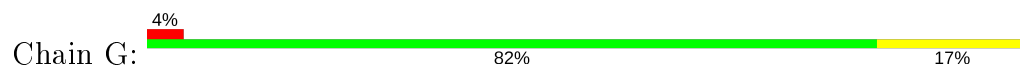


- Molecule 3: h128-3 Fab light chain

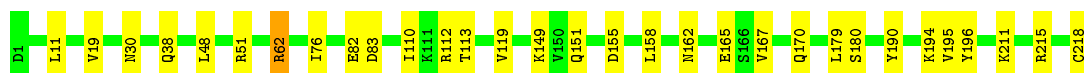
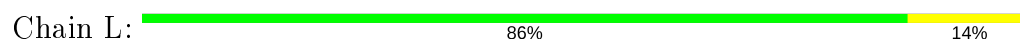




• Molecule 3: h128-3 Fab light chain



• Molecule 3: h128-3 Fab light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	187.28Å 187.28Å 183.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.21 – 3.00 44.21 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.4 (44.21-3.00) 96.5 (44.21-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.75 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.228 , 0.270 0.228 , 0.270	Depositor DCC
R_{free} test set	3459 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	59.1	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	16436	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.96% 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	A	0.27	0/790	0.46	0/1080
1	P	0.29	0/790	0.50	0/1080
1	Q	0.29	0/790	0.49	0/1080
1	R	0.26	0/790	0.47	0/1080
2	B	0.27	0/1716	0.48	0/2336
2	D	0.28	0/1716	0.48	0/2336
2	F	0.28	0/1716	0.47	0/2336
2	H	0.29	0/1716	0.49	0/2336
3	C	0.28	0/1705	0.50	0/2314
3	E	0.28	0/1705	0.49	0/2314
3	G	0.26	0/1705	0.47	0/2314
3	L	0.28	0/1705	0.49	0/2314
All	All	0.28	0/16844	0.48	0/22920

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	A	763	0	729	17	0
1	P	763	0	729	8	0
1	Q	763	0	729	16	0
1	R	763	0	729	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1676	0	1624	27	0
2	D	1676	0	1624	27	0
2	F	1676	0	1624	42	0
2	H	1676	0	1624	21	0
3	C	1670	0	1609	19	0
3	E	1670	0	1609	28	0
3	G	1670	0	1609	25	0
3	L	1670	0	1609	19	0
All	All	16436	0	15848	247	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 8.

All (247) 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:A:40:GLU:OE2	1:A:72:ARG:NH1	2.18	0.76
1:Q:39:LYS:NZ	1:Q:70:ALA:O	2.18	0.75
3:E:155:ASP:OD2	3:E:193:HIS:ND1	2.22	0.73
2:H:69:ARG:NH1	2:H:92:ASP:OD2	2.16	0.72
3:E:149:LYS:NZ	3:E:151:GLN:OE1	2.21	0.72
2:D:100:ARG:NH2	2:D:110:ASP:OD2	2.22	0.72
1:P:40:GLU:OE2	1:P:74:ARG:NH2	2.24	0.71
2:D:93:THR:HG23	2:D:119:THR:HA	1.73	0.70
2:B:128:PRO:HB3	2:B:154:TYR:HB3	1.73	0.70
2:F:135:PRO:HG2	2:F:222:PRO:HG3	1.74	0.70
2:F:6:GLU:OE2	2:F:98:CYS:N	2.24	0.69
2:B:152:LYS:NZ	2:B:153:ASP:OD1	2.26	0.69
2:B:69:ARG:NH1	2:B:92:ASP:OD2	2.23	0.69
2:F:69:ARG:NH2	2:F:92:ASP:OD2	2.26	0.68
2:F:128:PRO:HB3	2:F:154:TYR:HB3	1.76	0.67
1:A:39:LYS:NZ	1:A:71:GLY:HA3	2.10	0.67
1:P:74:ARG:NH1	1:P:89:PRO:HG3	2.09	0.67
2:B:223:LYS:NZ	3:C:126:ASP:OD1	2.27	0.67
3:C:193:HIS:O	3:C:215:ARG:NE	2.25	0.66
3:G:112:ARG:NH2	3:G:113:THR:O	2.28	0.66
3:C:62:ARG:NH2	3:C:83:ASP:OD1	2.28	0.65
3:E:40:LYS:NZ	3:E:82:GLU:O	2.23	0.65
2:D:11:LEU:HG	2:D:156:PRO:HG3	1.77	0.65
3:E:114:VAL:HG13	3:E:145:PRO:HD3	1.77	0.65
2:H:53:PHE:O	2:H:74:ARG:NH2	2.30	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:100:ARG:NH2	2:F:110:ASP:OD2	2.30	0.64
2:D:6:GLU:OE2	2:D:97:TYR:HA	1.96	0.64
1:A:40:GLU:OE2	1:A:74:ARG:NH2	2.31	0.63
1:Q:6:PRO:HG2	1:Q:87:SER:HB3	1.79	0.63
3:G:32:ILE:HA	3:G:51:ARG:HA	1.80	0.63
2:H:128:PRO:HB3	2:H:154:TYR:HB3	1.80	0.63
1:A:35:TYR:OH	1:A:55:LYS:O	2.15	0.63
1:R:67:GLU:OE1	1:R:67:GLU:N	2.31	0.62
2:F:104:THR:O	3:G:51:ARG:NH2	2.32	0.62
3:E:159:GLN:HB3	3:E:162:ASN:HD21	1.65	0.62
1:Q:52:LEU:HD13	1:Q:58:ALA:HA	1.81	0.62
3:L:38:GLN:HB2	3:L:48:LEU:HD11	1.82	0.61
2:H:3:GLN:HB3	2:H:25:SER:HB3	1.81	0.61
1:Q:10:ALA:HB2	1:Q:90:LEU:HD21	1.84	0.60
2:B:53:PHE:O	2:B:74:ARG:NH2	2.34	0.60
2:H:6:GLU:OE2	2:H:97:TYR:HA	2.01	0.60
1:A:6:PRO:HG2	1:A:87:SER:HB3	1.84	0.60
2:B:31:ASN:HD22	2:B:32:HIS:H	1.50	0.60
2:F:53:PHE:O	2:F:74:ARG:NH2	2.34	0.60
3:C:158:LEU:HD12	3:L:158:LEU:HD12	1.84	0.59
3:E:191:GLU:O	3:E:215:ARG:NH2	2.34	0.59
3:G:38:GLN:O	3:G:46:LYS:N	2.34	0.59
1:P:17:SER:OG	1:P:20:ASN:OD1	2.21	0.58
1:R:51:PRO:HB2	1:R:55:LYS:HG3	1.85	0.58
2:F:161:VAL:HG22	2:F:207:VAL:HG22	1.86	0.58
3:E:30:ASN:HB3	3:E:33:TYR:HD2	1.69	0.57
1:R:39:LYS:NZ	1:R:70:ALA:O	2.31	0.57
1:R:74:ARG:HG2	1:R:86:PRO:HB2	1.86	0.57
1:A:31:GLU:OE2	2:H:34:TYR:OH	2.16	0.57
2:B:130:VAL:O	2:B:218:LYS:NZ	2.34	0.57
3:L:190:TYR:O	3:L:196:TYR:OH	2.21	0.57
1:Q:17:SER:OG	1:Q:20:ASN:OD1	2.22	0.56
3:L:149:LYS:HZ2	3:L:151:GLN:HG3	1.69	0.56
3:G:82:GLU:N	3:G:82:GLU:OE2	2.26	0.56
2:D:218:LYS:NZ	3:E:127:GLU:OE1	2.29	0.56
3:C:162:ASN:N	3:C:162:ASN:OD1	2.39	0.56
2:D:2:VAL:HB	2:D:111:LEU:HD11	1.86	0.56
2:F:93:THR:HG23	2:F:119:THR:HA	1.87	0.56
3:E:151:GLN:NE2	3:E:199:GLU:OE1	2.39	0.56
3:E:62:ARG:NH2	3:E:83:ASP:OD1	2.38	0.56
1:Q:40:GLU:CD	1:Q:72:ARG:HH11	2.08	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:194:PRO:O	2:F:197:SER:OG	2.22	0.56
2:D:64:ASP:HA	2:D:67:LYS:HG3	1.88	0.55
1:R:16:ILE:HG13	1:R:22:VAL:HB	1.88	0.55
1:R:39:LYS:NZ	1:R:71:GLY:HA3	2.21	0.55
2:D:40:GLN:NE2	3:E:39:GLN:OE1	2.39	0.55
3:E:138:CYS:HB2	3:E:152:TRP:CH2	2.42	0.55
3:E:197:ALA:HB1	3:E:210:THR:HG22	1.88	0.55
2:H:135:PRO:HG3	2:H:147:LEU:HD23	1.88	0.54
3:L:62:ARG:NH2	3:L:83:ASP:OD1	2.40	0.54
3:C:141:ASN:OD1	3:C:142:ASN:ND2	2.40	0.54
1:A:20:ASN:ND2	2:F:84:GLN:OE1	2.41	0.54
3:L:149:LYS:NZ	3:L:151:GLN:HG3	2.21	0.54
2:D:2:VAL:HG11	2:D:28:ASP:OD1	2.06	0.54
1:P:14:SER:OG	1:P:91:GLU:O	2.24	0.54
3:E:13:ALA:HB3	3:E:79:LEU:HD22	1.89	0.54
1:Q:33:ARG:NH1	1:Q:80:PRO:HG3	2.22	0.54
2:F:177:ALA:HA	2:F:187:LEU:HB3	1.89	0.53
1:Q:74:ARG:NH1	1:Q:89:PRO:HG3	2.24	0.53
3:G:80:GLN:HB2	3:G:83:ASP:OD2	2.09	0.53
3:G:112:ARG:HD2	3:G:175:SER:HB2	1.90	0.53
2:H:221:GLU:OE2	2:H:222:PRO:HD2	2.09	0.52
3:L:110:ILE:O	3:L:170:GLN:NE2	2.42	0.52
1:R:6:PRO:HG2	1:R:87:SER:HB3	1.90	0.52
3:G:153:LYS:HB2	3:G:197:ALA:HB3	1.90	0.52
3:C:30:ASN:HB3	3:C:33:TYR:CD2	2.44	0.52
2:F:140:THR:HG22	2:F:145:ALA:HA	1.92	0.52
2:F:2:VAL:HA	2:F:26:GLY:HA3	1.90	0.52
2:H:29:PHE:CG	2:H:29:PHE:O	2.63	0.52
2:B:31:ASN:ND2	2:B:32:HIS:H	2.08	0.51
3:C:153:LYS:NZ	3:C:199:GLU:OE1	2.34	0.51
3:L:194:LYS:O	3:L:215:ARG:N	2.37	0.51
2:H:136:SER:OG	2:H:139:SER:N	2.44	0.51
3:E:19:VAL:HG22	3:E:76:ILE:HB	1.92	0.51
2:F:85:MET:HB3	2:F:88:LEU:HD21	1.92	0.51
2:B:197:SER:HB2	2:B:201:GLN:HB2	1.93	0.51
2:B:62:TYR:O	2:B:67:LYS:NZ	2.43	0.51
3:G:109:GLU:OE1	3:G:177:TYR:OH	2.27	0.50
2:D:40:GLN:OE1	3:E:39:GLN:NE2	2.39	0.50
1:R:40:GLU:OE2	1:R:74:ARG:NH2	2.44	0.50
2:D:214:THR:HG22	2:D:216:VAL:HG23	1.94	0.50
2:H:20:LEU:HD12	2:H:83:LEU:HD23	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:145:ALA:N	2:F:193:VAL:O	2.35	0.49
1:Q:33:ARG:CZ	1:Q:80:PRO:HG3	2.42	0.49
1:A:36:ARG:HA	1:A:48:ARG:HA	1.94	0.49
1:P:76:TYR:CZ	1:P:86:PRO:HB3	2.47	0.49
2:B:137:SER:O	2:B:140:THR:OG1	2.26	0.49
3:C:30:ASN:HB3	3:C:33:TYR:HD2	1.76	0.49
2:B:75:ASP:HB2	2:B:82:TYR:HE2	1.77	0.49
3:C:196:TYR:HB2	3:C:213:PHE:CE1	2.47	0.49
2:B:99:ALA:HB1	2:B:109:SER:HB3	1.95	0.49
2:F:35:MET:HG2	2:F:81:LEU:HG	1.94	0.49
1:A:16:ILE:HG13	1:A:22:VAL:HB	1.94	0.48
3:E:86:THR:HG22	3:E:107:LYS:HG3	1.95	0.48
3:E:193:HIS:O	3:E:215:ARG:NE	2.33	0.48
1:R:24:ILE:HB	1:R:60:PHE:HB2	1.95	0.48
3:G:86:THR:HG22	3:G:107:LYS:HG3	1.96	0.48
2:H:36:TYR:O	2:H:98:CYS:HA	2.13	0.48
2:B:89:ARG:HG3	2:B:91:GLU:HG2	1.96	0.48
3:L:167:VAL:HG22	3:L:179:LEU:HD12	1.94	0.48
3:L:112:ARG:NH2	3:L:113:THR:O	2.43	0.48
2:F:3:GLN:N	2:F:25:SER:O	2.31	0.48
3:L:19:VAL:HG22	3:L:76:ILE:HB	1.94	0.48
1:R:33:ARG:CZ	1:R:80:PRO:HG3	2.44	0.48
3:G:202:HIS:CD2	3:G:203:GLN:H	2.32	0.48
1:R:8:LEU:HD13	1:R:75:CYS:HB2	1.96	0.48
1:A:17:SER:OG	1:A:20:ASN:OD1	2.21	0.47
2:D:212:SER:OG	2:D:214:THR:OG1	2.28	0.47
2:F:31:ASN:HD22	2:F:32:HIS:H	1.62	0.47
2:B:136:SER:H	2:B:139:SER:HB3	1.79	0.47
3:G:117:PRO:HD3	3:G:202:HIS:ND1	2.30	0.47
3:C:29:ILE:HD11	3:C:34:LEU:HD23	1.96	0.47
2:H:62:TYR:HE1	2:H:72:ILE:HG13	1.79	0.47
3:C:156:ASN:O	3:C:156:ASN:ND2	2.44	0.47
3:G:162:ASN:OD1	3:G:162:ASN:N	2.48	0.47
1:A:51:PRO:HB2	1:A:55:LYS:HG3	1.97	0.47
1:A:39:LYS:HZ1	1:A:71:GLY:HA3	1.79	0.47
2:B:64:ASP:OD1	3:C:97:ASP:HA	2.15	0.47
2:D:134:ALA:HB3	2:D:223:LYS:HB2	1.95	0.46
1:R:35:TYR:CD1	1:R:58:ALA:HB2	2.50	0.46
1:A:76:TYR:CZ	1:A:86:PRO:HB3	2.50	0.46
3:G:155:ASP:HA	3:G:195:VAL:HG13	1.97	0.46
3:L:162:ASN:N	3:L:162:ASN:OD1	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:2:ILE:HD12	3:E:94:ASP:HB3	1.97	0.46
1:P:16:ILE:O	1:P:94:MET:HA	2.16	0.46
2:F:195:SER:HA	2:F:198:LEU:HG	1.97	0.46
2:B:20:LEU:HD12	2:B:83:LEU:HD23	1.98	0.46
2:B:147:LEU:HD13	2:B:220:VAL:HG11	1.96	0.46
2:H:194:PRO:O	2:H:197:SER:OG	2.25	0.46
2:B:85:MET:HB3	2:B:88:LEU:HD21	1.98	0.45
3:G:174:ASP:N	3:G:174:ASP:OD1	2.45	0.45
2:H:85:MET:HB3	2:H:88:LEU:HD21	1.98	0.45
1:Q:76:TYR:CZ	1:Q:86:PRO:HB3	2.51	0.45
3:G:11:LEU:HD11	3:G:108:VAL:HG22	1.98	0.45
2:D:201:GLN:OE1	2:D:202:THR:N	2.49	0.45
1:A:3:LEU:HD12	1:A:3:LEU:HA	1.74	0.45
2:F:204:ILE:HG12	2:F:219:LYS:HA	1.99	0.45
2:F:52:ILE:HG13	2:F:60:THR:HG22	1.97	0.45
2:F:62:TYR:HE1	2:F:72:ILE:HG13	1.82	0.45
2:D:128:PRO:HB3	2:D:154:TYR:HB3	1.98	0.45
2:B:138:LYS:HB2	2:B:138:LYS:HE2	1.88	0.44
2:D:209:HIS:CE1	2:D:211:PRO:HB2	2.52	0.44
2:F:138:LYS:HE2	2:F:138:LYS:HB2	1.71	0.44
3:G:112:ARG:HG2	3:G:113:THR:N	2.32	0.44
2:D:159:VAL:HG22	2:D:187:LEU:HD21	1.98	0.44
2:F:75:ASP:OD2	2:F:78:LYS:HG3	2.16	0.44
2:H:104:THR:O	3:L:51:ARG:NH2	2.50	0.44
1:R:76:TYR:CZ	1:R:86:PRO:HB3	2.52	0.44
2:F:132:PRO:HB3	2:F:220:VAL:HG22	1.99	0.44
1:Q:16:ILE:HG13	1:Q:22:VAL:HB	1.99	0.44
2:B:204:ILE:HG12	2:B:219:LYS:HA	1.98	0.44
2:F:41:ALA:HB3	2:F:44:LYS:HB2	1.99	0.44
1:Q:74:ARG:CZ	1:Q:89:PRO:HG3	2.48	0.44
3:G:128:GLN:O	3:G:131:SER:OG	2.34	0.44
3:C:158:LEU:HD13	3:C:159:GLN:N	2.32	0.43
2:D:104:THR:O	3:E:51:ARG:NH2	2.51	0.43
2:F:143:GLY:O	2:F:195:SER:N	2.44	0.43
3:E:135:SER:HA	3:E:183:LEU:O	2.18	0.43
2:D:12:VAL:HG11	2:D:88:LEU:HD13	1.99	0.43
3:G:107:LYS:NZ	3:G:169:GLU:OE2	2.50	0.43
3:C:8:PRO:HB3	3:L:11:LEU:HD13	2.00	0.43
2:F:17:SER:OG	2:F:84:GLN:OE1	2.35	0.43
2:F:11:LEU:HD23	2:F:119:THR:O	2.19	0.43
3:G:1:ASP:HB2	3:G:2:ILE:H	1.63	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:152:LYS:NZ	2:D:153:ASP:OD2	2.49	0.43
2:F:64:ASP:OD1	3:G:97:ASP:HA	2.19	0.43
2:B:159:VAL:HG22	2:B:187:LEU:HD21	2.01	0.42
3:L:155:ASP:HA	3:L:195:VAL:HG13	2.01	0.42
2:D:157:GLU:OE2	2:D:177:ALA:HB3	2.19	0.42
2:D:29:PHE:HZ	2:D:79:ASN:HD21	1.66	0.42
3:G:120:PHE:HB2	3:G:139:LEU:HB3	2.01	0.42
3:L:119:VAL:HG12	3:L:211:LYS:HG3	2.00	0.42
1:A:50:ASN:OD1	3:L:30:ASN:ND2	2.46	0.42
3:C:1:ASP:HB2	3:C:98:VAL:HA	2.01	0.42
3:G:81:PRO:HA	3:G:84:PHE:CE2	2.54	0.42
1:R:52:LEU:HD13	1:R:58:ALA:HA	2.00	0.42
3:E:21:ILE:HG12	3:E:106:THR:HG21	2.01	0.42
2:H:93:THR:HG23	2:H:119:THR:HA	2.01	0.42
1:P:22:VAL:HG13	1:P:62:ILE:HB	2.00	0.42
2:F:31:ASN:ND2	2:F:32:HIS:H	2.17	0.42
2:D:6:GLU:HA	2:D:21:SER:O	2.19	0.42
3:G:2:ILE:HD12	3:G:94:ASP:HB3	2.02	0.42
2:B:136:SER:OG	2:B:139:SER:N	2.50	0.41
2:D:93:THR:HA	2:D:118:VAL:O	2.20	0.41
3:E:187:LYS:HD3	3:E:187:LYS:O	2.20	0.41
2:F:88:LEU:HD23	2:F:88:LEU:HA	1.91	0.41
1:A:35:TYR:CD1	1:A:58:ALA:HB2	2.54	0.41
3:C:154:VAL:HG22	3:C:196:TYR:CD2	2.55	0.41
2:D:171:GLY:O	2:D:191:VAL:HA	2.20	0.41
2:B:168:LEU:HD21	2:B:191:VAL:HG21	2.01	0.41
1:R:47:ASP:OD1	1:R:48:ARG:N	2.53	0.41
3:C:136:VAL:HB	3:C:183:LEU:HB3	2.02	0.41
3:E:196:TYR:HB2	3:E:213:PHE:CE1	2.55	0.41
2:F:111:LEU:HA	2:F:111:LEU:HD23	1.94	0.41
3:L:165:GLU:HA	3:L:180:SER:O	2.20	0.41
3:E:61:SER:OG	3:L:82:GLU:OE2	2.31	0.41
1:Q:40:GLU:OE1	1:Q:72:ARG:NE	2.38	0.41
3:E:30:ASN:HB3	3:E:33:TYR:CD2	2.53	0.41
2:H:89:ARG:HG3	2:H:91:GLU:HG2	2.02	0.41
2:B:4:LEU:HG	2:B:111:LEU:HD22	2.02	0.41
2:D:36:TYR:O	2:D:98:CYS:HA	2.20	0.41
2:H:135:PRO:HD3	2:H:147:LEU:HB3	2.03	0.41
1:Q:35:TYR:CD1	1:Q:58:ALA:HB2	2.55	0.41
2:B:36:TYR:CD1	2:B:51:SER:HB3	2.55	0.41
3:E:112:ARG:NH2	3:E:113:THR:O	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:5:LYS:HB3	1:P:85:GLN:NE2	2.36	0.41
1:A:10:ALA:HB2	1:A:90:LEU:HD21	2.03	0.41
3:E:55:LEU:HD11	3:E:63:PHE:O	2.21	0.41
2:F:180:GLN:N	2:F:184:LEU:O	2.48	0.41
2:F:161:VAL:HA	2:F:206:ASN:O	2.21	0.41
2:H:30:SER:C	2:H:32:HIS:H	2.25	0.41
2:F:37:TRP:HD1	2:F:72:ILE:HD13	1.86	0.40
2:B:103:SER:HB2	2:B:107:TRP:CH2	2.57	0.40
3:C:149:LYS:HB3	3:C:201:THR:HB	2.02	0.40
2:D:61:TYR:HE2	1:Q:81:VAL:HG23	1.85	0.40
2:F:175:PHE:CE2	3:G:180:SER:HB3	2.56	0.40
1:Q:72:ARG:NH1	1:Q:74:ARG:NH2	2.70	0.40
2:F:162:SER:OG	2:F:206:ASN:HB2	2.21	0.40
2:H:140:THR:HB	2:H:195:SER:OG	2.22	0.40
2:F:11:LEU:HD21	2:F:155:PHE:HE2	1.85	0.40
2:F:209:HIS:ND1	2:F:212:SER:OG	2.34	0.40
2:F:96:TYR:CE1	2:F:118:VAL:HB	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	92/95 (97%)	90 (98%)	2 (2%)	0	100	100
1	P	92/95 (97%)	91 (99%)	1 (1%)	0	100	100
1	Q	92/95 (97%)	89 (97%)	3 (3%)	0	100	100
1	R	92/95 (97%)	89 (97%)	3 (3%)	0	100	100
2	B	223/228 (98%)	217 (97%)	6 (3%)	0	100	100
2	D	223/228 (98%)	216 (97%)	7 (3%)	0	100	100
2	F	223/228 (98%)	215 (96%)	8 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	223/228 (98%)	211 (95%)	12 (5%)	0	100	100
3	C	216/218 (99%)	209 (97%)	7 (3%)	0	100	100
3	E	216/218 (99%)	209 (97%)	7 (3%)	0	100	100
3	G	216/218 (99%)	208 (96%)	8 (4%)	0	100	100
3	L	216/218 (99%)	211 (98%)	5 (2%)	0	100	100
All	All	2124/2164 (98%)	2055 (97%)	69 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	84/84 (100%)	82 (98%)	2 (2%)	49	79
1	P	84/84 (100%)	81 (96%)	3 (4%)	35	70
1	Q	84/84 (100%)	82 (98%)	2 (2%)	49	79
1	R	84/84 (100%)	84 (100%)	0	100	100
2	B	187/190 (98%)	184 (98%)	3 (2%)	62	86
2	D	187/190 (98%)	184 (98%)	3 (2%)	62	86
2	F	187/190 (98%)	184 (98%)	3 (2%)	62	86
2	H	187/190 (98%)	182 (97%)	5 (3%)	44	77
3	C	190/190 (100%)	183 (96%)	7 (4%)	34	70
3	E	190/190 (100%)	186 (98%)	4 (2%)	53	82
3	G	190/190 (100%)	187 (98%)	3 (2%)	62	86
3	L	190/190 (100%)	188 (99%)	2 (1%)	73	90
All	All	1844/1856 (99%)	1807 (98%)	37 (2%)	55	83

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	SER
1	A	57	LYS
2	B	31	ASN
2	B	206	ASN
2	B	225	CYS
3	C	18	ARG
3	C	62	ARG
3	C	94	ASP
3	C	97	ASP
3	C	156	ASN
3	C	158	LEU
3	C	180	SER
2	D	25	SER
2	D	29	PHE
2	D	35	MET
3	E	62	ARG
3	E	78	SER
3	E	111	LYS
3	E	217	GLU
2	F	31	ASN
2	F	111	LEU
2	F	136	SER
3	G	26	SER
3	G	147	GLU
3	G	180	SER
2	H	5	LEU
2	H	111	LEU
2	H	136	SER
2	H	205	CYS
2	H	225	CYS
3	L	62	ARG
3	L	218	CYS
1	P	55	LYS
1	P	57	LYS
1	P	74	ARG
1	Q	5	LYS
1	Q	48	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	G	142	ASN
3	L	151	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 carbohydrates 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	94/95 (98%)	-0.11	0 100 100	43, 66, 82, 97	0
1	P	94/95 (98%)	-0.32	1 (1%) 80 56	30, 44, 67, 83	0
1	Q	94/95 (98%)	-0.09	0 100 100	32, 53, 80, 92	0
1	R	94/95 (98%)	-0.26	0 100 100	50, 65, 89, 100	0
2	B	225/228 (98%)	-0.04	9 (4%) 38 15	31, 57, 99, 126	0
2	D	225/228 (98%)	-0.15	5 (2%) 62 33	29, 63, 94, 117	0
2	F	225/228 (98%)	0.26	16 (7%) 16 5	57, 78, 124, 141	0
2	H	225/228 (98%)	-0.27	0 100 100	31, 43, 85, 105	0
3	C	218/218 (100%)	-0.23	1 (0%) 91 75	28, 51, 88, 124	0
3	E	218/218 (100%)	-0.06	2 (0%) 84 63	25, 48, 101, 122	0
3	G	218/218 (100%)	0.35	8 (3%) 41 17	67, 90, 107, 141	0
3	L	218/218 (100%)	-0.34	0 100 100	28, 43, 70, 117	0
All	All	2148/2164 (99%)	-0.08	42 (1%) 65 36	25, 60, 103, 141	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	139	SER	6.4
2	F	224	SER	6.2
2	F	145	ALA	4.4
3	G	218	CYS	3.8
2	F	28	ASP	3.7
3	G	12	SER	3.5
2	B	224	SER	3.3
2	F	200	THR	3.3
2	D	1	GLU	3.2
2	F	141	SER	3.2
2	B	137	SER	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	27	ILE	3.0
2	D	137	SER	2.8
2	B	167	ALA	2.7
2	D	224	SER	2.7
2	F	136	SER	2.7
2	F	1	GLU	2.7
2	B	1	GLU	2.5
3	C	218	CYS	2.4
1	P	2	PRO	2.4
3	G	21	ILE	2.4
3	E	126	ASP	2.3
2	B	142	GLY	2.3
2	F	144	THR	2.3
2	D	225	CYS	2.3
3	E	217	GLU	2.3
2	B	200	THR	2.3
2	F	170	SER	2.3
2	F	142	GLY	2.3
3	G	203	GLN	2.2
2	B	141	SER	2.2
2	F	198	LEU	2.2
2	D	78	LYS	2.2
2	B	225	CYS	2.2
2	F	140	THR	2.1
3	G	81	PRO	2.1
3	G	19	VAL	2.1
2	F	138	LYS	2.1
2	B	140	THR	2.1
2	F	77	SER	2.0
3	G	111	LYS	2.0
3	G	205	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 carbohydrates 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.