



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 08:49 pm BST

PDB ID : 6N8D
Title : Crystal structure of GII.4 2002 norovirus P domain in complex with neutralizing human antibody A1431
Authors : Changela, A.; Verardi, R.; Kwong, P.D.
Deposited on : 2018-11-29
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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

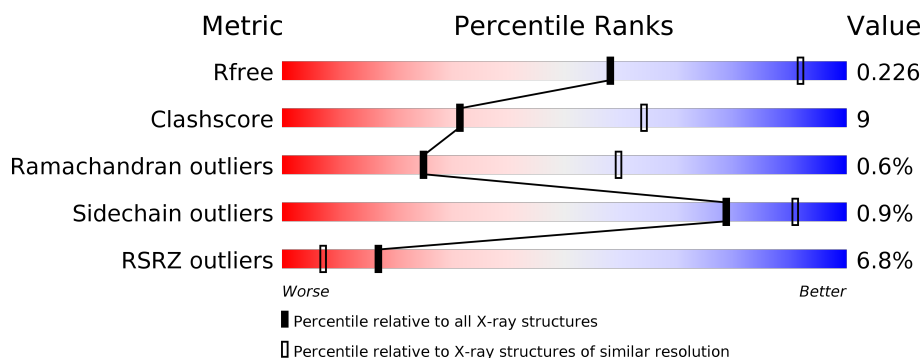
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	309	<div> <div></div> <div>90% 9% .</div> </div>
1	C	309	<div> <div></div> <div>91% 8% .</div> </div>
2	B	215	<div> <div>24%</div> <div>60% 36% ..</div> </div>
2	E	215	<div> <div>%</div> <div>68% 29% ..</div> </div>
3	D	238	<div> <div>19%</div> <div>70% 19% . 9%</div> </div>
3	F	238	<div> <div></div> <div>78% 12% . 9%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11214 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 Major capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	306	Total	C	N	O	S	0	0	0
			2375	1503	411	450	11			
1	A	306	Total	C	N	O	S	0	0	0
			2375	1503	411	450	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	222	GLY	-	expression tag	UNP R4I4P2
C	223	PRO	-	expression tag	UNP R4I4P2
C	224	SER	-	expression tag	UNP R4I4P2
A	222	GLY	-	expression tag	UNP R4I4P2
A	223	PRO	-	expression tag	UNP R4I4P2
A	224	SER	-	expression tag	UNP R4I4P2

- Molecule 2 is a protein called A1431 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	212	Total	C	N	O	S	0	0	0
			1636	1032	277	323	4			
2	B	212	Total	C	N	O	S	0	0	0
			1636	1032	277	323	4			

- Molecule 3 is a protein called A1431 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	216	Total	C	N	O	S	0	0	0
			1596	998	278	314	6			
3	D	216	Total	C	N	O	S	0	0	0
			1596	998	278	314	6			

3 Residue-property plots [i](#)

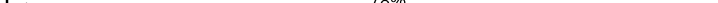
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

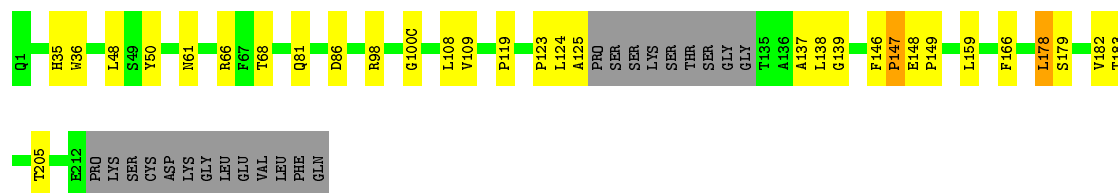
- Molecule 1: Major capsid protein

Chain C:  91% 8%



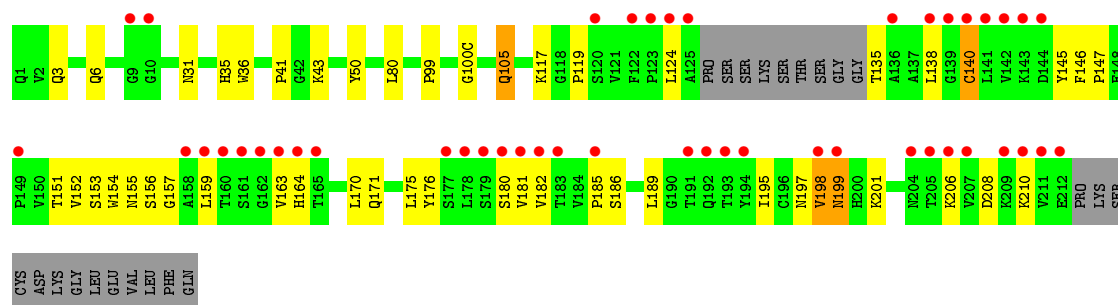
- Molecule 3: A1431 Fab heavy chain

Chain F:  78% 12% • 9%



- Molecule 3: A1431 Fab heavy chain

Chain D:  19% 70% 1% 9%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	147.37Å 157.36Å 110.36Å 90.00° 112.93° 90.00°	Depositor
Resolution (Å)	41.62 – 3.10 41.62 – 3.10	Depositor EDS
% Data completeness (in resolution range)	94.4 (41.62-3.10) 94.4 (41.62-3.10)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.45 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.176 , 0.227 0.176 , 0.226	Depositor DCC
R_{free} test set	1908 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	60.8	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 52.0	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	0.93	EDS
Total number of atoms	11214	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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	0.39	0/2446	0.59	0/3347
1	C	0.37	0/2446	0.55	0/3347
2	B	0.41	0/1674	0.63	0/2275
2	E	0.33	0/1674	0.59	0/2275
3	D	0.33	0/1634	0.58	0/2225
3	F	0.36	0/1634	0.58	1/2225 (0.0%)
All	All	0.37	0/11508	0.58	1/15694 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	178	LEU	CA-CB-CG	5.02	126.84	115.30

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	2375	0	2265	20	0
1	C	2375	0	2265	17	0
2	B	1636	0	1605	68	0
2	E	1636	0	1605	45	0
3	D	1596	0	1541	35	0
3	F	1596	0	1541	22	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11214	0	10822	199	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 9.

All (199) 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)
2:E:120:PRO:HG3	2:E:132:VAL:HG12	1.55	0.88
2:B:160:GLN:HB3	2:B:178:THR:HB	1.57	0.87
2:B:139:PHE:CZ	2:B:141:PRO:HD3	2.10	0.86
2:B:139:PHE:CE2	2:B:141:PRO:HD3	2.13	0.83
2:E:151:ASP:HA	2:E:191:VAL:HB	1.63	0.79
1:C:329:ARG:HH22	1:C:391:ASP:HB2	1.49	0.75
1:A:329:ARG:HH22	1:A:391:ASP:HB3	1.53	0.72
2:B:110:VAL:HG11	2:B:200:GLY:HA3	1.71	0.72
2:B:178:THR:HG22	2:B:180:THR:HG23	1.70	0.71
3:F:159:LEU:HD21	3:F:182:VAL:HG21	1.72	0.70
3:F:66:ARG:NH2	3:F:86:ASP:OD2	2.23	0.70
2:E:11:LEU:HD23	2:E:13:LEU:HD11	1.73	0.70
2:E:197:THR:HG22	2:E:204:PRO:HB3	1.73	0.70
2:B:178:THR:CG2	2:B:180:THR:HG23	2.22	0.69
3:D:199:ASN:HB3	3:D:206:LYS:HG2	1.74	0.68
1:A:412:THR:O	1:A:412:THR:HG22	1.93	0.67
2:B:201:LEU:HG	2:B:202:SER:H	1.58	0.67
3:F:137:ALA:HB2	3:F:183:THR:HG22	1.78	0.65
2:B:141:PRO:HG3	2:B:199:GLN:O	1.97	0.65
2:E:128:GLY:H	2:E:183:LYS:NZ	1.95	0.65
1:C:339:ARG:NH2	1:C:378:GLY:O	2.29	0.64
2:E:151:ASP:OD2	2:E:189:HIS:ND1	2.20	0.64
2:E:108:ARG:NH2	2:E:111:ALA:HB2	2.12	0.64
3:D:155:ASN:O	3:D:157:GLY:N	2.27	0.64
2:B:37:GLN:HG3	2:B:86:TYR:HE1	1.62	0.64
2:E:149:LYS:HB2	2:E:193:ALA:HB3	1.78	0.63
2:B:115:VAL:HG12	2:B:136:LEU:HA	1.79	0.63
2:B:187:GLU:OE2	2:B:211:ARG:NH2	2.31	0.63
2:B:121:SER:OG	2:B:123:GLU:OE2	2.16	0.63
3:F:178:LEU:HD23	3:F:179:SER:H	1.63	0.62
2:E:108:ARG:HH21	2:E:111:ALA:HB2	1.64	0.62
2:E:148:TRP:CZ2	2:E:177:SER:HB2	2.34	0.62
1:C:476:ARG:NH1	1:C:518:ASP:OD2	2.32	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:154:TRP:O	3:D:197:ASN:ND2	2.33	0.61
1:C:239:ASN:ND2	1:C:436:SER:OG	2.33	0.61
3:D:155:ASN:HB2	3:D:159:LEU:HD13	1.84	0.60
1:A:488:GLU:HG3	1:A:527:LEU:HD22	1.84	0.59
3:D:199:ASN:HB3	3:D:206:LYS:HA	1.84	0.59
3:D:195:ILE:HD11	3:D:208:ASP:HB3	1.84	0.59
1:A:307:ASN:OD1	1:A:309:ASN:ND2	2.37	0.58
1:A:341:ASP:N	1:A:341:ASP:OD1	2.34	0.58
2:B:132:VAL:HG11	2:B:209:PHE:HE2	1.68	0.58
2:B:117:ILE:HD12	2:B:118:PHE:H	1.69	0.58
2:B:154:LEU:H	2:B:154:LEU:HD12	1.69	0.58
2:B:145:LYS:HE2	2:B:197:THR:H	1.69	0.57
2:B:37:GLN:HG3	2:B:86:TYR:CE1	2.40	0.57
2:B:198:HIS:NE2	2:B:201:LEU:HD13	2.19	0.57
2:B:18:ARG:HD3	2:B:76:SER:HA	1.87	0.56
3:F:125:ALA:HA	3:F:138:LEU:HD23	1.87	0.56
2:E:113:PRO:HD2	2:E:201:LEU:HD21	1.86	0.56
3:D:154:TRP:CZ3	3:D:182:VAL:HB	2.40	0.56
2:E:148:TRP:HZ2	2:E:177:SER:HB2	1.71	0.56
2:E:148:TRP:CG	2:E:179:LEU:HD13	2.41	0.55
2:B:167:ASP:HB3	2:B:171:SER:H	1.72	0.55
3:D:153:SER:O	3:D:154:TRP:HD1	1.90	0.55
1:C:257:PHE:CE1	3:F:100(C):GLY:HA2	2.41	0.54
2:E:161:GLU:OE2	2:E:162:SER:N	2.38	0.54
1:C:329:ARG:NH2	1:C:391:ASP:HB2	2.21	0.54
1:A:433:PHE:HB3	1:A:450:ASP:HB3	1.88	0.54
2:B:111:ALA:O	2:B:139:PHE:HB2	2.08	0.54
3:D:145:TYR:O	3:D:176:TYR:N	2.41	0.53
3:D:31:ASN:HB3	3:D:99:PRO:HB3	1.91	0.53
1:C:280:PRO:HB3	1:C:455:GLN:HG2	1.91	0.53
3:D:154:TRP:CZ3	3:D:163:VAL:HG22	2.44	0.53
2:B:148:TRP:CD2	2:B:179:LEU:HD22	2.44	0.53
2:E:128:GLY:H	2:E:183:LYS:HZ1	1.56	0.53
2:B:187:GLU:HA	2:B:190:LYS:HE3	1.89	0.53
2:B:148:TRP:HE1	2:B:192:TYR:CB	2.22	0.52
2:B:190:LYS:NZ	2:B:211:ARG:HG2	2.24	0.52
3:F:148:GLU:HB3	3:F:149:PRO:HA	1.92	0.52
1:C:389:VAL:HG12	1:C:441:CYS:HB2	1.92	0.52
3:F:66:ARG:HH22	3:F:86:ASP:CG	2.13	0.51
2:B:198:HIS:CE1	2:B:201:LEU:HB2	2.45	0.51
1:C:329:ARG:HH12	1:C:391:ASP:HB2	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:170:LEU:HD22	3:D:171:GLN:H	1.75	0.51
3:D:164:HIS:HB2	3:D:181:VAL:HG12	1.93	0.51
2:E:149:LYS:HB3	2:E:152:ASN:HA	1.93	0.51
3:D:135:THR:HG22	3:D:185:PRO:HA	1.92	0.50
2:E:136:LEU:HD13	2:E:175:LEU:HB3	1.91	0.50
3:D:152:VAL:HG22	3:D:198:VAL:HG13	1.93	0.50
3:D:140:CYS:SG	3:D:180:SER:OG	2.69	0.50
1:A:257:PHE:CE1	3:D:100(C):GLY:HA2	2.47	0.50
1:A:280:PRO:HB3	1:A:455:GLN:HG2	1.92	0.50
2:B:140:TYR:HD2	2:B:173:TYR:HB2	1.75	0.50
3:D:36:TRP:CE2	3:D:80:LEU:HB2	2.47	0.50
3:D:41:PRO:O	3:D:43:LYS:NZ	2.43	0.50
2:E:76:SER:OG	2:E:77:ASN:N	2.45	0.50
2:E:132:VAL:HG22	2:E:179:LEU:HB3	1.94	0.49
2:E:190:LYS:HG3	2:E:211:ARG:HB3	1.94	0.49
2:E:121:SER:OG	3:F:123:PRO:O	2.29	0.49
1:C:470:SER:OG	1:C:471:ASP:N	2.46	0.49
2:B:110:VAL:HG13	2:B:139:PHE:HE1	1.78	0.49
2:B:163:VAL:HG22	2:B:175:LEU:HD13	1.94	0.49
3:D:135:THR:HA	3:D:186:SER:HB2	1.93	0.49
2:E:176:SER:HB3	3:F:166:PHE:CE2	2.48	0.49
1:A:297:HIS:ND1	1:A:372:ASN:HB3	2.28	0.49
2:B:4:LEU:HD13	2:B:90:HIS:HD2	1.78	0.48
2:E:61:ARG:NE	2:E:82:ASP:OD2	2.45	0.48
2:B:117:ILE:CD1	2:B:133:VAL:HB	2.43	0.48
1:C:488:GLU:HG3	1:C:527:LEU:HD22	1.95	0.48
1:A:297:HIS:CE1	1:A:372:ASN:HB3	2.49	0.48
2:B:133:VAL:HG13	2:B:177:SER:O	2.13	0.48
2:B:17:GLU:CD	2:B:18:ARG:H	2.17	0.48
3:D:154:TRP:CH2	3:D:182:VAL:HB	2.48	0.48
2:B:166:GLN:HG3	2:B:173:TYR:CE1	2.49	0.47
2:B:188:LYS:HD3	2:B:188:LYS:HA	1.67	0.47
1:C:433:PHE:HB3	1:C:450:ASP:HB3	1.96	0.47
3:F:68:THR:HB	3:F:81:GLN:HB3	1.96	0.47
2:B:148:TRP:CZ2	2:B:192:TYR:HB2	2.50	0.47
2:B:37:GLN:O	2:B:45:ARG:N	2.43	0.47
3:F:61:ASN:HB3	3:D:3:GLN:OE1	2.15	0.47
2:B:140:TYR:HE1	2:B:143:GLU:C	2.18	0.47
2:B:170:ASP:OD1	2:B:172:THR:N	2.48	0.46
2:B:119:PRO:HG3	2:B:209:PHE:HB3	1.97	0.46
2:E:50:ASP:HB2	2:E:53:TYR:HD2	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:138:ASN:ND2	2:B:138:ASN:O	2.49	0.46
2:E:192:TYR:O	2:E:208:SER:HB3	2.16	0.46
3:D:117:LYS:HD2	3:D:175:LEU:HD13	1.98	0.46
2:B:145:LYS:HG3	2:B:145:LYS:O	2.16	0.46
2:E:8:PRO:HD2	2:E:11:LEU:HD11	1.97	0.46
3:D:119:PRO:HA	3:D:145:TYR:HB2	1.98	0.45
1:C:397:GLN:HB3	3:F:98:ARG:HG2	1.98	0.45
2:E:21:LEU:HD23	2:E:102:THR:HB	1.99	0.45
2:B:108:ARG:HG2	2:B:109:THR:H	1.81	0.45
2:E:94:TRP:CG	2:E:95:PRO:HA	2.51	0.45
2:B:21:LEU:HD23	2:B:102:THR:HB	1.98	0.45
1:C:397:GLN:O	1:C:446:ASN:ND2	2.49	0.45
2:B:148:TRP:HE1	2:B:192:TYR:HB2	1.82	0.45
2:B:56:ILE:HA	2:B:56:ILE:HD13	1.85	0.45
2:E:148:TRP:O	2:E:149:LYS:HD2	2.17	0.45
3:F:178:LEU:HD23	3:F:179:SER:N	2.31	0.44
3:F:36:TRP:O	3:F:48:LEU:HB2	2.17	0.44
2:B:12:SER:OG	2:B:105:GLU:OE1	2.31	0.44
3:D:154:TRP:CZ2	3:D:163:VAL:HG13	2.52	0.44
2:B:108:ARG:NH2	2:B:170:ASP:O	2.48	0.44
2:B:155:GLN:NE2	2:B:158:ASN:OD1	2.51	0.44
2:E:140:TYR:CD1	2:E:141:PRO:HA	2.53	0.44
2:B:151:ASP:OD2	2:B:189:HIS:ND1	2.48	0.44
2:B:190:LYS:HZ3	2:B:211:ARG:HG2	1.83	0.44
3:D:35:HIS:CE1	3:D:50:TYR:HD1	2.36	0.44
2:E:187:GLU:O	2:E:211:ARG:NH2	2.51	0.44
2:E:6:GLN:HE21	2:E:6:GLN:HB3	1.59	0.44
1:A:308:TRP:CH2	1:A:380:ASN:HB3	2.53	0.43
2:B:132:VAL:O	2:B:178:THR:HA	2.18	0.43
2:B:89:GLN:NE2	2:B:96:LEU:HD22	2.33	0.43
3:F:124:LEU:HB2	3:F:139:GLY:H	1.83	0.43
2:B:125:LEU:HG	2:B:183:LYS:HE3	1.99	0.43
2:E:192:TYR:HB2	2:E:209:PHE:HB3	2.01	0.43
2:E:118:PHE:CE1	3:F:138:LEU:HA	2.54	0.43
2:B:169:LYS:HB3	2:B:169:LYS:HE2	1.84	0.43
3:D:124:LEU:HD23	3:D:138:LEU:HB2	2.01	0.43
3:D:35:HIS:CE1	3:D:50:TYR:CD1	3.07	0.43
2:B:61:ARG:NH2	2:B:82:ASP:OD1	2.50	0.43
3:D:154:TRP:HB3	3:D:155:ASN:H	1.54	0.43
3:D:151:THR:OG1	3:D:201:LYS:NZ	2.37	0.43
2:E:17:GLU:HG2	2:E:18:ARG:H	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:6:GLN:HG3	3:D:105:GLN:OE1	2.18	0.42
2:B:4:LEU:HG	2:B:23:CYS:SG	2.58	0.42
3:D:199:ASN:OD1	3:D:199:ASN:N	2.51	0.42
3:F:119:PRO:HD2	3:F:205:THR:HB	2.01	0.42
3:F:146:PHE:CD2	3:F:147:PRO:HA	2.55	0.42
3:D:152:VAL:HG13	3:D:198:VAL:HG22	2.00	0.42
3:F:108:LEU:HD23	3:F:109:VAL:N	2.34	0.42
2:B:83:PHE:CE1	2:B:106:ILE:HG12	2.54	0.42
2:E:145:LYS:HA	2:E:145:LYS:HD2	1.80	0.42
2:B:125:LEU:HD11	2:B:186:TYR:CZ	2.55	0.42
2:B:147:GLN:NE2	2:B:154:LEU:HD23	2.34	0.42
2:B:177:SER:O	2:B:178:THR:OG1	2.35	0.42
2:E:142:ARG:HB2	2:E:173:TYR:CE1	2.54	0.41
2:E:4:LEU:HG	2:E:90:HIS:HD2	1.85	0.41
1:A:337:THR:HG23	1:A:344:THR:HG22	2.02	0.41
1:A:329:ARG:NH2	1:A:391:ASP:HB3	2.29	0.41
1:A:412:THR:O	1:A:412:THR:CG2	2.65	0.41
1:A:389:VAL:HG12	1:A:441:CYS:HB2	2.03	0.41
2:E:19:ALA:HB2	2:E:78:LEU:HD11	2.02	0.41
3:F:35:HIS:CE1	3:F:50:TYR:CD1	3.08	0.41
1:A:500:ALA:HB2	1:A:527:LEU:HB2	2.02	0.41
2:B:76:SER:OG	2:B:77:ASN:N	2.53	0.41
1:C:231:ILE:H	1:C:231:ILE:HG13	1.64	0.41
2:B:117:ILE:HG12	2:B:133:VAL:O	2.21	0.41
2:B:81:GLU:HG3	2:B:81:GLU:H	1.63	0.41
1:C:529:PRO:O	1:A:411:ARG:NH1	2.53	0.41
2:B:24:LYS:HA	2:B:69:THR:O	2.20	0.41
2:E:182:SER:OG	2:E:183:LYS:N	2.54	0.41
2:B:108:ARG:HG2	2:B:109:THR:N	2.35	0.41
2:E:201:LEU:HB3	2:E:202:SER:H	1.75	0.41
2:B:170:ASP:OD1	2:B:172:THR:OG1	2.25	0.41
1:C:434:PHE:HB2	1:C:451:CYS:SG	2.61	0.41
2:E:193:ALA:HA	2:E:208:SER:OG	2.20	0.41
2:E:167:ASP:HB3	2:E:171:SER:H	1.86	0.40
3:D:198:VAL:O	3:D:199:ASN:HB2	2.21	0.40
1:A:227:PHE:CE1	1:A:268:THR:HB	2.57	0.40
1:A:287:ARG:HD2	1:A:306:GLN:HA	2.02	0.40
1:A:347:HIS:HB3	1:A:370:ASP:OD1	2.22	0.40
2:B:148:TRP:CD1	2:B:149:LYS:N	2.89	0.40
3:D:146:PHE:HB2	3:D:175:LEU:HA	2.03	0.40
2:E:83:PHE:CD1	2:E:104:VAL:HG12	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4:LEU:HD22	2:E:23:CYS:SG	2.62	0.40
3:F:147:PRO:HB2	3:F:148:GLU:H	1.67	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	304/309 (98%)	295 (97%)	9 (3%)	0	100	100
1	C	304/309 (98%)	293 (96%)	11 (4%)	0	100	100
2	B	210/215 (98%)	177 (84%)	31 (15%)	2 (1%)	15	49
2	E	210/215 (98%)	180 (86%)	28 (13%)	2 (1%)	15	49
3	D	212/238 (89%)	194 (92%)	14 (7%)	4 (2%)	8	33
3	F	212/238 (89%)	201 (95%)	10 (5%)	1 (0%)	29	64
All	All	1452/1524 (95%)	1340 (92%)	103 (7%)	9 (1%)	25	59

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	147	PRO
2	B	210	ASN
3	D	198	VAL
2	E	157	GLY
2	E	204	PRO
3	D	156	SER
2	B	157	GLY
3	D	199	ASN
3	F	147	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	263/265 (99%)	263 (100%)	0	100	100
1	C	263/265 (99%)	263 (100%)	0	100	100
2	B	183/185 (99%)	179 (98%)	4 (2%)	52	78
2	E	183/185 (99%)	180 (98%)	3 (2%)	62	84
3	D	175/194 (90%)	171 (98%)	4 (2%)	50	77
3	F	175/194 (90%)	175 (100%)	0	100	100
All	All	1242/1288 (96%)	1231 (99%)	11 (1%)	78	91

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	92	SER
2	E	149	LYS
2	E	182	SER
2	B	139	PHE
2	B	140	TYR
2	B	160	GLN
2	B	192	TYR
3	D	105	GLN
3	D	140	CYS
3	D	189	LEU
3	D	210	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	309	ASN

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 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	306/309 (99%)	-0.53	0	100	100	20, 43, 76, 105	0
1	C	306/309 (99%)	-0.50	0	100	100	24, 49, 90, 110	0
2	B	212/215 (98%)	0.97	51 (24%)	0	0	45, 132, 231, 250	0
2	E	212/215 (98%)	-0.14	3 (1%)	75	56	31, 88, 161, 178	0
3	D	216/238 (90%)	0.72	46 (21%)	0	0	35, 111, 220, 246	0
3	F	216/238 (90%)	-0.43	0	100	100	28, 68, 126, 147	0
All	All	1468/1524 (96%)	-0.05	100 (6%)	17	7	20, 66, 205, 250	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	181	LEU	10.1
3	D	162	GLY	8.1
2	B	135	LEU	7.6
3	D	183	THR	7.5
3	D	179	SER	7.4
3	D	210	LYS	7.2
2	B	134	CYS	7.0
2	B	118	PHE	6.8
2	B	182	SER	6.6
2	B	197	THR	6.2
3	D	125	ALA	6.0
3	D	136	ALA	5.7
2	B	185	ASP	5.5
2	B	119	PRO	5.5
3	D	120	SER	5.2
3	D	138	LEU	5.1
2	B	122	ASP	5.0
3	D	123	PRO	5.0
2	B	180	THR	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	156	SER	4.6
3	D	159	LEU	4.6
2	B	120	PRO	4.5
3	D	122	PHE	4.5
2	B	126	LYS	4.4
3	D	211	VAL	4.4
2	B	117	ILE	4.4
3	D	163	VAL	4.4
2	B	153	ALA	4.3
3	D	124	LEU	4.3
2	B	208	SER	4.2
2	B	177	SER	4.2
3	D	141	LEU	4.1
2	B	154	LEU	4.1
2	B	133	VAL	4.0
2	B	152	ASN	4.0
3	D	193	THR	4.0
3	D	180	SER	3.9
2	B	132	VAL	3.8
3	D	182	VAL	3.8
3	D	164	HIS	3.6
2	B	136	LEU	3.6
3	D	158	ALA	3.5
2	B	189	HIS	3.5
2	B	200	GLY	3.4
2	B	147	GLN	3.4
3	D	139	GLY	3.3
3	D	165	THR	3.3
3	D	149	PRO	3.2
2	B	201	LEU	3.1
2	B	159	SER	3.1
2	B	204	PRO	3.1
3	D	161	SER	3.1
2	B	121	SER	3.1
3	D	140	CYS	3.1
3	D	192	GLN	3.0
2	B	155	GLN	3.0
3	D	10	GLY	3.0
2	E	156	SER	3.0
3	D	144	ASP	2.9
2	B	191	VAL	2.9
2	B	184	ALA	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	D	160	THR	2.9
2	B	188	LYS	2.8
2	B	151	ASP	2.8
3	D	194	TYR	2.8
2	B	179	LEU	2.7
2	B	193	ALA	2.7
3	D	207	VAL	2.7
2	B	210	ASN	2.7
3	D	178	LEU	2.6
3	D	205	THR	2.6
2	B	194	CYS	2.6
3	D	206	LYS	2.6
3	D	191	THR	2.6
2	B	113	PRO	2.5
2	B	145	LYS	2.5
2	B	161	GLU	2.5
2	B	157	GLY	2.5
2	B	202	SER	2.5
2	E	157	GLY	2.5
3	D	142	VAL	2.4
2	B	112	ALA	2.4
3	D	181	VAL	2.4
3	D	185	PRO	2.4
3	D	9	GLY	2.4
2	B	190	LYS	2.4
3	D	199	ASN	2.4
3	D	177	SER	2.3
3	D	198	VAL	2.3
2	B	127	SER	2.3
2	B	144	ALA	2.3
2	B	187	GLU	2.3
2	E	148	TRP	2.3
3	D	209	LYS	2.2
3	D	143	LYS	2.2
2	B	116	PHE	2.2
3	D	204	ASN	2.1
3	D	212	GLU	2.0
2	B	167	ASP	2.0
2	B	138	ASN	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.