



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:26 PM GMT

PDB ID : 4RQP
Title : Crystal structure of the naturally occurring empty particle of a clinical C4 strain EV71
Authors : Chen, R.; Lyu, K.
Deposited on : 2014-11-04
Resolution : 3.15 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

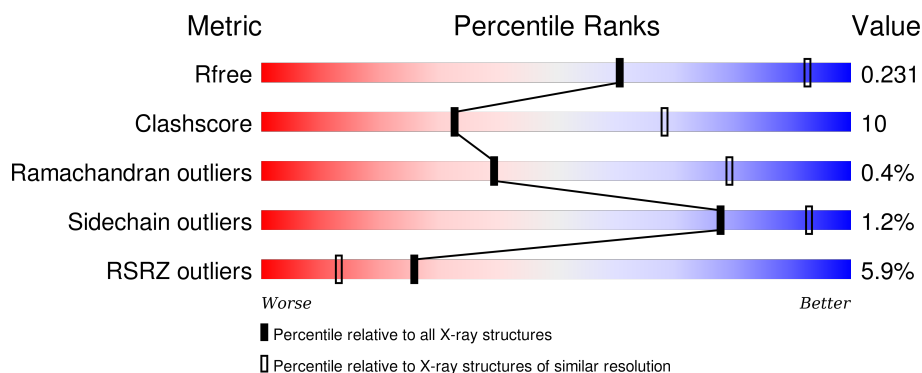
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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}	91344	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)

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. 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	297	<div> <div>3%</div> <div> <div></div> <div>55%</div> <div>19%</div> <div>•</div> <div>25%</div> </div> </div>
1	E	297	<div> <div>4%</div> <div> <div></div> <div>57%</div> <div>18%</div> <div>•</div> <div>25%</div> </div> </div>
1	I	297	<div> <div>4%</div> <div> <div></div> <div>57%</div> <div>18%</div> <div>•</div> <div>25%</div> </div> </div>
1	M	297	<div> <div>4%</div> <div> <div></div> <div>56%</div> <div>18%</div> <div>•</div> <div>25%</div> </div> </div>
1	Q	297	<div> <div>4%</div> <div> <div></div> <div>57%</div> <div>16%</div> <div>•</div> <div>25%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	B	242	
2	F	242	
2	J	242	
2	N	242	
2	R	242	
3	C	323	
3	G	323	
3	K	323	
3	O	323	
3	S	323	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26615 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 Capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	223	Total	C	N	O	S	0	0	0
			1764	1130	296	327	11			
1	Q	223	Total	C	N	O	S	0	0	0
			1764	1130	296	327	11			
1	I	223	Total	C	N	O	S	0	0	0
			1764	1130	296	327	11			
1	M	223	Total	C	N	O	S	0	0	0
			1764	1130	296	327	11			
1	A	223	Total	C	N	O	S	0	0	0
			1764	1130	296	327	11			

- Molecule 2 is a protein called Capsid protein VP3.

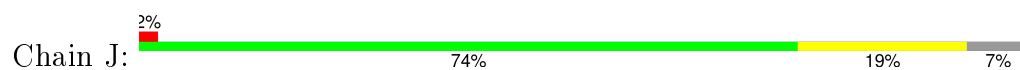
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	225	Total	C	N	O	S	0	0	0
			1718	1106	281	320	11			
2	R	225	Total	C	N	O	S	0	0	0
			1718	1106	281	320	11			
2	J	225	Total	C	N	O	S	0	0	0
			1718	1106	281	320	11			
2	N	225	Total	C	N	O	S	0	0	0
			1718	1106	281	320	11			
2	B	225	Total	C	N	O	S	0	0	0
			1718	1106	281	320	11			

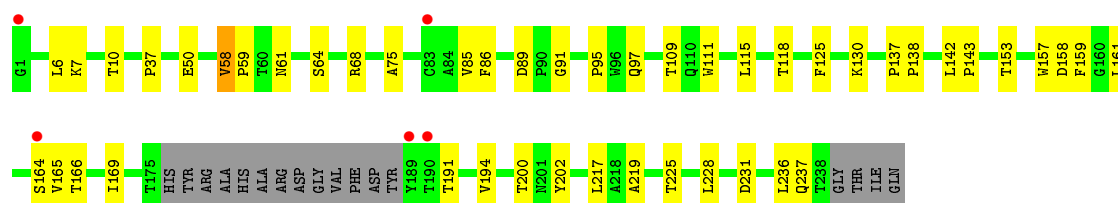
There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	227	GLN	LYS	engineered mutation	UNP F6KTB0
R	227	GLN	LYS	engineered mutation	UNP F6KTB0
J	227	GLN	LYS	engineered mutation	UNP F6KTB0
N	227	GLN	LYS	engineered mutation	UNP F6KTB0
B	227	GLN	LYS	engineered mutation	UNP F6KTB0

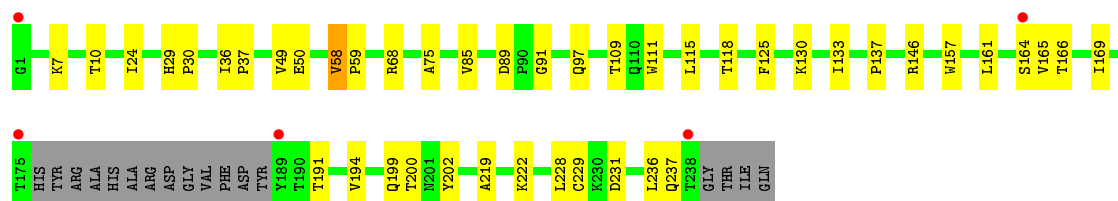
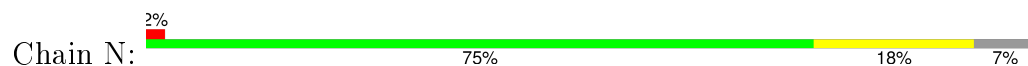
- Molecule 3 is a protein called Capsid protein VP0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	238	Total	C	N	O	S	0	0	0
			1841	1183	303	347	8			
3	S	238	Total	C	N	O	S	0	0	0
			1841	1183	303	347	8			
3	K	238	Total	C	N	O	S	0	0	0
			1841	1183	303	347	8			
3	O	238	Total	C	N	O	S	0	0	0
			1841	1183	303	347	8			
3	C	238	Total	C	N	O	S	0	0	0
			1841	1183	303	347	8			

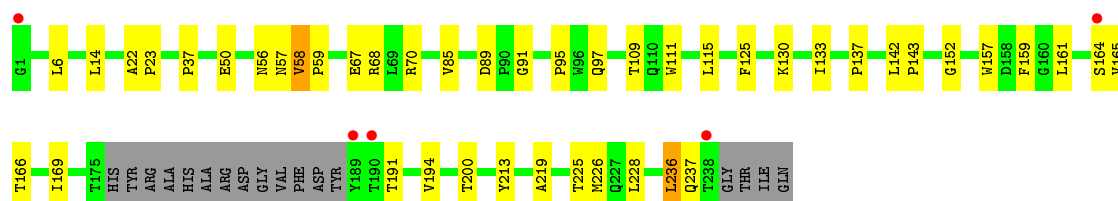
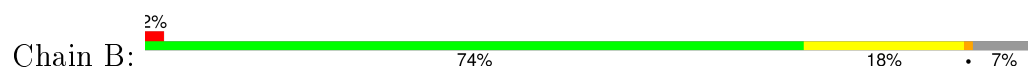




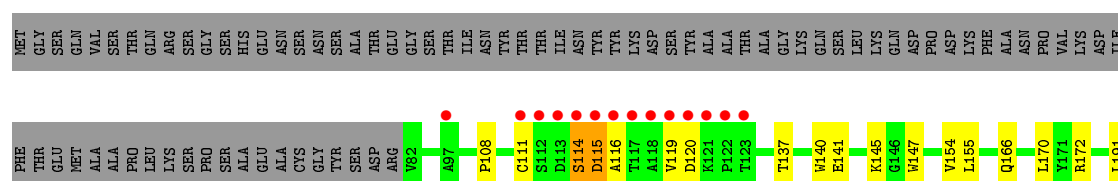
• Molecule 2: Capsid protein VP3



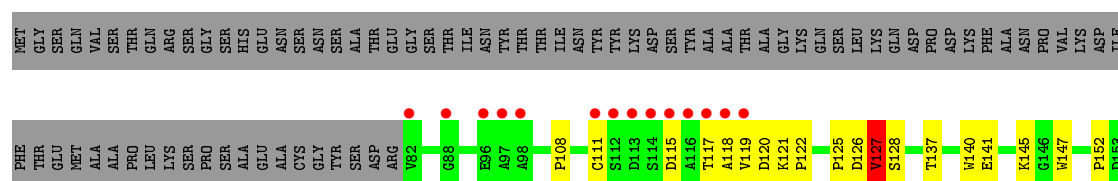
• Molecule 2: Capsid protein VP3



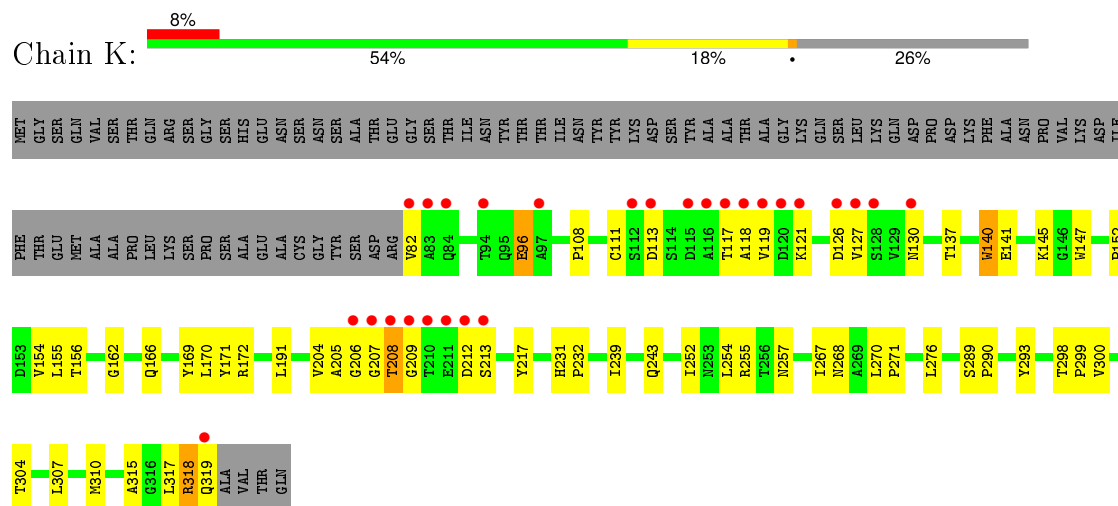
• Molecule 3: Capsid protein VP0



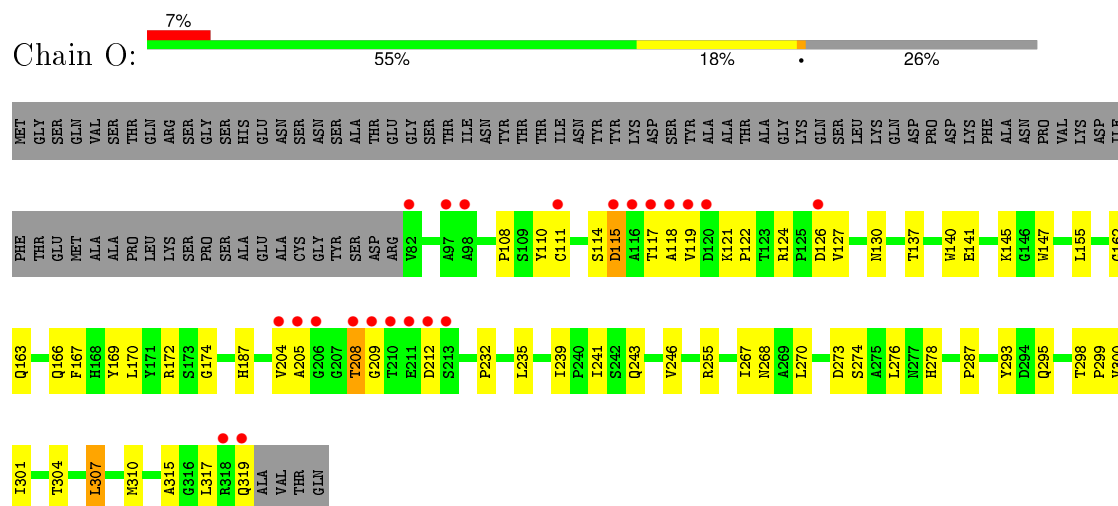
• Molecule 3: Capsid protein VP0



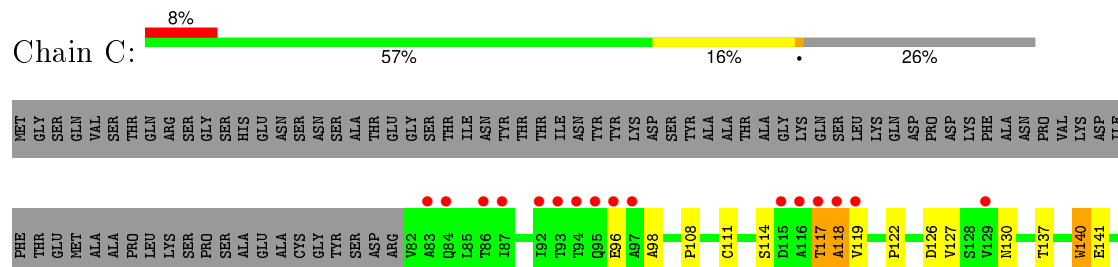
- Molecule 3: Capsid protein VP0

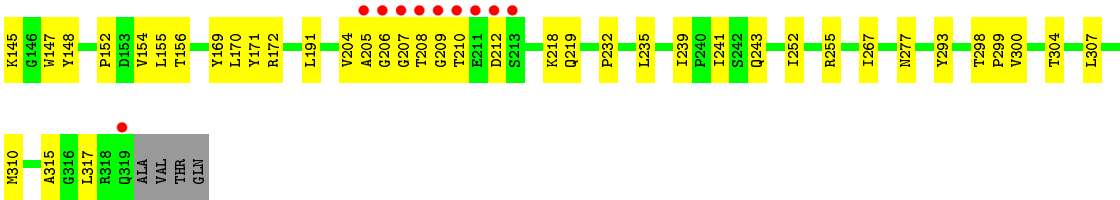


- Molecule 3: Capsid protein VP0



- Molecule 3: Capsid protein VP0





4 Data and refinement statistics

Property	Value	Source
Space group	P 4 ₂ 3 2	Depositor
Cell constants a, b, c, α , β , γ	352.98Å 352.98Å 352.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.92 – 3.15 49.92 – 3.15	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.92-3.15) 78.4 (49.92-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 3.12Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.216 , 0.234 0.207 , 0.231	Depositor DCC
R_{free} test set	1823 reflections (1.81%)	DCC
Wilson B-factor (Å ²)	59.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 20.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 110052 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	26615	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.32	0/1818	0.51	0/2478
1	E	0.31	0/1818	0.50	0/2478
1	I	0.36	0/1818	0.53	0/2478
1	M	0.31	0/1818	0.50	0/2478
1	Q	0.35	0/1818	0.56	0/2478
2	B	0.31	0/1764	0.47	0/2415
2	F	0.27	0/1764	0.47	0/2415
2	J	0.30	0/1764	0.47	0/2415
2	N	0.29	0/1764	0.47	0/2415
2	R	0.28	0/1764	0.48	0/2415
3	C	0.31	0/1896	0.51	1/2602 (0.0%)
3	G	0.28	0/1896	0.50	1/2602 (0.0%)
3	K	0.30	0/1896	0.52	1/2602 (0.0%)
3	O	0.29	0/1896	0.51	1/2602 (0.0%)
3	S	0.32	0/1896	0.55	1/2602 (0.0%)
All	All	0.31	0/27390	0.50	5/37475 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	1
3	G	0	1
All	All	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	115	ASP	CB-CG-OD1	5.60	123.34	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	115	ASP	N-CA-C	5.37	125.50	111.00
3	S	127	VAL	CG1-CB-CG2	-5.30	102.42	110.90
3	C	140	TRP	CA-CB-CG	5.02	123.23	113.70
3	K	140	TRP	CA-CB-CG	5.00	123.20	113.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	G	114	SER	Peptide
1	I	216	GLN	Peptide

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	1764	0	1712	54	0
1	E	1764	0	1712	47	0
1	I	1764	0	1712	44	0
1	M	1764	0	1712	55	0
1	Q	1764	0	1712	55	0
2	B	1718	0	1707	33	0
2	F	1718	0	1707	38	0
2	J	1718	0	1707	37	0
2	N	1718	0	1707	39	0
2	R	1718	0	1707	40	0
3	C	1841	0	1780	42	0
3	G	1841	0	1780	41	0
3	K	1841	0	1780	51	0
3	O	1841	0	1780	46	0
3	S	1841	0	1780	42	0
All	All	26615	0	25995	549	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 10.

The worst 5 of 549 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:I:210:THR:HG22	1:I:211:PHE:HA	1.29	1.15
1:Q:213:GLU:HB2	1:Q:214:HIS:HA	1.34	1.05
1:A:215:LYS:H	1:A:216:GLN:HA	1.29	0.96
1:M:86:ARG:NH2	2:N:229:CYS:SG	2.42	0.92
1:Q:213:GLU:CB	1:Q:214:HIS:HA	2.03	0.88

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	221/297 (74%)	207 (94%)	13 (6%)	1 (0%)	34	76
1	E	221/297 (74%)	206 (93%)	14 (6%)	1 (0%)	34	76
1	I	221/297 (74%)	208 (94%)	12 (5%)	1 (0%)	34	76
1	M	221/297 (74%)	207 (94%)	13 (6%)	1 (0%)	34	76
1	Q	221/297 (74%)	207 (94%)	12 (5%)	2 (1%)	21	65
2	B	221/242 (91%)	202 (91%)	18 (8%)	1 (0%)	34	76
2	F	221/242 (91%)	201 (91%)	20 (9%)	0	100	100
2	J	221/242 (91%)	201 (91%)	20 (9%)	0	100	100
2	N	221/242 (91%)	200 (90%)	21 (10%)	0	100	100
2	R	221/242 (91%)	201 (91%)	20 (9%)	0	100	100
3	C	236/323 (73%)	219 (93%)	16 (7%)	1 (0%)	39	79
3	G	236/323 (73%)	219 (93%)	17 (7%)	0	100	100
3	K	236/323 (73%)	220 (93%)	15 (6%)	1 (0%)	39	79
3	O	236/323 (73%)	219 (93%)	17 (7%)	0	100	100
3	S	236/323 (73%)	218 (92%)	15 (6%)	3 (1%)	15	57
All	All	3390/4310 (79%)	3135 (92%)	243 (7%)	12 (0%)	39	79

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	S	127	VAL
1	Q	288	GLY
1	M	288	GLY
1	A	288	GLY
3	K	113	ASP

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	191/251 (76%)	190 (100%)	1 (0%)	92	97
1	E	191/251 (76%)	189 (99%)	2 (1%)	82	94
1	I	191/251 (76%)	189 (99%)	2 (1%)	82	94
1	M	191/251 (76%)	188 (98%)	3 (2%)	70	90
1	Q	191/251 (76%)	184 (96%)	7 (4%)	41	78
2	B	189/202 (94%)	188 (100%)	1 (0%)	92	97
2	F	189/202 (94%)	187 (99%)	2 (1%)	80	93
2	J	189/202 (94%)	188 (100%)	1 (0%)	92	97
2	N	189/202 (94%)	188 (100%)	1 (0%)	92	97
2	R	189/202 (94%)	188 (100%)	1 (0%)	92	97
3	C	202/272 (74%)	199 (98%)	3 (2%)	72	91
3	G	202/272 (74%)	201 (100%)	1 (0%)	92	97
3	K	202/272 (74%)	198 (98%)	4 (2%)	63	88
3	O	202/272 (74%)	197 (98%)	5 (2%)	55	85
3	S	202/272 (74%)	201 (100%)	1 (0%)	92	97
All	All	2910/3625 (80%)	2875 (99%)	35 (1%)	78	93

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	123	VAL
2	J	58	VAL
3	C	117	THR
1	M	211	PHE
1	A	123	VAL

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

Mol	Chain	Res	Type
3	G	277	ASN
1	I	189	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	223/297 (75%)	-0.30	10 (4%) 37 21	28, 37, 132, 220	0
1	E	223/297 (75%)	-0.24	13 (5%) 26 13	27, 37, 133, 222	0
1	I	223/297 (75%)	-0.29	11 (4%) 33 19	29, 38, 132, 219	0
1	M	223/297 (75%)	-0.29	12 (5%) 29 15	28, 38, 132, 219	0
1	Q	223/297 (75%)	-0.24	11 (4%) 33 19	28, 38, 133, 219	0
2	B	225/242 (92%)	-0.36	5 (2%) 65 49	30, 42, 79, 153	0
2	F	225/242 (92%)	-0.41	4 (1%) 71 56	30, 41, 77, 151	0
2	J	225/242 (92%)	-0.40	5 (2%) 65 49	30, 42, 79, 153	0
2	N	225/242 (92%)	-0.47	5 (2%) 65 49	30, 42, 81, 155	0
2	R	225/242 (92%)	-0.43	4 (1%) 71 56	30, 42, 79, 152	0
3	C	238/323 (73%)	0.21	26 (10%) 7 3	30, 50, 166, 220	0
3	G	238/323 (73%)	0.04	23 (9%) 10 5	30, 49, 161, 218	0
3	K	238/323 (73%)	0.28	27 (11%) 7 3	30, 50, 163, 218	0
3	O	238/323 (73%)	0.06	22 (9%) 11 5	31, 50, 163, 217	0
3	S	238/323 (73%)	0.25	25 (10%) 8 4	31, 52, 164, 221	0
All	All	3430/4310 (79%)	-0.17	203 (5%) 26 13	27, 42, 137, 222	0

The worst 5 of 203 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	210	THR	14.4
3	O	210	THR	11.8
3	S	210	THR	10.6
3	K	115	ASP	8.3
1	Q	212	GLY	8.3

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.