Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 11:44 AM EDT

PDB ID	:	7JTF
Title	:	Structure of Hepatitis C Virus Envelope Glycoprotein E2 core from genotype 6a bound to broadly neutralizing antibody RM2-01
Authors	:	Tzarum, N.; Wilson, I.A.; Law, M.
Deposited on	:	2020-08-17
Resolution	:	3.35 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

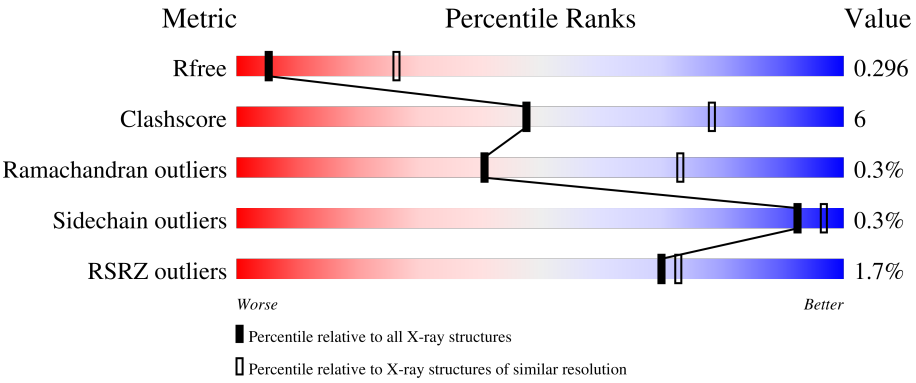
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

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 <=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	229	% 77% 15% 8%
1	C	229	79% 14% 7%
2	B	214	3% 85% 12%
2	D	214	82% 16%
3	E	189	2% 60% 14% 25%

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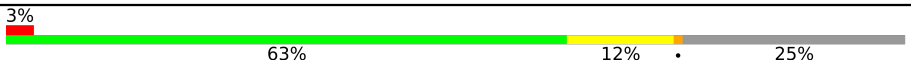
Mol	Chain	Length	Quality of chain
3	F	189	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8617 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 RM2-01 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1583	1010	266	301	6			
1	C	212	Total	C	N	O	S	0	0	0
			1588	1013	267	302	6			

- Molecule 2 is a protein called RM2-01 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	206	Total	C	N	O	S	0	0	0
			1594	1000	267	322	5			
2	D	211	Total	C	N	O	S	0	0	0
			1624	1017	272	330	5			

- Molecule 3 is a protein called Envelope glycoprotein E2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	141	Total	C	N	O	S	0	0	0
			1111	710	190	198	13			
3	F	142	Total	C	N	O	S	0	0	0
			1117	713	191	200	13			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	448	ASP	ASN	engineered mutation	UNP B9V0E2
E	482	GLY	-	linker	UNP B9V0E2
E	483	SER	-	linker	UNP B9V0E2
E	484	SER	-	linker	UNP B9V0E2
E	485	GLY	-	linker	UNP B9V0E2
E	592	GLY	-	linker	UNP B9V0E2
E	593	GLY	-	linker	UNP B9V0E2
E	597	GLY	-	linker	UNP B9V0E2

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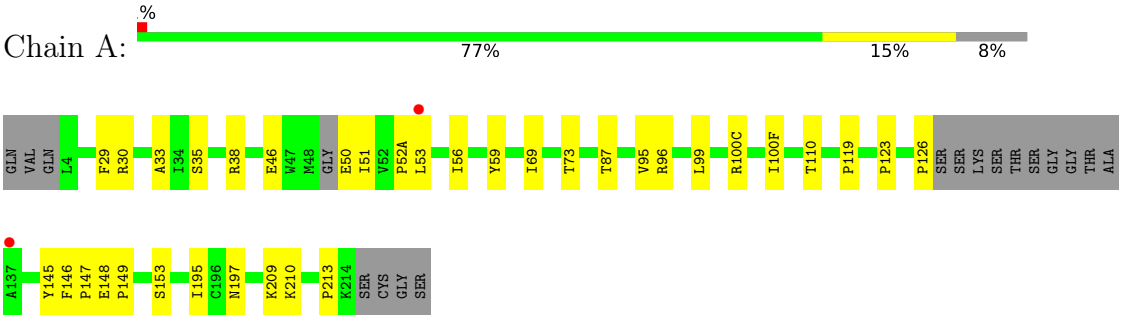
Chain	Residue	Modelled	Actual	Comment	Reference
F	448	ASP	ASN	engineered mutation	UNP B9V0E2
F	482	GLY	-	linker	UNP B9V0E2
F	483	SER	-	linker	UNP B9V0E2
F	484	SER	-	linker	UNP B9V0E2
F	485	GLY	-	linker	UNP B9V0E2
F	592	GLY	-	linker	UNP B9V0E2
F	593	GLY	-	linker	UNP B9V0E2
F	597	GLY	-	linker	UNP B9V0E2

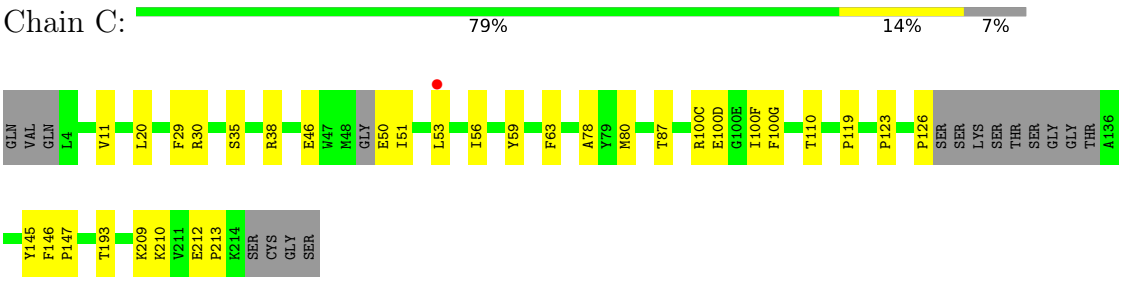
3 Residue-property plots (i)

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.

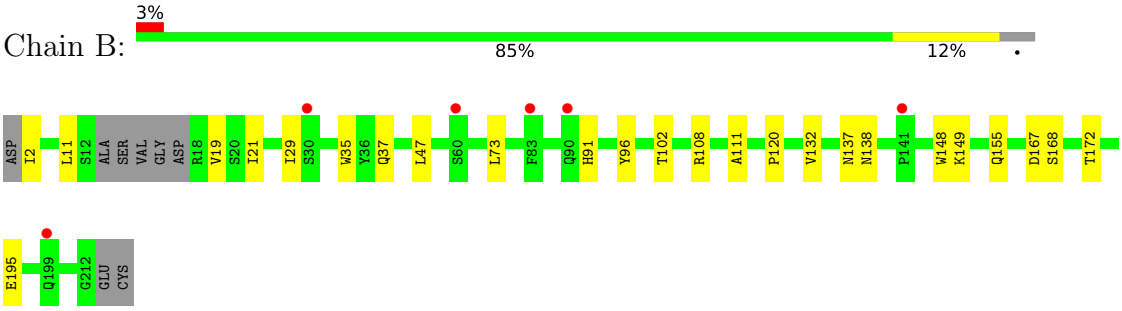
• Molecule 1: RM2-01 Fab heavy chain



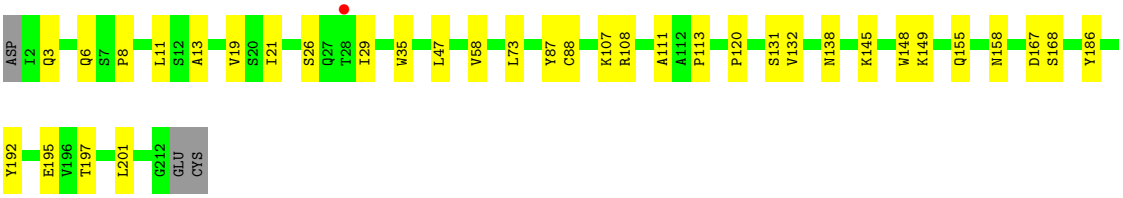
• Molecule 1: RM2-01 Fab heavy chain



• Molecule 2: RM2-01 Fab light chain

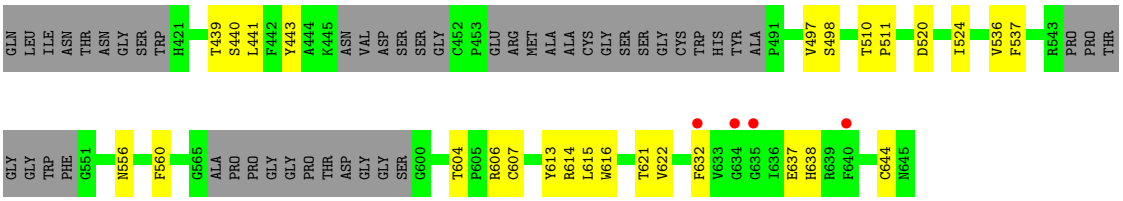


• Molecule 2: RM2-01 Fab light chain



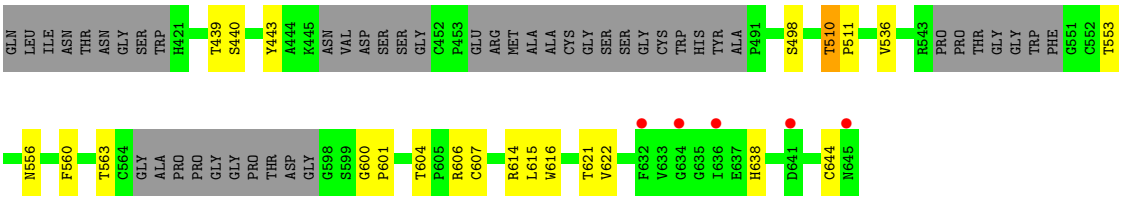
• Molecule 3: Envelope glycoprotein E2

Chain E:



• Molecule 3: Envelope glycoprotein E2

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.73Å 64.89Å 145.21Å 90.00° 105.16° 90.00°	Depositor
Resolution (Å)	29.86 – 3.35 29.86 – 3.35	Depositor EDS
% Data completeness (in resolution range)	91.2 (29.86-3.35) 91.2 (29.86-3.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 3.31Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.242 , 0.296 0.242 , 0.296	Depositor DCC
R_{free} test set	1077 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	101.6	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 58.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8617	wwPDB-VP
Average B, all atoms (Å^2)	117.0	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 34.04 % 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 7.2707e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.24	0/1619	0.44	0/2205
1	C	0.25	0/1624	0.45	0/2212
2	B	0.24	0/1629	0.43	0/2211
2	D	0.25	0/1660	0.43	0/2255
3	E	0.24	0/1143	0.44	0/1556
3	F	0.24	0/1149	0.42	0/1564
All	All	0.24	0/8824	0.44	0/12003

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

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	1583	0	1578	23	0
1	C	1588	0	1583	20	0
2	B	1594	0	1551	14	0
2	D	1624	0	1578	20	0
3	E	1111	0	1056	17	0
3	F	1117	0	1061	14	0
All	All	8617	0	8407	104	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 6.

All (104) 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:C:30:ARG:HG2	1:C:53:LEU:HD21	1.59	0.83
1:A:30:ARG:HG2	1:A:53:LEU:HD21	1.60	0.83
2:D:108:ARG:HH12	2:D:111:ALA:HB2	1.51	0.75
3:E:604:THR:HG22	3:E:606:ARG:H	1.55	0.71
2:B:137:ASN:OD1	2:B:138:ASN:ND2	2.26	0.69
1:C:38:ARG:HB3	1:C:46:GLU:HB3	1.77	0.66
1:A:100(C):ARG:HB2	1:A:100(F):ILE:HD11	1.80	0.63
1:C:100(C):ARG:HB2	1:C:100(F):ILE:HD11	1.79	0.63
1:A:29:PHE:HD2	1:A:53:LEU:HD23	1.66	0.60
3:F:604:THR:HG22	3:F:606:ARG:H	1.67	0.59
1:C:29:PHE:HD2	1:C:53:LEU:HD23	1.65	0.59
1:C:35:SER:HB2	1:C:51:ILE:HG22	1.86	0.58
3:F:614:ARG:NH1	3:F:621:THR:O	2.35	0.57
2:D:47:LEU:HA	2:D:58:VAL:HG21	1.86	0.57
2:D:113:PRO:HD2	2:D:201:LEU:HG	1.86	0.57
2:D:145:LYS:HB3	2:D:197:THR:HB	1.86	0.57
1:A:50:GLU:HB3	1:A:51:ILE:HG23	1.87	0.56
1:A:87:THR:HG23	1:A:110:THR:HA	1.86	0.56
3:E:498:SER:HA	3:E:536:VAL:HG12	1.88	0.56
1:C:126:PRO:HG2	1:C:213:PRO:HB3	1.87	0.55
3:F:556:ASN:OD1	3:F:560:PHE:N	2.36	0.55
1:A:35:SER:HB2	1:A:51:ILE:HG22	1.89	0.54
1:C:210:LYS:NZ	1:C:212:GLU:OE2	2.28	0.54
1:C:87:THR:HG23	1:C:110:THR:HA	1.90	0.54
3:F:553:THR:HG22	3:F:563:THR:HG22	1.91	0.53
1:A:126:PRO:HG2	1:A:213:PRO:HB3	1.91	0.52
2:B:11:LEU:HD11	2:B:19:VAL:HG21	1.90	0.52
1:C:29:PHE:HZ	1:C:78:ALA:HB2	1.74	0.52
1:A:38:ARG:HB3	1:A:46:GLU:HB3	1.92	0.52
3:F:511:PRO:HB2	3:F:638:HIS:CG	2.46	0.51
2:B:167:ASP:OD1	2:B:168:SER:N	2.43	0.51
1:C:123:PRO:HD3	1:C:209:LYS:HE2	1.91	0.51
3:E:604:THR:HB	3:E:607:CYS:HB2	1.94	0.50
3:E:614:ARG:NH1	3:E:621:THR:O	2.39	0.50
1:C:30:ARG:HA	1:C:53:LEU:HG	1.93	0.50
2:D:13:ALA:HA	2:D:107:LYS:HE3	1.92	0.50
1:A:59:TYR:HE1	1:A:69:ILE:HG13	1.76	0.50
1:A:195:ILE:HG12	1:A:210:LYS:HA	1.92	0.50
2:D:167:ASP:OD1	2:D:168:SER:N	2.44	0.50
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:11:LEU:HD22	2:B:21:ILE:HD11	1.93	0.49
2:D:35:TRP:CE2	2:D:73:LEU:HB2	2.48	0.49
2:D:120:PRO:HD3	2:D:132:VAL:HG22	1.94	0.49
3:F:615:LEU:HD22	3:F:622:VAL:HG22	1.95	0.49
2:B:138:ASN:OD1	2:B:172:THR:OG1	2.23	0.49
3:E:615:LEU:HD22	3:E:622:VAL:HG22	1.95	0.49
2:B:21:ILE:HD12	2:B:102:THR:HG21	1.93	0.48
2:B:108:ARG:HH12	2:B:111:ALA:HB2	1.79	0.48
2:D:108:ARG:NH1	2:D:111:ALA:HB2	2.26	0.48
2:D:149:LYS:NZ	2:D:195:GLU:HB2	2.27	0.48
2:B:120:PRO:HD3	2:B:132:VAL:HG22	1.95	0.48
1:A:153:SER:O	1:A:197:ASN:N	2.39	0.47
3:E:556:ASN:OD1	3:E:560:PHE:N	2.44	0.47
1:C:20:LEU:HB2	1:C:80:MET:HB3	1.95	0.47
1:C:38:ARG:HH21	1:C:63:PHE:HZ	1.62	0.47
1:C:119:PRO:HB3	1:C:145:TYR:HB3	1.97	0.46
3:E:607:CYS:HA	3:E:644:CYS:HA	1.96	0.46
2:D:186:TYR:O	2:D:192:TYR:OH	2.34	0.46
3:F:607:CYS:HA	3:F:644:CYS:HA	1.98	0.45
1:A:148:GLU:HG3	1:A:149:PRO:HA	1.98	0.45
3:F:498:SER:HA	3:F:536:VAL:HG12	1.98	0.45
1:C:193:THR:HG23	1:C:210:LYS:HE2	1.98	0.45
3:F:510:THR:HB	3:F:511:PRO:HD2	1.99	0.45
3:F:556:ASN:HD21	3:F:560:PHE:HD2	1.65	0.45
2:D:11:LEU:HD21	2:D:19:VAL:HB	1.99	0.45
1:A:119:PRO:HB3	1:A:145:TYR:HB3	1.98	0.44
3:E:556:ASN:HD21	3:E:560:PHE:HD2	1.64	0.44
1:C:56:ILE:HG23	3:F:439:THR:HG22	1.99	0.44
1:A:33:ALA:HB3	1:A:95:VAL:HG13	2.00	0.44
3:F:604:THR:HB	3:F:607:CYS:HB2	1.98	0.44
1:C:50:GLU:N	1:C:59:TYR:HA	2.33	0.44
1:C:35:SER:HB3	1:C:100(G):PHE:HE2	1.82	0.44
2:D:29:ILE:HD12	2:D:29:ILE:HA	1.90	0.43
1:A:99:LEU:HD12	3:E:441:LEU:HD21	2.01	0.43
2:D:148:TRP:HB2	2:D:155:GLN:HB2	2.01	0.43
2:B:2:ILE:HD11	2:B:29:ILE:HD11	2.01	0.43
2:D:158:ASN:OD1	2:D:158:ASN:N	2.50	0.43
3:F:440:SER:HG	3:F:616:TRP:HD1	1.66	0.43
1:A:96:ARG:HB2	1:A:100(F):ILE:H	1.84	0.42
1:A:123:PRO:HD3	1:A:209:LYS:HE2	2.01	0.42
3:E:440:SER:HG	3:E:616:TRP:HD1	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ARG:HG2	1:A:53:LEU:CD2	2.39	0.42
1:A:56:ILE:HG23	3:E:439:THR:HG22	2.02	0.42
2:B:91:HIS:HA	2:B:96:TYR:HD1	1.84	0.42
3:E:511:PRO:HB2	3:E:638:HIS:CG	2.54	0.42
2:D:120:PRO:HB3	2:D:131:SER:H	1.83	0.42
2:B:149:LYS:NZ	2:B:195:GLU:OE1	2.49	0.42
2:D:6:GLN:HE22	2:D:87:TYR:HA	1.84	0.42
2:D:3:GLN:HG2	2:D:26:SER:HB3	2.01	0.42
3:E:510:THR:HB	3:E:511:PRO:HD2	2.02	0.41
3:E:520:ASP:OD1	3:E:524:ILE:N	2.52	0.41
1:C:146:PHE:HA	1:C:147:PRO:HA	1.83	0.41
2:B:35:TRP:CE2	2:B:73:LEU:HB2	2.55	0.41
1:C:11:VAL:HG22	1:C:110:THR:HB	2.02	0.41
3:F:600:GLY:HA3	3:F:601:PRO:HD3	1.85	0.41
1:A:29:PHE:CD2	1:A:53:LEU:HD23	2.53	0.41
1:A:99:LEU:HA	3:E:613:TYR:OH	2.21	0.41
1:A:146:PHE:HA	1:A:147:PRO:HA	1.84	0.41
1:A:53:LEU:HD22	1:A:73:THR:CB	2.51	0.41
2:B:148:TRP:HB2	2:B:155:GLN:HB2	2.02	0.41
2:D:35:TRP:CZ3	2:D:88:CYS:HB3	2.56	0.40
3:E:497:VAL:HG23	3:E:537:PHE:HB2	2.03	0.40
3:E:632:PHE:CE2	3:E:637:GLU:HB2	2.56	0.40
2:D:8:PRO:HG2	2:D:21:ILE:HG23	2.03	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	205/229 (90%)	186 (91%)	19 (9%)	0	100 100
1	C	206/229 (90%)	193 (94%)	12 (6%)	1 (0%)	29 63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	202/214 (94%)	188 (93%)	14 (7%)	0	100 100
2	D	209/214 (98%)	199 (95%)	9 (4%)	1 (0%)	29 63
3	E	131/189 (69%)	121 (92%)	10 (8%)	0	100 100
3	F	132/189 (70%)	123 (93%)	8 (6%)	1 (1%)	19 53
All	All	1085/1264 (86%)	1010 (93%)	72 (7%)	3 (0%)	41 73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	100(D)	GLU
2	D	138	ASN
3	F	510	THR

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	A	175/188 (93%)	174 (99%)	1 (1%)	86 93
1	C	175/188 (93%)	175 (100%)	0	100 100
2	B	184/190 (97%)	184 (100%)	0	100 100
2	D	187/190 (98%)	187 (100%)	0	100 100
3	E	125/159 (79%)	124 (99%)	1 (1%)	81 91
3	F	126/159 (79%)	125 (99%)	1 (1%)	81 91
All	All	972/1074 (90%)	969 (100%)	3 (0%)	92 97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52(A)	PRO
3	E	443	TYR
3	F	443	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	211/229 (92%)	-0.02	2 (0%)	84	87	71, 112, 154, 184	0
1	C	212/229 (92%)	-0.04	1 (0%)	91	93	48, 97, 150, 168	0
2	B	206/214 (96%)	0.11	6 (2%)	51	54	80, 133, 183, 204	0
2	D	211/214 (98%)	-0.15	1 (0%)	91	93	58, 92, 133, 163	0
3	E	141/189 (74%)	0.15	4 (2%)	53	55	73, 128, 180, 204	0
3	F	142/189 (75%)	0.32	5 (3%)	44	46	69, 140, 193, 273	0
All	All	1123/1264 (88%)	0.04	19 (1%)	70	73	48, 114, 174, 273	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	199	GLN	4.6
3	F	645	ASN	4.4
3	E	634	GLY	4.4
3	F	632	PHE	4.3
2	D	28	THR	3.6
2	B	83	PHE	3.1
1	C	53	LEU	2.9
3	E	635	GLY	2.8
1	A	137	ALA	2.5
2	B	30	SER	2.5
3	F	636	ILE	2.4
2	B	90	GLN	2.4
2	B	60	SER	2.4
3	E	640	PHE	2.3
3	F	634	GLY	2.3
2	B	141	PRO	2.3
3	E	632	PHE	2.2
1	A	53	LEU	2.1
3	F	641	ASP	2.1

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.