



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 07:39 pm GMT

PDB ID : 4CS8  
Title : Crystal structure of the asymmetric human metapneumovirus M2-1 tetramer, form 2  
Authors : Leyrat, C.; Renner, M.; Harlos, K.; Grimes, J.M.  
Deposited on : 2014-03-05  
Resolution : 2.10 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](mailto: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>.

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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 : 2.36  
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) : 2.36

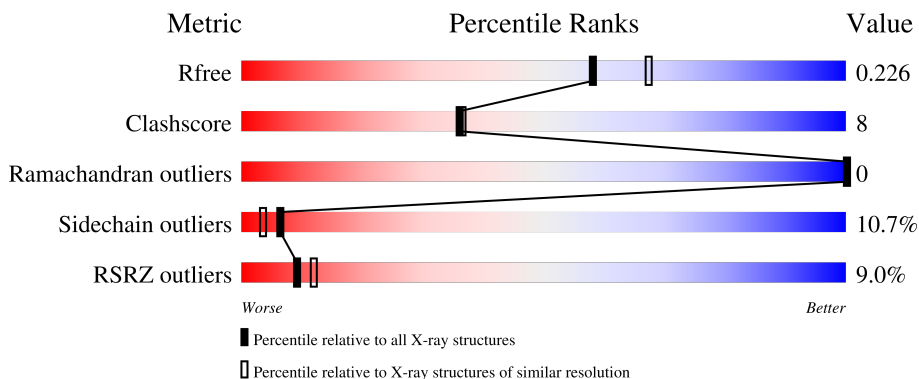
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	189	 7% 60% 21% • 16%
1	B	189	 5% 68% 16% • 13%
1	E	189	 16% 66% 17% • 15%
2	C	189	 3% 71% 12% • 14%

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 5536 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 M2-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	159	1288	803	242	237	6	0	0	0
1	B	164	1319	822	247	244	6	0	0	0
1	E	161	1302	812	239	245	6	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q8QN58
A	0	PRO	-	expression tag	UNP Q8QN58
B	-1	GLY	-	expression tag	UNP Q8QN58
B	0	PRO	-	expression tag	UNP Q8QN58
E	-1	GLY	-	expression tag	UNP Q8QN58
E	0	PRO	-	expression tag	UNP Q8QN58

- Molecule 2 is a protein called M2-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	162	1309	814	245	244	6	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP Q8QN58
C	0	PRO	-	expression tag	UNP Q8QN58
C	49	ASP	ASN	conflict	UNP Q8QN58

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Zn 1	0	0
3	B	1	Total 1	Zn 1	0	0
3	C	1	Total 1	Zn 1	0	0
3	E	1	Total 1	Zn 1	0	0

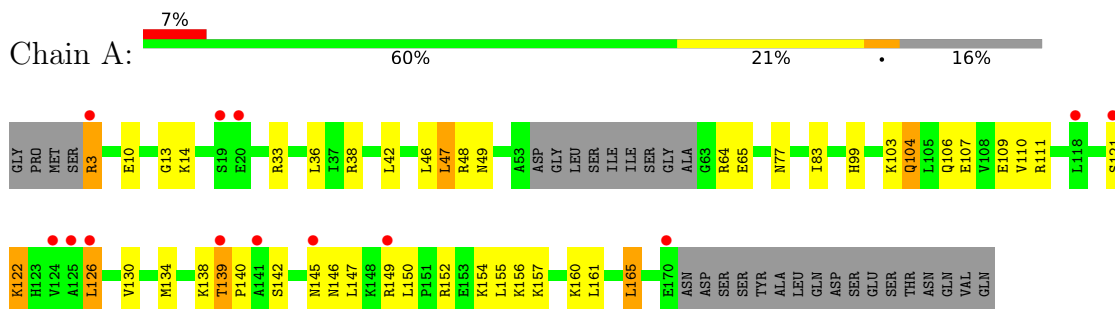
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	64	Total 64	O 64	0	0
4	B	100	Total 100	O 100	0	0
4	C	112	Total 112	O 112	0	0
4	E	38	Total 38	O 38	0	0

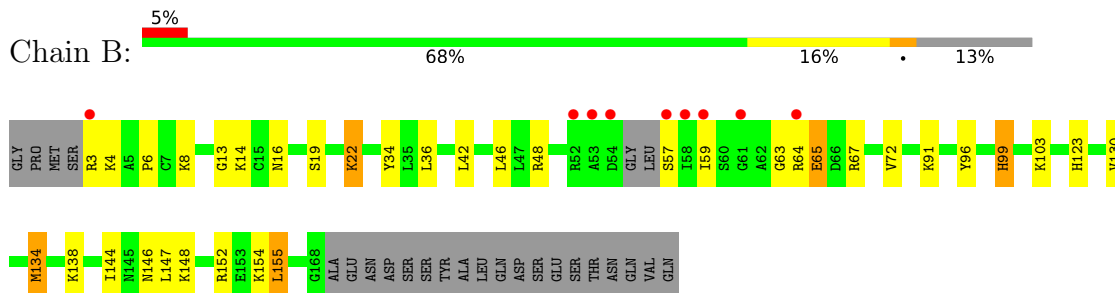
### 3 Residue-property plots [i](#)

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.

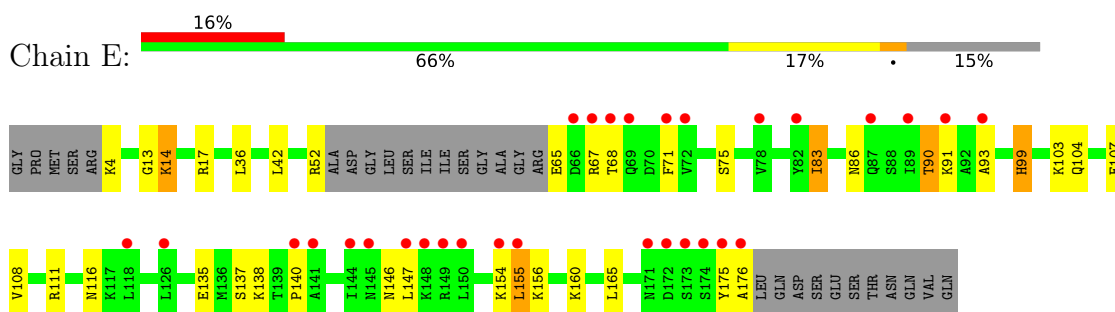
- Molecule 1: M2-1



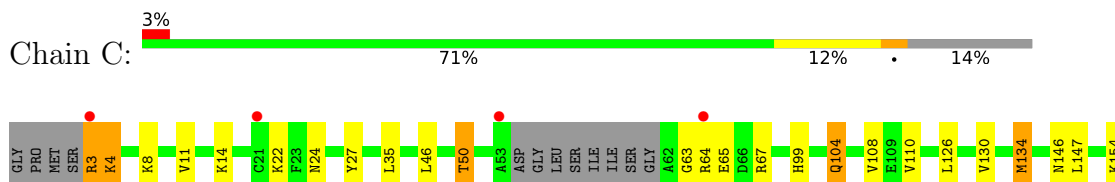
- Molecule 1: M2-1



- Molecule 1: M2-1



- Molecule 2: M2-1



L155	
L165	
E170	
H171	
D172	
SER	
SER	
TYR	
ALA	
LEU	
GLN	
ASP	
SER	
GLU	
SER	
THR	
ASN	
GLN	
VAL	
GLN	

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.98Å 93.42Å 85.21Å 90.00° 95.44° 90.00°	Depositor
Resolution (Å)	30.75 – 2.10 44.81 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.75-2.10) 99.8 (44.81-2.10)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.03 (at 2.10Å)	Xtrriage
Refinement program	BUSTER 2.11.4	Depositor
R, $R_{free}$	0.192 , 0.222 0.195 , 0.226	Depositor DCC
$R_{free}$ test set	2296 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.2	Xtrriage
Anisotropy	0.183	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 64.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5536	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section:  
ZN

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	0.45	0/1307	0.66	1/1757 (0.1%)
1	B	0.46	1/1338 (0.1%)	0.60	0/1799
1	E	0.41	0/1322	0.61	0/1780
2	C	0.47	1/1328 (0.1%)	0.60	0/1786
All	All	0.45	2/5295 (0.0%)	0.62	1/7122 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	134	MET	SD-CE	-5.75	1.45	1.77
2	C	134	MET	SD-CE	-5.34	1.48	1.77

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	THR	CB-CA-C	5.09	125.33	111.60

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	1288	0	1307	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1319	0	1340	25	0
1	E	1302	0	1307	28	0
2	C	1309	0	1320	18	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
4	A	64	0	0	0	0
4	B	100	0	0	1	0
4	C	112	0	0	2	0
4	E	38	0	0	1	0
All	All	5536	0	5274	84	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 8.

All (84) 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:14:LYS:H	1:E:104:GLN:HE22	1.06	1.00
1:B:64:ARG:NH1	1:E:146:ASN:HD21	1.61	0.97
2:C:64:ARG:HH21	2:C:67:ARG:HD2	1.40	0.85
2:C:110:VAL:HG21	2:C:134:MET:HE1	1.65	0.78
1:A:104:GLN:HE22	1:E:14:LYS:H	1.30	0.77
1:B:14:LYS:H	1:E:104:GLN:NE2	1.84	0.76
2:C:130:VAL:HG12	2:C:134:MET:CE	2.16	0.74
1:A:122:LYS:O	1:A:122:LYS:HD3	1.87	0.74
2:C:130:VAL:HG12	2:C:134:MET:HE2	1.71	0.73
2:C:64:ARG:NH2	2:C:67:ARG:HD2	2.03	0.73
2:C:108:VAL:HG21	4:E:2024:HOH:O	1.90	0.71
1:E:13:GLY:HA2	1:E:42:LEU:HD11	1.75	0.69
1:B:130:VAL:HG12	1:B:134:MET:CE	2.23	0.67
1:B:14:LYS:N	1:E:104:GLN:HE22	1.87	0.65
1:B:13:GLY:HA2	1:B:42:LEU:HD11	1.79	0.64
2:C:4:LYS:HG2	2:C:24:ASN:HB2	1.81	0.63
1:E:68:THR:HA	1:E:71:PHE:CE2	2.36	0.61
1:B:130:VAL:HG12	1:B:134:MET:HE2	1.82	0.60
1:A:130:VAL:HG12	1:A:134:MET:HE3	1.83	0.60
1:B:3:ARG:HA	1:B:22:LYS:O	2.00	0.60
1:A:77:ASN:HD21	1:E:17:ARG:HH11	1.50	0.59
1:A:110:VAL:HG21	1:A:134:MET:CE	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:135:GLU:O	1:E:138:LYS:HD2	2.03	0.58
1:B:22:LYS:HA	1:B:22:LYS:HE3	1.86	0.58
2:C:64:ARG:CD	4:C:2030:HOH:O	2.52	0.58
1:A:13:GLY:HA2	1:A:42:LEU:HD11	1.86	0.57
1:A:122:LYS:NZ	1:A:126:LEU:HD23	2.20	0.57
1:B:16:ASN:HB3	1:E:75:SER:HB2	1.85	0.57
1:B:72:VAL:HA	1:E:154:LYS:HD2	1.86	0.57
1:B:34:TYR:OH	1:E:175:TYR:HA	2.06	0.56
1:A:3:ARG:O	1:A:3:ARG:HG3	2.05	0.56
1:A:107:GLU:OE2	1:A:111:ARG:HD3	2.06	0.55
1:B:64:ARG:NH1	1:E:146:ASN:ND2	2.44	0.55
1:B:96:TYR:O	1:B:99:HIS:HD2	1.90	0.55
1:A:122:LYS:HD3	1:A:122:LYS:C	2.24	0.55
2:C:64:ARG:HD2	4:C:2030:HOH:O	2.06	0.55
1:A:106:GLN:HB2	1:A:109:GLU:HG3	1.88	0.55
2:C:27:TYR:HB3	2:C:35:LEU:HD21	1.89	0.55
1:A:130:VAL:HG12	1:A:134:MET:CE	2.38	0.54
1:B:48:ARG:HG2	1:E:138:LYS:HE2	1.91	0.52
1:E:107:GLU:HB3	1:E:111:ARG:HH12	1.75	0.52
1:A:49:ASN:HD22	2:C:50:THR:CG2	2.23	0.51
1:A:83:ILE:HA	1:A:156:LYS:HE3	1.93	0.50
1:E:83:ILE:HA	1:E:156:LYS:HD2	1.93	0.50
1:A:49:ASN:HB3	2:C:50:THR:HG23	1.92	0.50
1:B:130:VAL:HG12	1:B:134:MET:HE3	1.91	0.50
2:C:63:GLY:C	2:C:65:GLU:H	2.14	0.50
1:E:91:LYS:HE2	1:E:155:LEU:HD12	1.93	0.49
1:A:110:VAL:HG21	1:A:134:MET:HE2	1.94	0.49
1:B:48:ARG:HD2	1:E:138:LYS:HG3	1.94	0.49
1:A:46:LEU:HD23	2:C:50:THR:HG21	1.95	0.48
1:A:110:VAL:HG21	1:A:134:MET:HE1	1.95	0.48
1:E:90:THR:HG23	1:E:93:ALA:HB2	1.97	0.47
1:B:6:PRO:HD3	1:E:176:ALA:C	2.35	0.47
1:B:63:GLY:O	1:B:67:ARG:HG3	2.14	0.47
1:A:150:LEU:HD22	1:A:154:LYS:HD3	1.95	0.47
1:B:144:ILE:HG22	1:B:148:LYS:HE2	1.97	0.47
2:C:8:LYS:HA	2:C:11:VAL:HG22	1.97	0.47
1:A:161:LEU:HG	1:A:165:LEU:HD22	1.96	0.46
1:E:13:GLY:HA2	1:E:42:LEU:CD1	2.45	0.46
1:A:104:GLN:HG3	1:A:104:GLN:O	2.15	0.46
2:C:46:LEU:O	2:C:50:THR:HB	2.14	0.46
1:A:10:GLU:O	1:A:38:ARG:HD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:THR:HG23	1:A:142:SER:OG	2.17	0.45
1:B:91:LYS:HE3	1:B:155:LEU:HD12	1.98	0.45
1:B:64:ARG:NH2	1:B:65:GLU:HA	2.31	0.45
1:A:138:LYS:O	1:A:140:PRO:HD3	2.16	0.45
1:A:64:ARG:HA	1:A:64:ARG:HD2	1.80	0.45
1:B:99:HIS:CE1	1:B:103:LYS:HE3	2.52	0.45
1:A:14:LYS:H	2:C:104:GLN:HE22	1.65	0.44
1:A:36:LEU:HD11	1:E:36:LEU:HD13	1.99	0.44
1:E:99:HIS:NE2	1:E:140:PRO:HB3	2.32	0.44
2:C:3:ARG:HA	2:C:3:ARG:HD3	1.39	0.44
1:A:142:SER:O	1:A:146:ASN:HB2	2.18	0.43
1:B:123:HIS:HD2	4:B:2071:HOH:O	2.00	0.43
1:E:175:TYR:CD1	1:E:175:TYR:N	2.86	0.43
1:A:146:ASN:HA	1:A:149:ARG:NH1	2.34	0.42
1:B:36:LEU:HD13	1:E:36:LEU:HD11	2.02	0.42
1:A:126:LEU:HD22	1:A:126:LEU:HA	1.90	0.41
1:E:103:LYS:HG2	1:E:137:SER:HB3	2.03	0.41
1:A:104:GLN:NE2	1:E:13:GLY:HA3	2.36	0.41
1:E:107:GLU:HB3	1:E:111:ARG:NH1	2.35	0.41
1:A:47:LEU:HD13	1:A:47:LEU:HA	1.96	0.40
1:A:3:ARG:O	1:A:3:ARG:CG	2.69	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	155/189 (82%)	151 (97%)	4 (3%)	0	100	100
1	B	160/189 (85%)	156 (98%)	4 (2%)	0	100	100
1	E	157/189 (83%)	155 (99%)	2 (1%)	0	100	100
2	C	158/189 (84%)	154 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	630/756 (83%)	616 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	142/167 (85%)	124 (87%)	18 (13%)	4	2
1	B	146/167 (87%)	131 (90%)	15 (10%)	7	4
1	E	145/167 (87%)	130 (90%)	15 (10%)	7	4
2	C	144/167 (86%)	130 (90%)	14 (10%)	8	5
All	All	577/668 (86%)	515 (89%)	62 (11%)	6	3

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	33	ARG
1	A	47	LEU
1	A	48	ARG
1	A	65	GLU
1	A	99	HIS
1	A	103	LYS
1	A	104	GLN
1	A	121	SER
1	A	122	LYS
1	A	126	LEU
1	A	145	ASN
1	A	147	LEU
1	A	152	ARG
1	A	155	LEU
1	A	157	LYS
1	A	160	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	165	LEU
1	B	4	LYS
1	B	8	LYS
1	B	19	SER
1	B	22	LYS
1	B	46	LEU
1	B	57	SER
1	B	59	ILE
1	B	65	GLU
1	B	99	HIS
1	B	138	LYS
1	B	146	ASN
1	B	147	LEU
1	B	152	ARG
1	B	154	LYS
1	B	155	LEU
2	C	3	ARG
2	C	4	LYS
2	C	14	LYS
2	C	22	LYS
2	C	50	THR
2	C	99	HIS
2	C	104	GLN
2	C	126	LEU
2	C	146	ASN
2	C	147	LEU
2	C	154	LYS
2	C	155	LEU
2	C	165	LEU
2	C	170	GLU
1	E	4	LYS
1	E	14	LYS
1	E	52	ARG
1	E	65	GLU
1	E	67	ARG
1	E	83	ILE
1	E	86	ASN
1	E	90	THR
1	E	99	HIS
1	E	108	VAL
1	E	116	ASN
1	E	147	LEU

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Mol	Chain	Res	Type
1	E	155	LEU
1	E	160	LYS
1	E	165	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	77	ASN
1	A	104	GLN
1	A	112	GLN
1	A	123	HIS
1	A	145	ASN
1	B	77	ASN
1	B	99	HIS
1	B	112	GLN
2	C	77	ASN
2	C	104	GLN
2	C	145	ASN
2	C	171	ASN
1	E	45	GLN
1	E	49	ASN
1	E	69	GLN
1	E	77	ASN
1	E	80	GLN
1	E	86	ASN
1	E	104	GLN
1	E	123	HIS
1	E	146	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	159/189 (84%)	0.76	13 (8%) 11 15	35, 63, 101, 117	0
1	B	164/189 (86%)	0.40	9 (5%) 25 31	34, 52, 94, 134	0
1	E	161/189 (85%)	1.19	30 (18%) 1 1	38, 70, 119, 129	0
2	C	162/189 (85%)	0.25	6 (3%) 41 48	35, 49, 87, 106	0
All	All	646/756 (85%)	0.65	58 (8%) 9 12	34, 57, 101, 134	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	176	ALA	13.6
1	E	173	SER	6.2
1	E	175	TYR	5.8
1	B	3	ARG	5.8
1	E	174	SER	5.2
1	E	89	ILE	4.9
1	A	118	LEU	4.9
1	E	72	VAL	4.8
1	A	139	THR	4.5
1	E	172	ASP	4.5
1	A	141	ALA	4.3
1	E	155	LEU	4.3
1	A	121	SER	4.2
1	E	71	PHE	4.1
1	A	126	LEU	4.0
1	E	141	ALA	4.0
1	E	68	THR	3.9
1	E	149	ARG	3.9
1	B	58	ILE	3.9
1	A	19	SER	3.8
1	E	93	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	144	ILE	3.6
1	E	118	LEU	3.5
1	B	53	ALA	3.5
2	C	170	GLU	3.5
1	B	64	ARG	3.5
1	E	66	ASP	3.4
1	B	57	SER	3.4
1	E	145	ASN	3.4
2	C	3	ARG	3.3
1	E	148	LYS	3.2
2	C	53	ALA	3.2
1	E	150	LEU	3.2
1	E	154	LYS	3.1
1	A	3	ARG	3.1
1	E	147	LEU	3.1
1	E	91	LYS	2.9
1	E	171	ASN	2.8
1	A	170	GLU	2.8
1	B	59	ILE	2.7
1	E	69	GLN	2.7
1	E	87	GLN	2.7
1	E	126	LEU	2.7
1	E	82	TYR	2.6
1	A	145	ASN	2.5
1	E	67	ARG	2.5
1	E	140	PRO	2.5
1	A	149	ARG	2.4
1	A	124	VAL	2.4
1	A	125	ALA	2.3
1	A	20	GLU	2.3
2	C	21	CYS	2.3
1	B	61	GLY	2.2
1	B	52	ARG	2.2
1	B	54	ASP	2.1
2	C	64	ARG	2.0
2	C	171	ASN	2.0
1	E	78	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	C	1173	1/1	0.96	0.10	51,51,51,51	1
3	ZN	B	1169	1/1	0.97	0.13	61,61,61,61	0
3	ZN	A	1171	1/1	0.99	0.11	49,49,49,49	0
3	ZN	E	1177	1/1	1.00	0.16	37,37,37,37	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.