



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 13, 2022 – 12:03 PM EST

PDB ID : 7RYV
Title : Anti-HIV neutralizing antibody Ab1573 Fab isolated from sequentially immunized macaques
Authors : Yang, Z.; Bjorkman, P.J.
Deposited on : 2021-08-26
Resolution : 2.50 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	:	2.25
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)	:	2.25

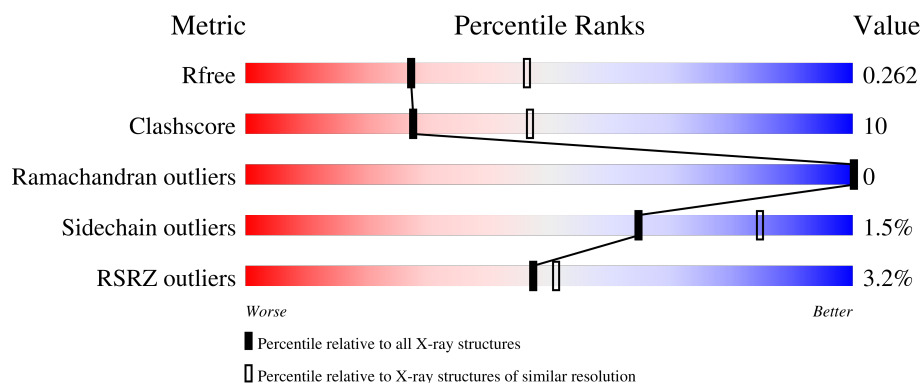
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	E	228	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>.</div> </div> </div>
1	H	228	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>..</div> </div> </div>
1	I	228	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>.</div> </div> </div>
1	P	228	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>.</div> </div> </div>
2	F	216	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>19%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	J	216	<div><div></div><div>2%</div><div>81%</div><div>16%</div><div></div></div>
2	L	216	<div><div></div><div>3%</div><div>80%</div><div>18%</div><div></div></div>
2	Q	216	<div><div></div><div>8%</div><div>70%</div><div>28%</div><div></div></div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13616 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 Ab1573 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	218	Total	C	N	O	S	0	0	0
			1616	1023	276	311	6			
1	H	220	Total	C	N	O	S	0	0	0
			1628	1029	278	315	6			
1	I	219	Total	C	N	O	S	0	0	0
			1622	1026	277	313	6			
1	P	219	Total	C	N	O	S	0	0	0
			1622	1026	277	313	6			

- Molecule 2 is a protein called Ab1573 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	213	Total	C	N	O	S	0	0	0
			1615	1015	265	330	5			
2	J	211	Total	C	N	O	S	0	0	0
			1599	1006	262	326	5			
2	L	212	Total	C	N	O	S	0	0	0
			1608	1011	264	328	5			
2	Q	213	Total	C	N	O	S	0	0	0
			1615	1015	265	330	5			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	113	Total	O	0	0
			113	113		
3	F	106	Total	O	0	0
			106	106		
3	H	92	Total	O	0	0
			92	92		
3	I	75	Total	O	0	0
			75	75		

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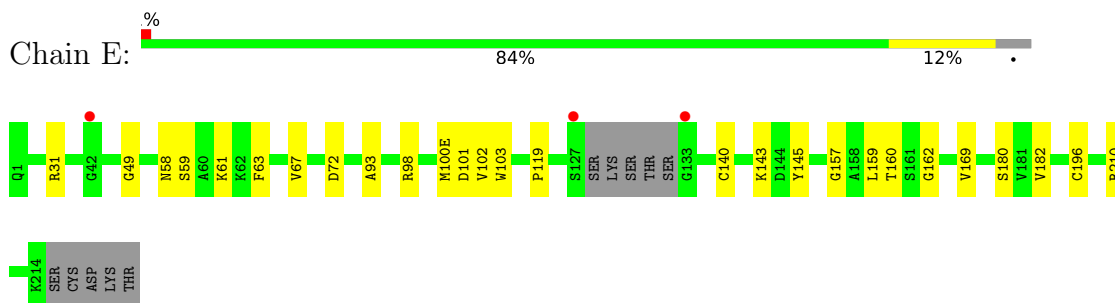
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	70	Total 70	O 70	0	0
3	L	79	Total 79	O 79	0	0
3	P	64	Total 64	O 64	0	0
3	Q	92	Total 92	O 92	0	0

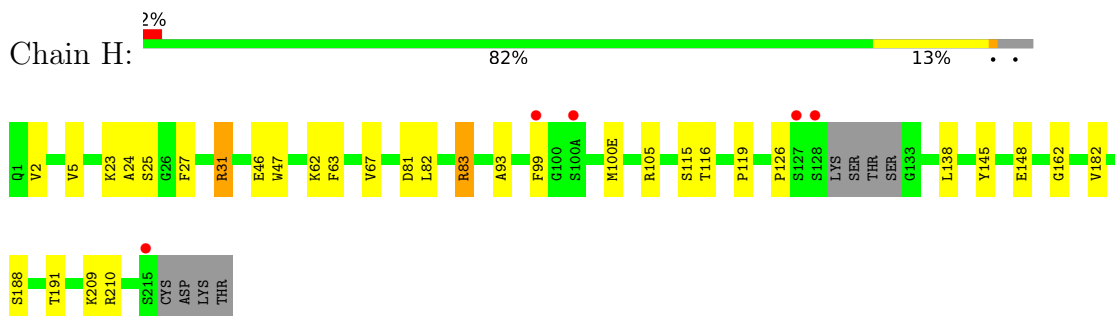
3 Residue-property plots [i](#)

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.

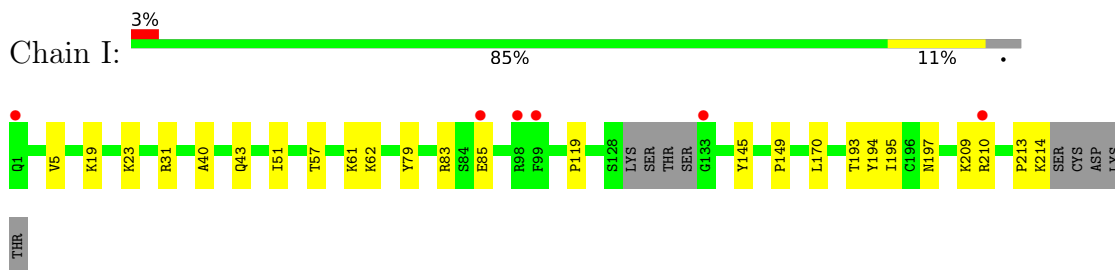
- Molecule 1: Ab1573 Fab heavy chain



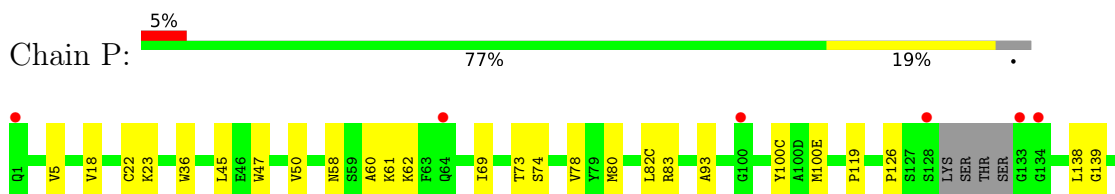
- Molecule 1: Ab1573 Fab heavy chain

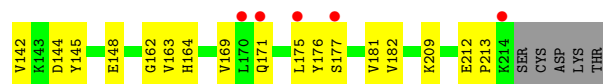


- Molecule 1: Ab1573 Fab heavy chain

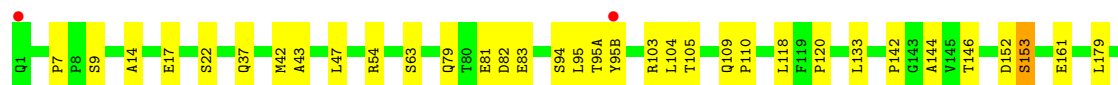
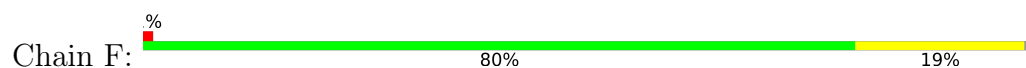


- Molecule 1: Ab1573 Fab heavy chain

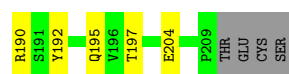
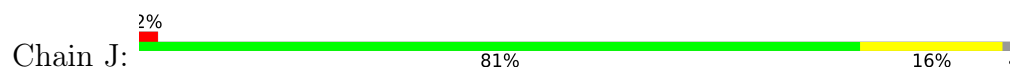




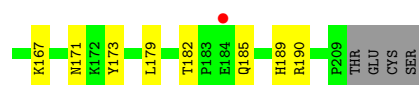
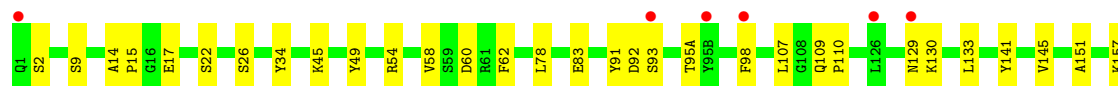
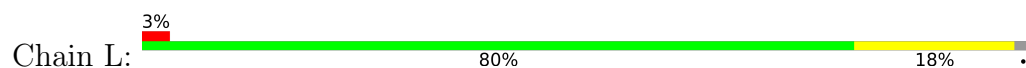
- Molecule 2: Ab1573 Fab light chain



- Molecule 2: Ab1573 Fab light chain



- Molecule 2: Ab1573 Fab light chain



- Molecule 2: Ab1573 Fab light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.50Å 138.40Å 83.73Å 90.00° 95.71° 90.00°	Depositor
Resolution (Å)	38.65 – 2.50 38.91 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.3 (38.65-2.50) 94.9 (38.91-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.216 , 0.254 0.224 , 0.262	Depositor DCC
R_{free} test set	1993 reflections (3.15%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	1.286	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13616	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 55.34 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.2091e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	E	0.32	0/1652	0.57	0/2250
1	H	0.29	0/1664	0.56	0/2266
1	I	0.33	0/1658	0.56	0/2258
1	P	0.35	0/1658	0.57	0/2258
2	F	0.36	0/1658	0.57	0/2264
2	J	0.34	0/1642	0.53	0/2242
2	L	0.35	0/1651	0.54	0/2254
2	Q	0.46	0/1658	0.59	0/2264
All	All	0.35	0/13241	0.56	0/18056

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	E	1616	0	1613	20	0
1	H	1628	0	1621	24	0
1	I	1622	0	1616	15	0
1	P	1622	0	1616	49	0
2	F	1615	0	1546	44	0
2	J	1599	0	1528	24	0
2	L	1608	0	1539	34	0
2	Q	1615	0	1546	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	113	0	0	6	0
3	F	106	0	0	22	1
3	H	92	0	0	8	0
3	I	75	0	0	4	0
3	J	70	0	0	8	1
3	L	79	0	0	14	1
3	P	64	0	0	16	0
3	Q	92	0	0	17	1
All	All	13616	0	12625	255	2

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 10.

All (255) 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:E:140:CYS:HB3	3:E:393:HOH:O	1.13	1.28
2:Q:190:ARG:HB3	3:Q:302:HOH:O	1.28	1.26
1:P:213:PRO:CD	3:P:302:HOH:O	1.91	1.15
1:P:73:THR:CA	3:P:301:HOH:O	1.95	1.12
1:P:213:PRO:HD2	3:P:302:HOH:O	1.50	1.09
1:P:73:THR:N	3:P:301:HOH:O	1.83	1.09
1:P:213:PRO:N	3:P:302:HOH:O	1.83	1.09
2:F:95:LEU:HD23	3:F:303:HOH:O	1.54	1.07
2:L:54:ARG:NE	3:L:301:HOH:O	1.81	1.07
1:E:31:ARG:NH1	3:E:301:HOH:O	1.83	1.06
2:F:95:LEU:N	3:F:303:HOH:O	1.94	1.01
1:P:73:THR:CB	3:P:301:HOH:O	2.10	0.98
2:F:95:LEU:CG	3:F:303:HOH:O	2.11	0.97
2:L:54:ARG:NH2	3:L:301:HOH:O	1.96	0.97
2:J:93:SER:O	3:J:301:HOH:O	1.82	0.97
2:L:109:GLN:NE2	3:L:304:HOH:O	1.99	0.95
1:H:24:ALA:O	3:H:302:HOH:O	1.84	0.94
1:H:148:GLU:OE2	3:H:301:HOH:O	1.84	0.94
2:F:95:LEU:CA	3:F:303:HOH:O	2.16	0.93
2:F:144:ALA:O	3:F:301:HOH:O	1.86	0.92
2:F:94:SER:C	3:F:303:HOH:O	2.07	0.91
1:H:116:THR:O	3:H:303:HOH:O	1.87	0.91
1:H:105:ARG:NH1	3:H:304:HOH:O	2.04	0.90
2:J:195:GLN:HG2	2:J:204:GLU:HG3	1.53	0.89
2:Q:124:GLU:OE1	3:Q:301:HOH:O	1.93	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:195:GLN:HG2	2:Q:204:GLU:HG3	1.62	0.82
1:P:73:THR:HB	3:P:301:HOH:O	1.77	0.81
2:F:103:ARG:NE	3:F:302:HOH:O	1.89	0.81
2:L:145:VAL:O	3:L:303:HOH:O	1.99	0.80
1:E:103:TRP:O	3:E:303:HOH:O	1.99	0.80
1:P:100(C):TYR:HB3	2:Q:96:TRP:HE1	1.47	0.79
2:J:133:LEU:HD12	2:J:179:LEU:HD23	1.63	0.79
2:J:93:SER:HA	3:J:301:HOH:O	1.83	0.78
1:P:148:GLU:OE1	3:P:304:HOH:O	2.01	0.78
1:P:74:SER:N	3:P:301:HOH:O	2.14	0.78
2:F:95:LEU:CD2	3:F:303:HOH:O	2.12	0.78
1:H:25:SER:HA	3:H:302:HOH:O	1.84	0.77
2:Q:47:LEU:HD11	2:Q:62:PHE:CG	2.20	0.77
1:E:140:CYS:CB	3:E:393:HOH:O	1.91	0.76
2:Q:152:ASP:OD1	3:Q:302:HOH:O	2.04	0.75
2:L:9:SER:O	3:L:305:HOH:O	2.03	0.75
1:P:144:ASP:HA	1:P:175:LEU:HB3	1.69	0.75
2:F:142:PRO:O	3:F:301:HOH:O	2.04	0.73
2:L:167:LYS:NZ	3:L:308:HOH:O	2.20	0.73
1:I:193:THR:HB	1:I:210:ARG:HD2	1.71	0.73
1:P:213:PRO:O	3:P:302:HOH:O	2.05	0.73
2:F:43:ALA:O	3:F:304:HOH:O	2.06	0.71
2:L:54:ARG:CZ	3:L:301:HOH:O	2.13	0.71
1:P:212:GLU:OE2	3:P:305:HOH:O	2.08	0.71
2:L:17:GLU:OE1	3:L:306:HOH:O	2.07	0.71
2:L:133:LEU:HD12	2:L:179:LEU:HD23	1.71	0.70
2:J:150:LYS:NZ	3:J:302:HOH:O	1.94	0.70
1:I:149:PRO:O	3:I:301:HOH:O	2.08	0.70
1:P:119:PRO:HB3	1:P:145:TYR:HB3	1.72	0.70
2:F:133:LEU:HD12	2:F:179:LEU:HD23	1.74	0.69
2:F:152:ASP:O	3:F:306:HOH:O	2.10	0.69
2:F:118:LEU:O	3:F:305:HOH:O	2.08	0.69
1:P:144:ASP:HB3	1:P:175:LEU:HD13	1.74	0.69
2:F:146:THR:HG22	2:F:197:THR:HB	1.75	0.68
2:Q:190:ARG:CB	3:Q:302:HOH:O	2.06	0.68
2:Q:109:GLN:N	3:Q:304:HOH:O	2.10	0.68
2:Q:113:ALA:O	3:Q:306:HOH:O	2.12	0.68
2:J:93:SER:CA	3:J:301:HOH:O	2.39	0.67
2:F:95:LEU:HG	3:F:303:HOH:O	1.86	0.67
2:L:182:THR:OG1	2:L:185:GLN:HG3	1.97	0.65
1:E:143:LYS:NZ	3:E:312:HOH:O	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:133:LEU:HD12	2:Q:179:LEU:HD23	1.79	0.65
2:Q:190:ARG:CA	3:Q:302:HOH:O	2.40	0.64
1:P:163:VAL:HG22	1:P:182:VAL:HB	1.79	0.64
2:J:158:ALA:O	3:J:303:HOH:O	2.15	0.64
2:Q:47:LEU:CD2	2:Q:73:LEU:HD21	2.27	0.64
2:F:103:ARG:NH1	3:F:308:HOH:O	2.29	0.63
2:F:95:LEU:CB	3:F:303:HOH:O	2.34	0.63
1:P:209:LYS:NZ	3:Q:301:HOH:O	2.32	0.63
2:Q:42:MET:HB2	3:Q:318:HOH:O	1.98	0.62
2:Q:91:TYR:CE2	2:Q:93:SER:HA	2.34	0.62
2:F:42:MET:N	3:F:311:HOH:O	2.33	0.61
2:F:54:ARG:NH1	3:F:310:HOH:O	2.32	0.61
1:H:25:SER:CA	3:H:302:HOH:O	2.44	0.61
1:P:213:PRO:CA	3:P:302:HOH:O	2.35	0.60
2:Q:105:THR:OG1	3:Q:303:HOH:O	2.06	0.60
1:P:18:VAL:HG23	1:P:82(C):LEU:HD11	1.84	0.60
1:P:139:GLY:HA3	1:P:181:VAL:HG12	1.84	0.60
2:J:138:SER:HB2	2:J:168:GLN:OE1	2.01	0.60
1:I:119:PRO:HB3	1:I:145:TYR:HB3	1.84	0.59
1:E:140:CYS:SG	1:E:180:SER:HB3	2.41	0.59
1:E:169:VAL:HG21	2:F:161:GLU:HB3	1.86	0.58
2:Q:54:ARG:HG2	2:Q:58:VAL:HB	1.85	0.58
1:P:60:ALA:HA	2:Q:95(B):TYR:CE2	2.38	0.58
2:Q:47:LEU:HD12	2:Q:58:VAL:HG11	1.84	0.58
2:J:146:THR:HG22	2:J:197:THR:HB	1.86	0.58
2:Q:47:LEU:HD11	2:Q:62:PHE:CB	2.33	0.58
1:E:162:GLY:O	1:E:182:VAL:HA	2.04	0.58
2:F:81:GLU:OE2	2:L:157:LYS:HD2	2.02	0.58
2:F:7:PRO:HD3	2:F:22:SER:O	2.03	0.58
2:J:127:GLN:OE1	3:J:304:HOH:O	2.17	0.58
1:P:93:ALA:HB1	1:P:100(E):MET:HB3	1.85	0.57
1:E:58:ASN:HD22	2:F:95(A):THR:HB	1.68	0.57
2:Q:18:ARG:HE	2:Q:74:THR:HG21	1.70	0.57
2:J:123:SER:O	2:J:127:GLN:HG2	2.04	0.57
2:F:190:ARG:O	2:F:191:SER:HB3	2.05	0.56
2:Q:7:PRO:HD3	2:Q:22:SER:O	2.04	0.56
2:Q:18:ARG:HE	2:Q:74:THR:CG2	2.18	0.56
2:Q:47:LEU:HG	2:Q:48:ILE:HG13	1.88	0.56
2:Q:173:TYR:OH	3:Q:305:HOH:O	2.12	0.56
1:E:72:ASP:OD1	3:E:306:HOH:O	2.17	0.56
2:F:144:ALA:N	3:F:301:HOH:O	1.95	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:119:PRO:HB3	1:H:145:TYR:HB3	1.87	0.56
2:J:17:GLU:OE1	3:J:305:HOH:O	2.18	0.55
1:P:145:TYR:CZ	1:P:176:TYR:HB2	2.42	0.55
1:I:209:LYS:CD	3:I:308:HOH:O	2.55	0.55
2:Q:103:ARG:HG3	2:Q:103:ARG:HH11	1.72	0.55
2:Q:40:PRO:HD3	2:Q:84:SER:HA	1.89	0.54
2:F:81:GLU:CD	2:F:81:GLU:H	2.12	0.54
2:F:187:LYS:HA	3:F:307:HOH:O	2.07	0.54
2:L:110:PRO:HD2	3:L:344:HOH:O	2.07	0.54
1:P:169:VAL:HG11	2:Q:178:TYR:CD1	2.43	0.53
2:Q:121:PRO:O	3:Q:307:HOH:O	2.18	0.53
1:I:51:ILE:HG13	1:I:57:THR:HG22	1.89	0.53
1:I:213:PRO:O	1:I:214:LYS:HB2	2.07	0.53
1:P:169:VAL:CG2	2:Q:161:GLU:HG3	2.38	0.53
1:I:83:ARG:NH1	1:I:85:GLU:OE1	2.41	0.53
1:E:159:LEU:HD21	1:E:182:VAL:HG21	1.91	0.53
2:F:81:GLU:CD	2:L:157:LYS:HD2	2.30	0.52
2:F:153:SER:O	2:F:153:SER:OG	2.24	0.52
1:E:119:PRO:HB3	1:E:145:TYR:HB3	1.91	0.52
2:J:78:LEU:HD21	2:J:104:LEU:HD21	1.90	0.52
1:H:126:PRO:HG3	1:H:138:LEU:HB3	1.91	0.52
1:E:93:ALA:HB1	1:E:100(E):MET:HB3	1.92	0.52
2:L:91:TYR:CE2	2:L:93:SER:HA	2.45	0.52
1:H:83:ARG:HD3	1:H:83:ARG:N	2.25	0.51
2:L:167:LYS:HE3	2:L:171:ASN:HA	1.92	0.51
1:H:46:GLU:OE2	1:H:62:LYS:HE3	2.11	0.51
2:Q:4:LEU:HD13	2:Q:97:VAL:HG11	1.93	0.51
2:F:63:SER:HB3	3:F:310:HOH:O	2.11	0.51
2:Q:137:ILE:HG12	2:Q:196:VAL:HG21	1.92	0.51
2:L:2:SER:HB3	2:L:26:SER:HB2	1.93	0.51
2:L:173:TYR:OH	3:L:307:HOH:O	2.18	0.51
1:H:188:SER:O	1:H:191:THR:HG22	2.11	0.50
2:F:83:GLU:HG3	2:F:104:LEU:O	2.12	0.50
1:P:169:VAL:HG13	1:P:169:VAL:O	2.11	0.50
1:E:61:LYS:HG3	2:F:95(B):TYR:OH	2.12	0.50
2:Q:5:THR:O	2:Q:23:CYS:HA	2.11	0.50
1:E:140:CYS:HB3	1:E:196:CYS:SG	2.49	0.50
2:F:120:PRO:HA	2:F:133:LEU:HD23	1.94	0.50
1:I:40:ALA:HB3	1:I:43:GLN:HG3	1.94	0.50
2:J:11:VAL:HG23	2:J:104:LEU:HD13	1.93	0.50
1:H:24:ALA:C	3:H:302:HOH:O	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:47:TRP:HB2	2:L:98:PHE:CE1	2.47	0.49
1:I:209:LYS:HD3	3:I:308:HOH:O	2.11	0.49
2:Q:2:SER:O	2:Q:97:VAL:HG11	2.12	0.49
1:E:157:GLY:O	1:E:160:THR:HG23	2.13	0.49
2:F:182:THR:OG1	2:F:185:GLN:HG3	2.12	0.49
1:E:49:GLY:HA2	1:E:59:SER:HA	1.95	0.49
2:L:45:LYS:CE	3:L:313:HOH:O	2.61	0.49
1:H:2:VAL:HG13	1:H:27:PHE:CD1	2.49	0.48
1:P:45:LEU:HD21	2:Q:38:GLN:NE2	2.28	0.48
2:F:144:ALA:CA	3:F:301:HOH:O	2.56	0.48
2:Q:209:PRO:HD3	3:Q:314:HOH:O	2.12	0.48
1:H:67:VAL:HG12	1:H:82:LEU:HD13	1.96	0.48
1:P:126:PRO:HA	3:P:329:HOH:O	2.13	0.48
2:Q:190:ARG:HH11	2:Q:190:ARG:HG2	1.79	0.48
2:Q:47:LEU:HD21	2:Q:73:LEU:HD11	1.95	0.47
1:P:144:ASP:CA	1:P:175:LEU:HB3	2.43	0.47
2:Q:191:SER:N	3:Q:302:HOH:O	2.47	0.47
2:L:14:ALA:HB3	2:L:17:GLU:OE2	2.14	0.47
1:P:213:PRO:CB	3:P:302:HOH:O	2.62	0.47
2:J:37:GLN:HB2	2:J:47:LEU:HD11	1.96	0.47
1:P:126:PRO:HG3	1:P:138:LEU:HD23	1.97	0.47
1:I:170:LEU:HD23	3:I:374:HOH:O	2.15	0.46
2:Q:182:THR:OG1	2:Q:185:GLN:HG3	2.16	0.46
2:J:35:TRP:CZ3	2:J:88:CYS:HB3	2.50	0.46
2:J:114:PRO:HB3	2:J:137:ILE:CG2	2.46	0.46
2:Q:47:LEU:CD2	2:Q:73:LEU:HD11	2.45	0.46
2:Q:103:ARG:HD2	3:Q:384:HOH:O	2.14	0.46
1:E:63:PHE:HB3	1:E:67:VAL:HG13	1.98	0.46
2:F:144:ALA:C	3:F:301:HOH:O	2.40	0.46
2:J:121:PRO:HD3	2:J:133:LEU:HD23	1.98	0.45
1:P:47:TRP:HB2	2:Q:98:PHE:CE1	2.51	0.45
1:P:100(C):TYR:HB3	2:Q:96:TRP:NE1	2.26	0.45
2:F:14:ALA:O	2:F:17:GLU:HB2	2.15	0.45
2:J:190:ARG:HG2	2:J:190:ARG:HH11	1.81	0.45
2:Q:15:PRO:HD3	2:Q:107:LEU:O	2.16	0.45
2:F:146:THR:CG2	2:F:197:THR:HB	2.44	0.45
1:P:74:SER:OG	3:P:306:HOH:O	2.20	0.45
2:Q:39:VAL:HB	2:Q:42:MET:HG3	1.99	0.45
2:Q:120:PRO:HA	2:Q:133:LEU:HD23	1.98	0.45
1:E:140:CYS:CB	1:E:196:CYS:SG	3.03	0.45
2:L:109:GLN:HB3	3:L:304:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:167:LYS:HD2	2:J:173:TYR:CZ	2.52	0.44
2:L:15:PRO:HD3	2:L:107:LEU:O	2.17	0.44
2:F:79:GLN:HB3	2:L:157:LYS:NZ	2.32	0.44
2:F:83:GLU:OE2	2:F:105:THR:HG23	2.17	0.44
2:J:131:ALA:HB3	2:J:181:LEU:O	2.17	0.44
1:I:19:LYS:HD2	1:I:79:TYR:HB3	2.00	0.44
1:I:194:TYR:O	1:I:210:ARG:HG3	2.17	0.44
2:L:22:SER:OG	3:L:302:HOH:O	1.92	0.44
2:L:109:GLN:HB2	2:L:141:TYR:CE2	2.52	0.44
2:Q:190:ARG:C	3:Q:302:HOH:O	2.54	0.44
2:Q:95:LEU:O	2:Q:95(B):TYR:HD1	2.01	0.44
2:Q:4:LEU:HD13	2:Q:97:VAL:CG1	2.48	0.44
1:P:61:LYS:HG3	2:Q:95(B):TYR:OH	2.17	0.44
1:P:5:VAL:HG23	1:P:23:LYS:HB3	1.99	0.43
1:P:45:LEU:HD21	2:Q:38:GLN:CD	2.39	0.43
2:L:129:ASN:O	2:L:130:LYS:HD3	2.19	0.43
1:I:5:VAL:HG23	1:I:23:LYS:HB3	2.00	0.43
2:L:45:LYS:HE3	2:L:45:LYS:HB2	1.79	0.43
2:Q:91:TYR:CD1	2:Q:96:TRP:CE2	3.06	0.43
2:J:150:LYS:HD3	3:J:302:HOH:O	2.18	0.43
2:L:34:TYR:HD1	2:L:49:TYR:HA	1.84	0.43
1:H:47:TRP:HB2	2:L:98:PHE:HE1	1.83	0.43
2:Q:42:MET:CB	3:Q:318:HOH:O	2.60	0.43
2:Q:79:GLN:NE2	2:Q:81:GLU:OE1	2.52	0.43
1:H:162:GLY:O	1:H:182:VAL:HA	2.19	0.42
2:J:54:ARG:HG2	2:J:58:VAL:HB	2.00	0.42
2:F:9:SER:HB2	2:F:103:ARG:O	2.19	0.42
1:P:50:VAL:HG21	2:Q:96:TRP:CH2	2.54	0.42
2:Q:47:LEU:HD23	2:Q:73:LEU:CD2	2.50	0.42
2:Q:50:ASP:O	2:Q:51:ASN:HB2	2.18	0.42
1:H:93:ALA:HB1	1:H:100(E):MET:HB3	2.01	0.42
1:P:69:ILE:N	3:P:303:HOH:O	2.01	0.42
2:F:109:GLN:HG3	2:F:110:PRO:HD2	2.01	0.42
1:I:193:THR:CB	1:I:210:ARG:HD2	2.47	0.42
2:Q:91:TYR:CE1	2:Q:95(A):THR:HA	2.55	0.42
2:Q:103:ARG:HG3	2:Q:103:ARG:NH1	2.34	0.42
1:H:5:VAL:HG23	1:H:23:LYS:HB3	2.01	0.42
1:P:36:TRP:CE2	1:P:80:MET:HB2	2.54	0.42
1:P:47:TRP:HB2	2:Q:98:PHE:CD1	2.55	0.42
1:P:142:VAL:O	1:P:177:SER:HA	2.20	0.42
1:P:22:CYS:HB3	1:P:78:VAL:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:82:ASP:O	2:F:104:LEU:HD23	2.20	0.41
2:L:151:ALA:HB1	2:L:189:HIS:CD2	2.55	0.41
2:Q:150:LYS:HD3	2:Q:155:PRO:HA	2.02	0.41
2:Q:6:GLN:OE1	2:Q:99:GLY:HA3	2.20	0.41
1:P:58:ASN:HD21	2:Q:95(B):TYR:HE1	1.68	0.41
2:Q:47:LEU:HD12	2:Q:58:VAL:CG1	2.50	0.41
1:H:31:ARG:HD3	1:H:99:PHE:HA	2.01	0.41
1:H:115:SER:HA	3:H:338:HOH:O	2.20	0.41
2:J:151:ALA:HB2	2:J:192:TYR:CE2	2.56	0.41
1:P:171:GLN:HE21	1:P:171:GLN:HB2	1.60	0.41
1:P:209:LYS:HA	1:P:209:LYS:HD3	1.71	0.41
2:L:58:VAL:HA	3:L:341:HOH:O	2.21	0.41
1:P:169:VAL:HG22	2:Q:161:GLU:HG3	2.01	0.41
2:Q:111:LYS:HE2	2:Q:111:LYS:HB3	1.71	0.41
1:I:195:ILE:HA	1:I:210:ARG:HA	2.03	0.41
2:L:60:ASP:C	2:L:62:PHE:N	2.74	0.41
2:L:92:ASP:O	2:L:95(A):THR:N	2.53	0.41
1:P:50:VAL:HG21	2:Q:96:TRP:HH2	1.85	0.41
1:P:162:GLY:O	1:P:182:VAL:HA	2.21	0.41
1:H:63:PHE:HB3	1:H:67:VAL:HG13	2.02	0.41
2:L:78:LEU:HD23	2:L:78:LEU:HA	1.94	0.41
2:F:37:GLN:HB2	2:F:47:LEU:HD11	2.03	0.40
1:E:101:ASP:OD1	1:E:102:VAL:N	2.53	0.40
1:H:209:LYS:HA	1:H:209:LYS:HD3	1.74	0.40
1:H:67:VAL:HA	1:H:81:ASP:O	2.22	0.40

All (2) 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)
3:F:362:HOH:O	3:Q:383:HOH:O[1_554]	2.15	0.05
3:J:357:HOH:O	3:L:376:HOH:O[1_556]	2.19	0.01

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	E	214/228 (94%)	211 (99%)	3 (1%)	0	100	100
1	H	216/228 (95%)	212 (98%)	4 (2%)	0	100	100
1	I	215/228 (94%)	207 (96%)	8 (4%)	0	100	100
1	P	215/228 (94%)	212 (99%)	3 (1%)	0	100	100
2	F	211/216 (98%)	203 (96%)	8 (4%)	0	100	100
2	J	209/216 (97%)	204 (98%)	5 (2%)	0	100	100
2	L	210/216 (97%)	205 (98%)	5 (2%)	0	100	100
2	Q	211/216 (98%)	199 (94%)	12 (6%)	0	100	100
All	All	1701/1776 (96%)	1653 (97%)	48 (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	E	180/190 (95%)	178 (99%)	2 (1%)	73	89
1	H	182/190 (96%)	179 (98%)	3 (2%)	62	84
1	I	181/190 (95%)	177 (98%)	4 (2%)	52	77
1	P	181/190 (95%)	178 (98%)	3 (2%)	60	82
2	F	182/185 (98%)	180 (99%)	2 (1%)	73	89
2	J	180/185 (97%)	177 (98%)	3 (2%)	60	82
2	L	181/185 (98%)	179 (99%)	2 (1%)	73	89
2	Q	182/185 (98%)	179 (98%)	3 (2%)	62	84
All	All	1449/1500 (97%)	1427 (98%)	22 (2%)	65	85

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	98	ARG
1	E	210	ARG
2	F	153	SER
2	F	188	SER
1	H	31	ARG
1	H	83	ARG
1	H	210	ARG
1	I	31	ARG
1	I	61	LYS
1	I	62	LYS
1	I	197	ASN
2	J	54	ARG
2	J	72	SER
2	J	152	ASP
2	L	83	GLU
2	L	190	ARG
1	P	62	LYS
1	P	83	ARG
1	P	164	HIS
2	Q	78	LEU
2	Q	81	GLU
2	Q	180	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	3	GLN
2	L	109	GLN
1	P	58	ASN
2	Q	79	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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, 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	E	218/228 (95%)	-0.10	3 (1%) 75 77	13, 24, 44, 56	0
1	H	220/228 (96%)	0.01	5 (2%) 60 63	13, 24, 50, 73	0
1	I	219/228 (96%)	-0.00	6 (2%) 54 58	16, 25, 50, 72	0
1	P	219/228 (96%)	0.12	11 (5%) 28 30	16, 27, 57, 73	0
2	F	213/216 (98%)	-0.05	2 (0%) 84 86	14, 28, 44, 64	0
2	J	211/216 (97%)	-0.00	4 (1%) 66 69	16, 30, 50, 61	0
2	L	212/216 (98%)	0.14	7 (3%) 46 50	14, 29, 47, 55	0
2	Q	213/216 (98%)	0.31	18 (8%) 10 10	16, 30, 53, 73	0
All	All	1725/1776 (97%)	0.05	56 (3%) 47 51	13, 27, 50, 73	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Q	41	GLY	4.8
2	Q	95(A)	THR	4.7
1	H	127	SER	4.6
2	Q	95	LEU	4.4
1	H	128	SER	4.4
2	Q	96	TRP	4.3
2	Q	95(B)	TYR	4.2
1	P	133	GLY	4.1
2	Q	42	MET	4.0
1	E	127	SER	4.0
2	F	1	GLN	3.9
2	L	95(B)	TYR	3.9
2	Q	2	SER	3.6
1	I	98	ARG	3.4
2	Q	38	GLN	3.4
2	F	95(B)	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	H	215	SER	3.3
2	Q	94	SER	3.3
2	Q	1	GLN	3.3
1	P	170	LEU	3.2
2	Q	98	PHE	3.1
1	H	99	PHE	3.0
1	I	133	GLY	2.9
1	P	134	GLY	2.9
1	I	1	GLN	2.9
2	J	93	SER	2.9
2	Q	27	GLY	2.9
2	Q	93	SER	2.8
1	E	42	GLY	2.7
1	P	175	LEU	2.7
1	H	100(A)	SER	2.7
2	Q	97	VAL	2.7
2	L	1	GLN	2.6
1	P	128	SER	2.5
1	P	100	GLY	2.5
2	Q	47	LEU	2.5
2	L	126	LEU	2.5
1	I	210	ARG	2.4
2	J	180	SER	2.4
2	Q	7	PRO	2.4
2	J	152	ASP	2.4
2	L	184	GLU	2.4
1	P	214	LYS	2.3
1	E	133	GLY	2.3
2	Q	39	VAL	2.3
2	L	93	SER	2.3
1	P	171	GLN	2.3
2	Q	210	THR	2.3
1	P	177	SER	2.1
2	J	94	SER	2.1
2	L	129	ASN	2.1
2	L	98	PHE	2.1
1	P	64	GLN	2.1
1	I	99	PHE	2.0
1	P	1	GLN	2.0
1	I	85	GLU	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.