Full wwPDB X-ray Structure Validation Report ⓘ

Nov 27, 2020 – 10:48 am GMT

PDB ID	:	6S8C
Title	:	Post-fusion conformation of the envelope protein of tick-borne encephalitis virus with longer stem
Authors	:	Vaney, M.C.; Rouvinski, A.; Rey, F.A.
Deposited on	:	2019-07-09
Resolution	:	2.57 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:

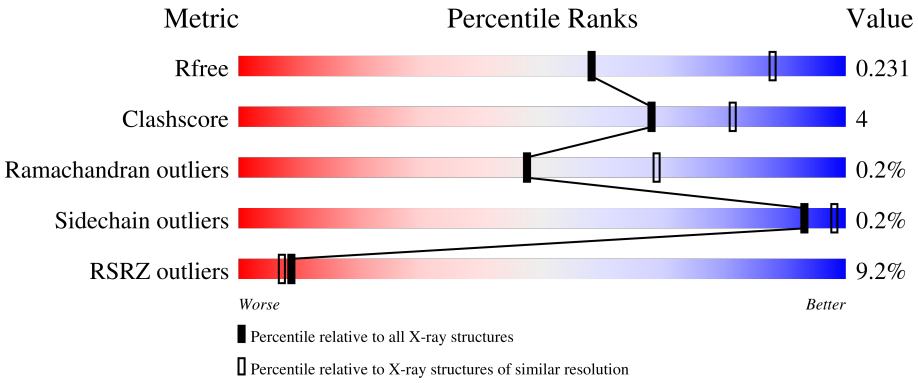
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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 2.57 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	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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 <=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	453	7% 68% 5% 27%
1	B	453	5% 72% 5% 23%
1	C	453	8% 68% 7% 25%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7833 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 Genome polyprotein,Genome polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2524	1595	439	474	16			
1	B	349	Total	C	N	O	S	0	0	1
			2643	1667	460	499	17			
1	C	339	Total	C	N	O	S	0	0	2
			2588	1634	449	488	17			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	101	HIS	TRP	engineered mutation	UNP P14336
A	405	GLY	-	linker	UNP P14336
A	406	GLY	-	linker	UNP P14336
A	407	GLY	-	linker	UNP P14336
A	408	SER	-	linker	UNP P14336
A	409	GLY	-	linker	UNP P14336
A	410	GLY	-	linker	UNP P14336
A	411	GLY	-	linker	UNP P14336
A	412	SER	-	linker	UNP P14336
A	435	GLY	-	expression tag	UNP P14336
A	436	PRO	-	expression tag	UNP P14336
A	437	PHE	-	expression tag	UNP P14336
A	438	GLU	-	expression tag	UNP P14336
A	439	ASP	-	expression tag	UNP P14336
A	440	ASP	-	expression tag	UNP P14336
A	441	ASP	-	expression tag	UNP P14336
A	442	ASP	-	expression tag	UNP P14336
A	443	LYS	-	expression tag	UNP P14336
A	444	ALA	-	expression tag	UNP P14336
A	445	GLY	-	expression tag	UNP P14336
A	446	TRP	-	expression tag	UNP P14336
A	447	SER	-	expression tag	UNP P14336
A	448	HIS	-	expression tag	UNP P14336

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Chain	Residue	Modelled	Actual	Comment	Reference
A	449	PRO	-	expression tag	UNP P14336
A	450	GLN	-	expression tag	UNP P14336
A	451	PHE	-	expression tag	UNP P14336
A	452	GLU	-	expression tag	UNP P14336
A	453	LYS	-	expression tag	UNP P14336
B	101	HIS	TRP	engineered mutation	UNP P14336
B	405	GLY	-	linker	UNP P14336
B	406	GLY	-	linker	UNP P14336
B	407	GLY	-	linker	UNP P14336
B	408	SER	-	linker	UNP P14336
B	409	GLY	-	linker	UNP P14336
B	410	GLY	-	linker	UNP P14336
B	411	GLY	-	linker	UNP P14336
B	412	SER	-	linker	UNP P14336
B	435	GLY	-	expression tag	UNP P14336
B	436	PRO	-	expression tag	UNP P14336
B	437	PHE	-	expression tag	UNP P14336
B	438	GLU	-	expression tag	UNP P14336
B	439	ASP	-	expression tag	UNP P14336
B	440	ASP	-	expression tag	UNP P14336
B	441	ASP	-	expression tag	UNP P14336
B	442	ASP	-	expression tag	UNP P14336
B	443	LYS	-	expression tag	UNP P14336
B	444	ALA	-	expression tag	UNP P14336
B	445	GLY	-	expression tag	UNP P14336
B	446	TRP	-	expression tag	UNP P14336
B	447	SER	-	expression tag	UNP P14336
B	448	HIS	-	expression tag	UNP P14336
B	449	PRO	-	expression tag	UNP P14336
B	450	GLN	-	expression tag	UNP P14336
B	451	PHE	-	expression tag	UNP P14336
B	452	GLU	-	expression tag	UNP P14336
B	453	LYS	-	expression tag	UNP P14336
C	101	HIS	TRP	engineered mutation	UNP P14336
C	405	GLY	-	linker	UNP P14336
C	406	GLY	-	linker	UNP P14336
C	407	GLY	-	linker	UNP P14336
C	408	SER	-	linker	UNP P14336
C	409	GLY	-	linker	UNP P14336
C	410	GLY	-	linker	UNP P14336
C	411	GLY	-	linker	UNP P14336
C	412	SER	-	linker	UNP P14336

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Chain	Residue	Modelled	Actual	Comment	Reference
C	435	GLY	-	expression tag	UNP P14336
C	436	PRO	-	expression tag	UNP P14336
C	437	PHE	-	expression tag	UNP P14336
C	438	GLU	-	expression tag	UNP P14336
C	439	ASP	-	expression tag	UNP P14336
C	440	ASP	-	expression tag	UNP P14336
C	441	ASP	-	expression tag	UNP P14336
C	442	ASP	-	expression tag	UNP P14336
C	443	LYS	-	expression tag	UNP P14336
C	444	ALA	-	expression tag	UNP P14336
C	445	GLY	-	expression tag	UNP P14336
C	446	TRP	-	expression tag	UNP P14336
C	447	SER	-	expression tag	UNP P14336
C	448	HIS	-	expression tag	UNP P14336
C	449	PRO	-	expression tag	UNP P14336
C	450	GLN	-	expression tag	UNP P14336
C	451	PHE	-	expression tag	UNP P14336
C	452	GLU	-	expression tag	UNP P14336
C	453	LYS	-	expression tag	UNP P14336

- Molecule 2 is water.

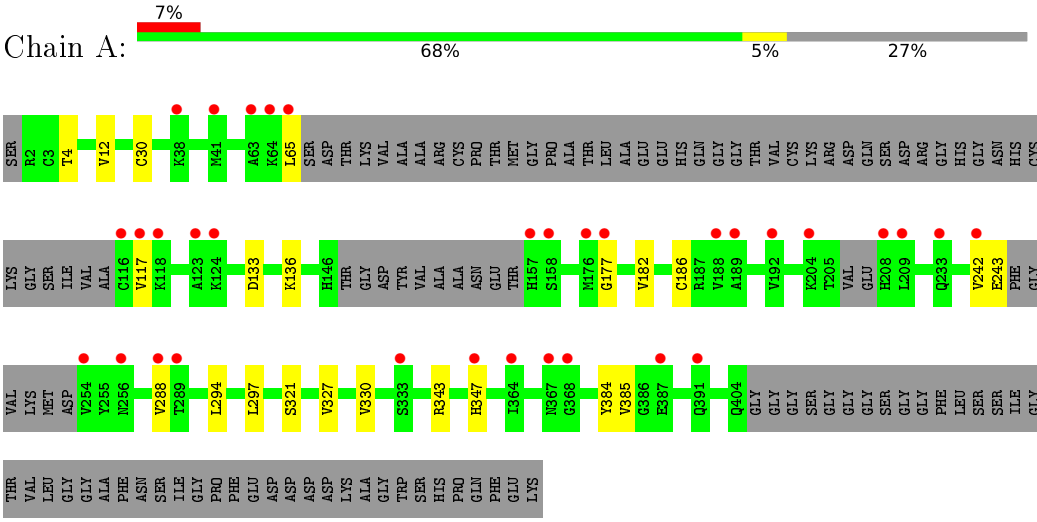
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	29	Total O 29 29	0	0
2	B	32	Total O 32 32	0	0
2	C	17	Total O 17 17	0	0

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.

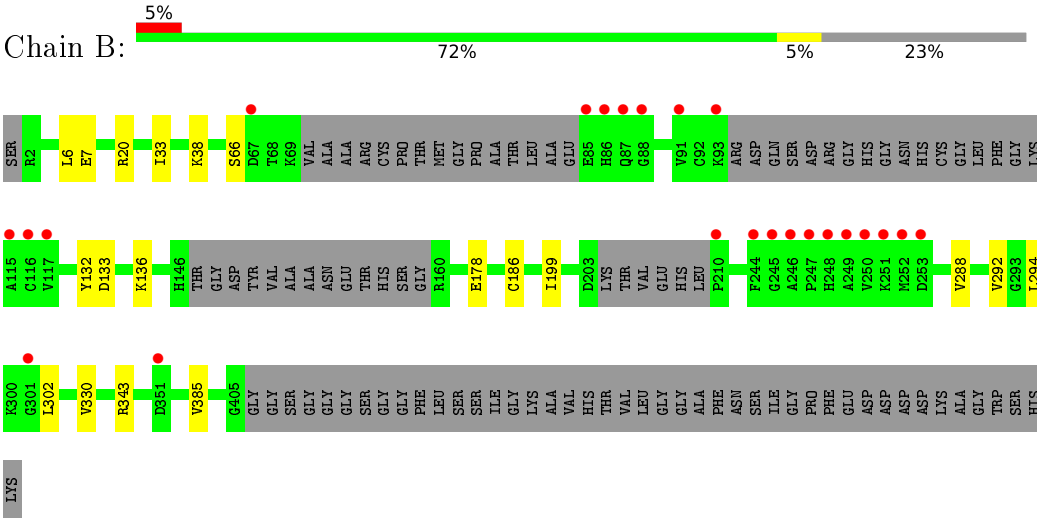
- Molecule 1: Genome polyprotein,Genome polyprotein

Chain A:



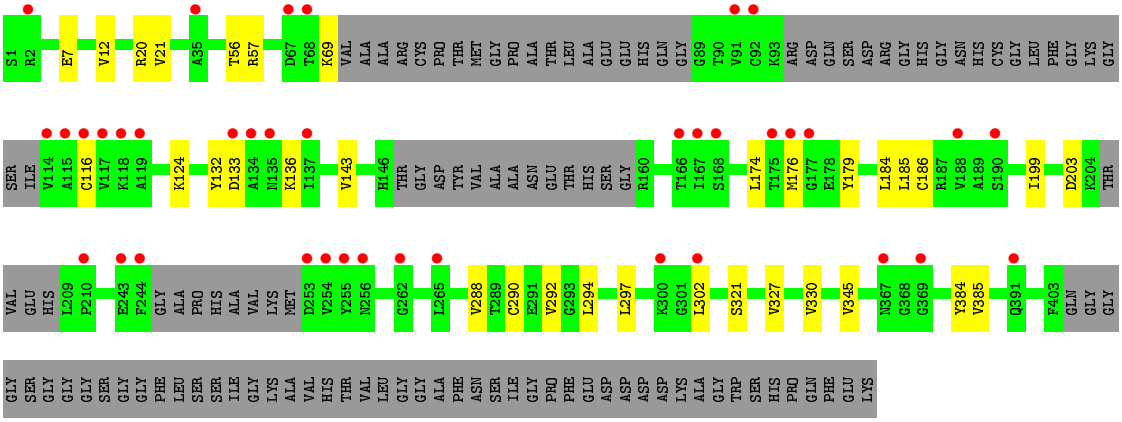
- Molecule 1: Genome polyprotein,Genome polyprotein

Chain B:



- Molecule 1: Genome polyprotein,Genome polyprotein

Chain C:


S1 R2 E7 V12 R20 V21 A35 T56 R57 D67 T68 K69 VAL ALA ALA ARG CYS PRO THR MET GLY PRO ALA THR LEU ALA GLU GLU HIS GLN GLY G89 T90 V91 C92 K93 ARG ASP GLN SER ASP ARG GLY HIS GLY ASN HIS CYS GLY LEU PHE GLY LYS GLY
SER ILE V114 A115 C116 V117 K118 A119 K124 Y132 D133 A134 N135 K136 I137 V143 H146 THR GLY ASP TYR VAL ALA ALA ASN GLU THR HIS SER GLY R160 T166 I167 S168 L174 T175 M176 G177 E178 Y179 L184 L185 C186 R187 V188 A189 S190 I199 D203 K204 THR
VAL GLU HIS L209 P210 E243 F244 GLY ALA PRO HIS ALA VAL LYS MET D253 V254 Y255 N256 G262 L265 V288 T289 C290 E291 V292 G293 L294 L297 K300 G301 L302 S321 V327 V330 V345 N367 G368 G369 Y384 V385 Q391 F403 GLN GLY GLY
GLY SER GLY GLY GLY SER GLY GLY PHE LEU SER SER ILE GLY LYS ALA VAL HIS THR VAL LEU GLY GLY ALA PHE ASN SER ILE GLY PRO PHE GLU ASP ASP ASP LYS ALA GLY TRP SER HIS PRO GLN PHE GLU LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	169.44Å 169.44Å 123.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.91 – 2.57 47.26 – 2.57	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.91-2.57) 99.6 (47.26-2.57)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 2.58Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.182 , 0.217 0.197 , 0.231	Depositor DCC
R_{free} test set	2028 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	54.7	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 45.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7833	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% of the height of the origin peak. No significant pseudotranslation is detected.*

[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	0.49	0/2575	0.73	0/3497
1	B	0.49	0/2696	0.70	0/3659
1	C	0.50	0/2638	0.71	0/3577
All	All	0.50	0/7909	0.71	0/10733

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	2524	0	2477	13	0
1	B	2643	0	2587	22	0
1	C	2588	0	2562	26	0
2	A	29	0	0	0	0
2	B	32	0	0	0	0
2	C	17	0	0	0	0
All	All	7833	0	7626	58	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 4.

All (58) 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:B:294:LEU:HD23	1:B:297:LEU:HD21	1.47	0.95
1:C:294:LEU:HD23	1:C:297:LEU:HD21	1.56	0.87
1:C:292:VAL:HG12	1:C:294:LEU:CD1	2.15	0.75
1:B:297:LEU:HD13	1:B:299:MET:HE2	1.72	0.71
1:A:186:CYS:HB3	1:A:288:VAL:HG22	1.75	0.69
1:B:186:CYS:HB3	1:B:288:VAL:HG22	1.75	0.69
1:C:186:CYS:HB3	1:C:288:VAL:HG22	1.75	0.67
1:B:297:LEU:CD1	1:B:299:MET:HE2	2.25	0.67
1:B:297:LEU:CD1	1:B:299:MET:CE	2.74	0.66
1:A:186:CYS:HB3	1:A:288:VAL:CG2	2.26	0.65
1:B:186:CYS:HB3	1:B:288:VAL:CG2	2.27	0.64
1:B:297:LEU:HD11	1:B:299:MET:HE3	1.78	0.64
1:C:186:CYS:HB3	1:C:288:VAL:CG2	2.27	0.63
1:B:297:LEU:HD11	1:B:299:MET:CE	2.30	0.62
1:A:65:LEU:HD21	1:A:117:VAL:HB	1.82	0.60
1:B:294:LEU:HD23	1:B:297:LEU:CD2	2.28	0.58
1:C:124:LYS:HD3	1:C:203:ASP:HB3	1.88	0.56
1:B:292:VAL:HG12	1:B:294:LEU:CD1	2.37	0.55
1:A:321:SER:HB3	1:A:327:VAL:HG13	1.88	0.54
1:A:12:VAL:HG21	1:C:20:ARG:HB2	1.92	0.52
1:C:176:MET:HB3	1:C:179:TYR:HB2	1.92	0.51
1:B:38:LYS:HD2	1:B:178:GLU:HB3	1.92	0.51
1:C:56:THR:HG23	1:C:57:ARG:N	2.26	0.50
1:C:294:LEU:HD23	1:C:297:LEU:CD2	2.37	0.50
1:B:294:LEU:CD2	1:B:297:LEU:HD21	2.32	0.50
1:C:7:GLU:HA	1:C:302:LEU:O	2.13	0.49
1:C:321:SER:HB3	1:C:327:VAL:HG13	1.95	0.49
1:A:182:VAL:HG22	1:A:294:LEU:HD23	1.94	0.48
1:B:20:ARG:HG3	1:C:12:VAL:HG21	1.95	0.48
1:A:343:ARG:HG2	1:A:384:TYR:HB2	1.94	0.48
1:C:185:LEU:O	1:C:290:CYS:HA	2.12	0.48
1:B:7:GLU:HA	1:B:302:LEU:O	2.14	0.47
1:C:56:THR:HG23	1:C:57:ARG:H	1.80	0.47
1:C:143:VAL:HG11	1:C:176:MET:SD	2.56	0.46
1:B:38:LYS:NZ	1:B:178:GLU:O	2.27	0.45
1:A:294:LEU:HB3	1:A:297:LEU:HD21	1.99	0.45
1:B:330:VAL:HG11	1:B:385:VAL:HG11	1.99	0.45
1:C:174:LEU:HD12	1:C:184:LEU:HD12	1.98	0.44
1:A:4:THR:HG22	1:A:30:CYS:O	2.17	0.44
1:C:345:VAL:HG22	1:C:384:TYR:HE2	1.82	0.44
1:B:132:TYR:CE2	1:B:199:ILE:HD11	2.53	0.44
1:B:297:LEU:HD13	1:B:299:MET:CE	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:VAL:HG11	1:A:385:VAL:HG11	2.01	0.43
1:B:294:LEU:HB3	1:B:297:LEU:HD21	2.00	0.43
1:C:69:LYS:HE3	1:C:116:CYS:HB2	2.01	0.42
1:B:6:LEU:HD22	1:B:33:ILE:HG22	2.01	0.42
1:C:330:VAL:HG11	1:C:385:VAL:HG11	2.02	0.42
1:C:132:TYR:CE2	1:C:199:ILE:HD11	2.54	0.42
1:C:133:ASP:HB3	1:C:136:LYS:HB2	2.01	0.42
1:A:242:VAL:CG1	1:A:243:GLU:N	2.82	0.42
1:B:133:ASP:HB3	1:B:136:LYS:HB2	2.02	0.42
1:C:294:LEU:HB3	1:C:297:LEU:HD21	2.02	0.41
1:B:20:ARG:HG3	1:C:12:VAL:CG2	2.50	0.41
1:C:292:VAL:HG12	1:C:294:LEU:HD12	2.01	0.41
1:A:182:VAL:HG22	1:A:294:LEU:CD2	2.50	0.41
1:A:133:ASP:HB3	1:A:136:LYS:HB2	2.02	0.41
1:C:292:VAL:CG1	1:C:294:LEU:CD1	2.95	0.41
1:C:21:VAL:HB	1:C:292:VAL:HB	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	321/453 (71%)	305 (95%)	15 (5%)	1 (0%)	41 62
1	B	339/453 (75%)	323 (95%)	15 (4%)	1 (0%)	41 62
1	C	327/453 (72%)	314 (96%)	13 (4%)	0	100 100
All	All	987/1359 (73%)	942 (95%)	43 (4%)	2 (0%)	47 69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	GLY

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Mol	Chain	Res	Type
1	B	66	SER

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	271/367 (74%)	270 (100%)	1 (0%)	91 97
1	B	282/367 (77%)	281 (100%)	1 (0%)	91 97
1	C	282/367 (77%)	282 (100%)	0	100 100
All	All	835/1101 (76%)	833 (100%)	2 (0%)	93 98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	347	HIS
1	B	343	ARG

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	214	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

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	331/453 (73%)	0.55	33 (9%) 7 5	33, 63, 100, 115	0
1	B	349/453 (77%)	0.17	23 (6%) 18 15	35, 58, 100, 125	0
1	C	339/453 (74%)	0.50	38 (11%) 5 4	36, 60, 105, 127	0
All	All	1019/1359 (74%)	0.40	94 (9%) 9 7	33, 60, 101, 127	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	248	HIS	9.2
1	A	176	MET	7.7
1	B	252	MET	6.8
1	B	250	VAL	6.7
1	C	91	VAL	6.6
1	B	249	ALA	6.6
1	C	176	MET	6.5
1	B	116	CYS	6.2
1	A	158	SER	5.7
1	A	116	CYS	5.4
1	B	86	HIS	5.3
1	B	246	ALA	5.1
1	B	251	LYS	5.1
1	B	247	PRO	5.0
1	C	254	VAL	4.9
1	C	210	PRO	4.9
1	B	210	PRO	4.8
1	B	115	ALA	4.8
1	C	244	PHE	4.6
1	A	157	HIS	4.4
1	A	117	VAL	4.0
1	C	255	TYR	3.9
1	C	115	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	253	ASP	3.8
1	B	253	ASP	3.8
1	A	209	LEU	3.7
1	C	67	ASP	3.7
1	A	208	HIS	3.7
1	A	347	HIS	3.5
1	B	244	PHE	3.5
1	C	177	GLY	3.5
1	C	68	THR	3.5
1	B	91	VAL	3.4
1	A	254	VAL	3.3
1	C	256	ASN	3.3
1	C	243	GLU	3.1
1	A	177	GLY	3.1
1	A	65	LEU	3.0
1	A	188	VAL	3.0
1	C	265	LEU	3.0
1	A	368	GLY	3.0
1	A	204	LYS	2.9
1	A	242	VAL	2.9
1	A	64	LYS	2.8
1	C	188	VAL	2.8
1	C	92	CYS	2.7
1	C	367	ASN	2.7
1	C	134	ALA	2.7
1	C	2	ARG	2.6
1	C	116	CYS	2.6
1	A	256	ASN	2.6
1	A	367	ASN	2.6
1	C	114	VAL	2.6
1	B	88	GLY	2.6
1	C	118	LYS	2.5
1	A	63	ALA	2.5
1	B	245	GLY	2.5
1	C	35	ALA	2.4
1	A	364	ILE	2.4
1	B	85	GLU	2.4
1	A	233	GLN	2.4
1	A	289	THR	2.4
1	C	391	GLN	2.4
1	A	38	LYS	2.3
1	C	175	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	117	VAL	2.3
1	C	137	ILE	2.3
1	A	124	LYS	2.3
1	C	133	ASP	2.3
1	C	135	ASN	2.3
1	A	189	ALA	2.3
1	A	41	MET	2.3
1	C	262	GLY	2.3
1	C	166	THR	2.3
1	A	192	VAL	2.2
1	B	301	GLY	2.2
1	C	168	SER	2.2
1	C	300	LYS	2.2
1	A	387	GLU	2.2
1	C	302	LEU	2.2
1	A	123	ALA	2.2
1	A	118	LYS	2.1
1	B	67	ASP	2.1
1	C	117	VAL	2.1
1	A	391	GLN	2.1
1	B	93	LYS	2.1
1	A	333	SER	2.1
1	C	167	ILE	2.1
1	B	351	ASP	2.1
1	C	119	ALA	2.0
1	A	288	VAL	2.0
1	C	190	SER	2.0
1	C	369	GLY	2.0
1	B	87	GLN	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.