



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2023 – 08:25 AM EDT

PDB ID : 7M3R  
Title : Crystallographic Structure of the Rhombohedral Crystal Form of STMV  
Grown from Bromide  
Authors : McPherson, A.  
Deposited on : 2021-03-18  
Resolution : 2.10 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](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 : 2.35.1  
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

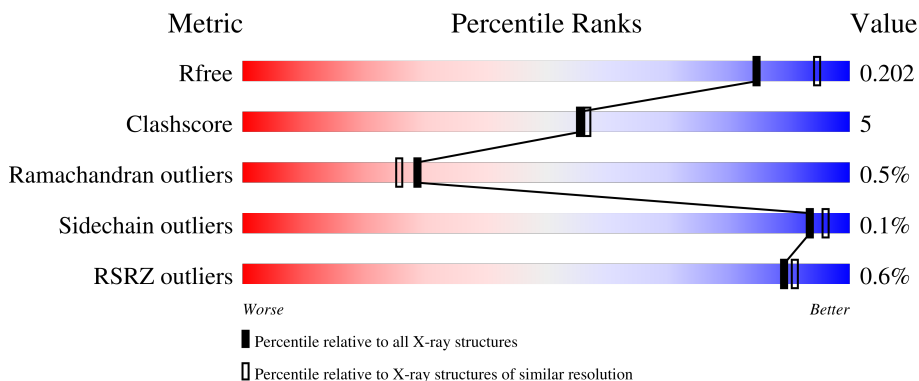
# 1 Overall quality at a glance

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	159	 86% 6% 8%
1	B	159	 84% 6% 10%
1	C	159	 83% 6% 11%
1	D	159	 84% 6% 9%
1	E	159	 83% 8% 9%

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Mol	Chain	Length	Quality of chain
1	F	159	
1	G	159	
1	GG	159	
1	H	159	
1	HH	159	
1	I	159	
1	II	159	
1	J	159	
1	JJ	159	
1	K	159	
1	KK	159	
1	L	159	
1	M	159	
1	N	159	
1	O	159	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BR	A	709	-	-	X	-
2	BR	B	201	-	-	X	-
2	BR	B	202	-	-	X	-
2	BR	B	206	-	-	X	-
2	BR	B	207	-	-	X	-
2	BR	B	211	-	-	X	-
2	BR	C	304	-	-	X	-
2	BR	C	306	-	-	X	-
2	BR	C	307	-	-	X	-
2	BR	C	308	-	-	X	-
2	BR	C	310	-	-	X	-
2	BR	C	312	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BR	D	301	-	-	X	-
2	BR	D	305	-	-	X	-
2	BR	D	306	-	-	X	-
2	BR	E	401	-	-	X	-
2	BR	F	601	-	-	X	-
2	BR	F	608	-	-	X	-
2	BR	G	504	-	-	X	-
2	BR	G	505	-	-	X	-
2	BR	G	509	-	-	X	-
2	BR	GG	203	-	-	X	-
2	BR	GG	215	-	-	X	-
2	BR	GG	216	-	-	X	-
2	BR	H	201	-	-	X	-
2	BR	H	206	-	-	X	-
2	BR	I	206	-	-	X	-
2	BR	I	207	-	-	X	-
2	BR	I	208	-	-	X	-
2	BR	I	209	-	-	X	-
2	BR	JJ	204	-	-	X	-
2	BR	K	202	-	-	X	-
2	BR	K	207	-	-	X	-
2	BR	KK	201	-	-	X	-
2	BR	KK	203	-	-	X	-
2	BR	L	1001	-	-	X	-
2	BR	L	1003	-	-	X	-
2	BR	L	1005	-	-	X	-
2	BR	M	503	-	-	X	-
2	BR	N	1303	-	-	X	-
2	BR	N	1309	-	-	X	-
2	BR	N	1310	-	-	X	-
2	BR	N	1311	-	-	X	-
2	BR	O	505	-	-	X	-
2	BR	O	507	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 49952 atoms, of which 22479 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 Coat protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	146	2257	713	1123	201	214	6	2	11	0
1	B	143	2212	703	1097	197	208	7	0	12	0
1	C	142	2206	696	1102	196	206	6	1	20	0
1	D	144	2264	712	1134	200	211	7	1	21	0
1	E	144	2212	703	1094	199	210	6	1	17	0
1	F	144	2238	705	1117	199	211	6	4	13	0
1	G	145	2242	711	1111	200	213	7	3	13	0
1	H	145	2268	716	1130	202	214	6	3	16	0
1	I	144	2256	710	1127	200	212	7	9	13	0
1	J	148	2259	721	1107	204	221	6	1	12	0
1	K	146	2311	726	1154	207	218	6	6	13	0
1	L	158	2435	792	1180	223	232	8	4	13	0
1	M	151	2371	755	1167	216	226	7	16	9	0
1	N	144	2296	721	1154	199	214	8	1	11	0
1	O	149	2297	731	1132	208	219	7	0	23	0
1	GG	145	2240	707	1114	200	213	6	1	18	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	HH	145	Total	C	H	N	O	S	0	14	0
			2251	711	1120	200	213	7			
1	II	144	Total	C	H	N	O	S	2	13	0
			2205	701	1089	199	210	6			
1	JJ	144	Total	C	H	N	O	S	1	16	0
			2230	703	1112	199	210	6			
1	KK	144	Total	C	H	N	O	S	2	13	0
			2233	703	1115	199	210	6			

- Molecule 2 is BROMIDE ION (three-letter code: BR) (formula: Br) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	9	Total	Br	0	0
			9	9		
2	B	11	Total	Br	0	0
			11	11		
2	C	13	Total	Br	0	0
			13	13		
2	D	8	Total	Br	0	0
			8	8		
2	E	10	Total	Br	0	0
			10	10		
2	F	8	Total	Br	0	0
			8	8		
2	G	8	Total	Br	0	0
			8	8		
2	H	12	Total	Br	0	0
			12	12		
2	I	9	Total	Br	0	0
			9	9		
2	J	10	Total	Br	0	0
			10	10		
2	K	6	Total	Br	0	0
			6	6		
2	L	8	Total	Br	0	0
			8	8		
2	M	8	Total	Br	0	0
			8	8		
2	N	13	Total	Br	0	0
			13	13		
2	O	10	Total	Br	0	0
			10	10		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	GG	18	Total 18	Br 18	0	0
2	HH	7	Total 7	Br 7	0	0
2	II	9	Total 9	Br 9	0	0
2	JJ	5	Total 5	Br 5	0	0
2	KK	9	Total 9	Br 9	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Mg 1	0	0
3	D	1	Total 1	Mg 1	0	0
3	F	1	Total 1	Mg 1	0	0
3	G	1	Total 1	Mg 1	0	0
3	H	1	Total 1	Mg 1	0	0
3	K	1	Total 1	Mg 1	0	0
3	O	1	Total 1	Mg 1	0	0
3	II	1	Total 1	Mg 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	231	Total 232	O 232	0	1
4	B	292	Total 292	O 292	0	1
4	C	165	Total 165	O 165	0	0
4	D	224	Total 224	O 224	0	0

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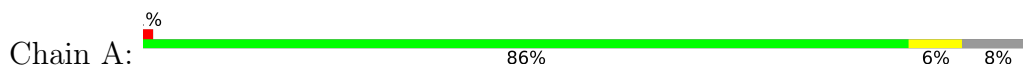
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	156	Total 156	O 156	0	0
4	F	169	Total 170	O 170	0	1
4	G	185	Total 185	O 185	0	0
4	H	343	Total 343	O 343	0	0
4	I	187	Total 187	O 187	0	1
4	J	252	Total 252	O 252	0	0
4	K	253	Total 253	O 253	0	0
4	L	220	Total 220	O 220	0	0
4	M	255	Total 255	O 255	0	0
4	N	170	Total 171	O 171	0	1
4	O	253	Total 253	O 253	0	1
4	GG	196	Total 196	O 196	0	0
4	HH	239	Total 239	O 239	0	0
4	II	209	Total 210	O 210	0	2
4	JJ	201	Total 202	O 202	0	1
4	KK	265	Total 265	O 265	0	0



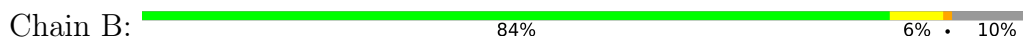
### 3 Residue-property plots [i](#)

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.

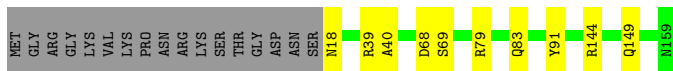
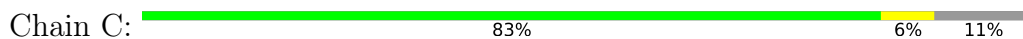
- Molecule 1: Coat protein



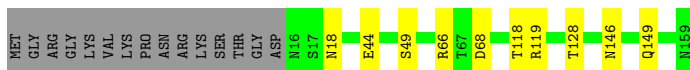
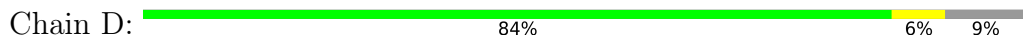
- Molecule 1: Coat protein



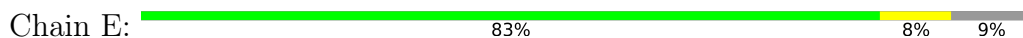
- Molecule 1: Coat protein



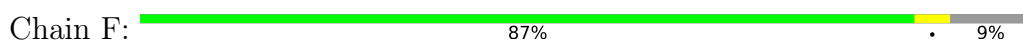
- Molecule 1: Coat protein



- Molecule 1: Coat protein

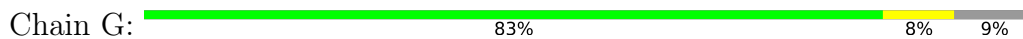


- Molecule 1: Coat protein

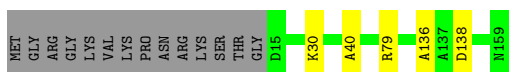
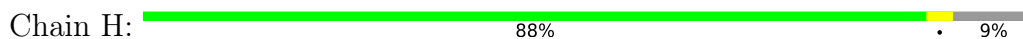




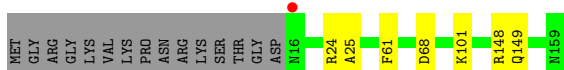
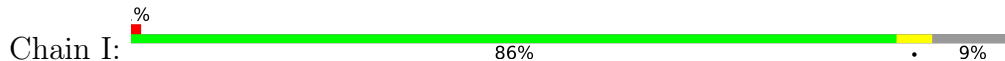
• Molecule 1: Coat protein



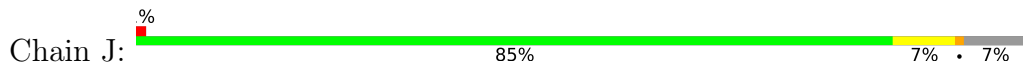
• Molecule 1: Coat protein



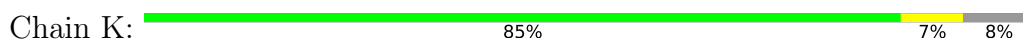
• Molecule 1: Coat protein



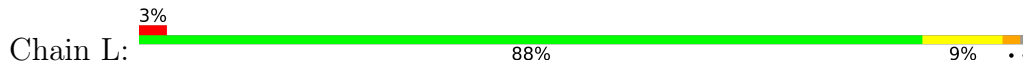
• Molecule 1: Coat protein



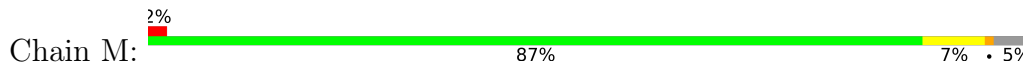
• Molecule 1: Coat protein

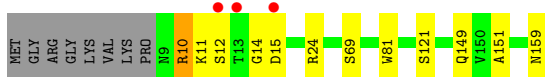


• Molecule 1: Coat protein



• Molecule 1: Coat protein

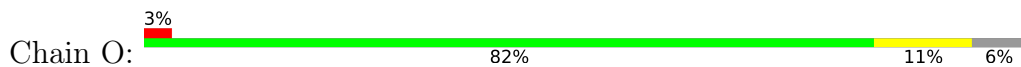




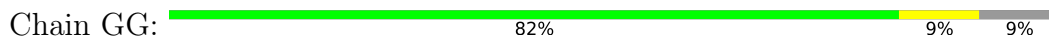
● Molecule 1: Coat protein



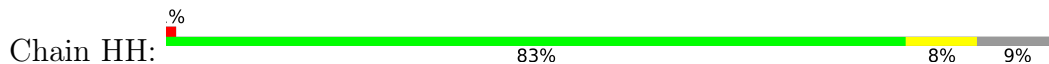
● Molecule 1: Coat protein



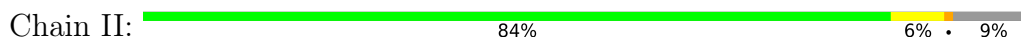
● Molecule 1: Coat protein



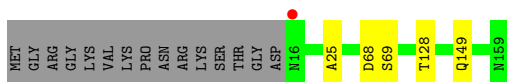
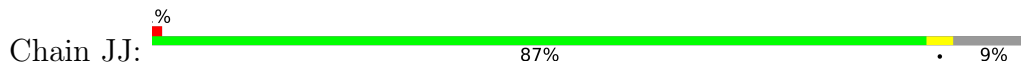
● Molecule 1: Coat protein



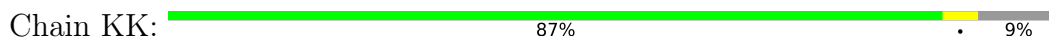
● Molecule 1: Coat protein



● Molecule 1: Coat protein



● Molecule 1: Coat protein



MET	GLY	ARG	GLY	LYS	VAL	LYS	PRO	ASN	ARG	LYS	SER	THR	GLY	ASP	N16	D68	F109	S121	T128	V140	Q149	N159
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## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	166.49Å 166.49Å 435.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	54.08 – 2.10 54.08 – 2.10	Depositor EDS
% Data completeness (in resolution range)	76.0 (54.08-2.10) 76.2 (54.08-2.10)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.10 (at 2.10Å)	Xtrriage
Refinement program	PHENIX 1.19_4092	Depositor
R, $R_{free}$	0.171 , 0.208 0.168 , 0.202	Depositor DCC
$R_{free}$ test set	10048 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.0	Xtrriage
Anisotropy	0.247	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 42.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	0.450 for -h-k,k,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	49952	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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

### 5.1 Standard geometry

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

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	0.25	0/1176	0.52	0/1603
1	B	0.25	0/1154	0.53	0/1571
1	C	0.26	0/1144	0.53	0/1559
1	D	0.25	0/1192	0.53	0/1624
1	E	0.26	0/1169	0.53	0/1592
1	F	0.25	0/1191	0.52	0/1623
1	G	0.31	0/1186	0.55	0/1615
1	GG	0.26	0/1166	0.53	0/1589
1	H	0.25	0/1196	0.53	0/1630
1	HH	0.25	0/1189	0.52	0/1620
1	I	0.25	0/1164	0.52	0/1585
1	II	0.25	0/1182	0.52	0/1610
1	J	0.25	0/1205	0.51	0/1641
1	JJ	0.25	0/1142	0.53	0/1556
1	K	0.25	0/1241	0.53	0/1690
1	KK	0.25	0/1169	0.53	0/1592
1	L	0.25	0/1342	0.53	0/1822
1	M	0.26	0/1268	0.54	0/1722
1	N	0.29	0/1227	0.56	0/1671
1	O	0.25	0/1195	0.53	0/1625
All	All	0.26	0/23898	0.53	0/32540

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

CLOSE-CONTACTS INFOmissingINFO

## 5.2 Torsion angles [i](#)

### 5.2.1 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	147/159 (92%)	139 (95%)	8 (5%)	0	100	100
1	B	143/159 (90%)	133 (93%)	9 (6%)	1 (1%)	22	18
1	C	142/159 (89%)	134 (94%)	8 (6%)	0	100	100
1	D	148/159 (93%)	141 (95%)	7 (5%)	0	100	100
1	E	145/159 (91%)	141 (97%)	3 (2%)	1 (1%)	22	18
1	F	148/159 (93%)	141 (95%)	7 (5%)	0	100	100
1	G	147/159 (92%)	140 (95%)	7 (5%)	0	100	100
1	GG	145/159 (91%)	137 (94%)	8 (6%)	0	100	100
1	H	149/159 (94%)	139 (93%)	10 (7%)	0	100	100
1	HH	148/159 (93%)	142 (96%)	6 (4%)	0	100	100
1	I	145/159 (91%)	137 (94%)	8 (6%)	0	100	100
1	II	147/159 (92%)	137 (93%)	8 (5%)	2 (1%)	11	6
1	J	150/159 (94%)	136 (91%)	12 (8%)	2 (1%)	12	7
1	JJ	142/159 (89%)	134 (94%)	8 (6%)	0	100	100
1	K	154/159 (97%)	144 (94%)	10 (6%)	0	100	100
1	KK	145/159 (91%)	136 (94%)	9 (6%)	0	100	100
1	L	169/159 (106%)	154 (91%)	12 (7%)	3 (2%)	8	4
1	M	158/159 (99%)	146 (92%)	9 (6%)	3 (2%)	8	3
1	N	153/159 (96%)	148 (97%)	4 (3%)	1 (1%)	22	18
1	O	149/159 (94%)	139 (93%)	8 (5%)	2 (1%)	12	7
All	All	2974/3180 (94%)	2798 (94%)	161 (5%)	15 (0%)	29	26

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	13	THR

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Mol	Chain	Res	Type
1	J	14	GLY
1	L	10	ARG
1	M	10	ARG
1	M	15	ASP

### 5.2.2 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	132/140 (94%)	132 (100%)	0	100	100
1	B	129/140 (92%)	129 (100%)	0	100	100
1	C	128/140 (91%)	128 (100%)	0	100	100
1	D	134/140 (96%)	134 (100%)	0	100	100
1	E	131/140 (94%)	131 (100%)	0	100	100
1	F	134/140 (96%)	134 (100%)	0	100	100
1	G	133/140 (95%)	132 (99%)	1 (1%)	81	86
1	GG	131/140 (94%)	131 (100%)	0	100	100
1	H	135/140 (96%)	135 (100%)	0	100	100
1	HH	134/140 (96%)	134 (100%)	0	100	100
1	I	131/140 (94%)	131 (100%)	0	100	100
1	II	132/140 (94%)	132 (100%)	0	100	100
1	J	135/140 (96%)	135 (100%)	0	100	100
1	JJ	128/140 (91%)	128 (100%)	0	100	100
1	K	139/140 (99%)	139 (100%)	0	100	100
1	KK	131/140 (94%)	131 (100%)	0	100	100
1	L	151/140 (108%)	151 (100%)	0	100	100
1	M	143/140 (102%)	143 (100%)	0	100	100
1	N	139/140 (99%)	138 (99%)	1 (1%)	84	88
1	O	134/140 (96%)	134 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2684/2800 (96%)	2682 (100%)	2 (0%)	93 96

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

Mol	Chain	Res	Type
1	G	38	VAL
1	N	16	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	149	GLN
1	J	149[A]	GLN
1	M	149	GLN
1	GG	149	GLN

### 5.2.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.4 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.5 Ligand geometry [i](#)

Of 199 ligands modelled in this entry, 199 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.

## 5.6 Other polymers [i](#)

There are no such residues in this entry.

## 5.7 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	146/159 (91%)	-0.58	1 (0%) 87 89	15, 20, 24, 43	4 (2%)
1	B	143/159 (89%)	-0.63	0 100 100	15, 19, 23, 26	3 (2%)
1	C	142/159 (89%)	-0.61	0 100 100	14, 19, 23, 32	3 (2%)
1	D	144/159 (90%)	-0.62	0 100 100	14, 18, 23, 67	3 (2%)
1	E	144/159 (90%)	-0.62	0 100 100	13, 19, 24, 44	3 (2%)
1	F	144/159 (90%)	-0.63	0 100 100	16, 20, 33, 60	4 (2%)
1	G	145/159 (91%)	-0.62	0 100 100	14, 19, 26, 50	2 (1%)
1	GG	145/159 (91%)	-0.50	0 100 100	17, 24, 32, 78	2 (1%)
1	H	145/159 (91%)	-0.58	0 100 100	16, 20, 25, 59	5 (3%)
1	HH	145/159 (91%)	-0.53	2 (1%) 75 78	16, 24, 31, 70	1 (0%)
1	I	144/159 (90%)	-0.61	1 (0%) 87 89	13, 20, 24, 38	1 (0%)
1	II	144/159 (90%)	-0.49	0 100 100	17, 24, 32, 62	4 (2%)
1	J	148/159 (93%)	-0.52	1 (0%) 87 89	14, 20, 25, 43	3 (2%)
1	JJ	144/159 (90%)	-0.54	1 (0%) 87 89	16, 23, 30, 87	2 (1%)
1	K	146/159 (91%)	-0.54	0 100 100	15, 21, 27, 34	1 (0%)
1	KK	144/159 (90%)	-0.59	0 100 100	17, 23, 32, 65	2 (1%)
1	L	158/159 (99%)	-0.18	5 (3%) 47 54	20, 25, 32, 35	2 (1%)
1	M	151/159 (94%)	-0.45	3 (1%) 65 69	17, 22, 32, 33	2 (1%)
1	N	144/159 (90%)	-0.51	0 100 100	17, 23, 31, 69	1 (0%)
1	O	149/159 (93%)	-0.35	4 (2%) 54 60	16, 25, 34, 119	0
All	All	2915/3180 (91%)	-0.53	18 (0%) 89 91	13, 21, 31, 119	48 (1%)

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	6	VAL	10.1
1	O	11	LYS	6.9
1	L	5	LYS	3.8
1	O	16	ASN	3.5
1	O	13	THR	3.2

## 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](#)

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
2	BR	O	505	1/1	0.74	0.35	129,129,129,129	0
2	BR	F	602	1/1	0.93	0.48	133,133,133,133	0
2	BR	GG	213	1/1	0.93	0.04	68,68,68,68	1
2	BR	N	1302	1/1	0.94	0.29	107,107,107,107	0
2	BR	D	301	1/1	0.95	0.39	101,101,101,101	0
2	BR	E	402	1/1	0.96	0.32	93,93,93,93	0
2	BR	L	1002	1/1	0.97	0.09	121,121,121,121	0
2	BR	F	601	1/1	0.97	0.29	75,75,75,75	0
2	BR	M	503	1/1	0.98	0.08	71,71,71,71	0
2	BR	C	308	1/1	0.98	0.03	54,54,54,54	0
2	BR	N	1309	1/1	0.98	0.03	61,61,61,61	0
2	BR	B	211	1/1	0.98	0.04	57,57,57,57	0
2	BR	C	302	1/1	0.98	0.38	114,114,114,114	0
2	BR	GG	215	1/1	0.98	0.04	79,79,79,79	0
2	BR	HH	202	1/1	0.98	0.04	40,40,40,40	0
2	BR	KK	202	1/1	0.98	0.03	44,44,44,44	0
3	MG	F	603	1/1	0.98	0.10	35,35,35,35	0
3	MG	H	202	1/1	0.98	0.04	25,25,25,25	0
2	BR	A	709	1/1	0.99	0.02	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BR	D	305	1/1	0.99	0.08	42,42,42,42	0
2	BR	D	306	1/1	0.99	0.07	52,52,52,52	0
2	BR	D	307	1/1	0.99	0.07	46,46,46,46	0
2	BR	A	710	1/1	0.99	0.06	50,50,50,50	0
2	BR	E	403	1/1	0.99	0.08	43,43,43,43	0
2	BR	E	404	1/1	0.99	0.08	45,45,45,45	0
2	BR	E	405	1/1	0.99	0.03	44,44,44,44	0
2	BR	E	406	1/1	0.99	0.05	51,51,51,51	0
2	BR	E	407	1/1	0.99	0.06	48,48,48,48	0
2	BR	E	408	1/1	0.99	0.04	45,45,45,45	0
2	BR	E	409	1/1	0.99	0.04	57,57,57,57	0
2	BR	E	410	1/1	0.99	0.03	51,51,51,51	0
2	BR	B	202	1/1	0.99	0.07	43,43,43,43	0
2	BR	B	206	1/1	0.99	0.04	69,69,69,69	0
2	BR	F	606	1/1	0.99	0.05	48,48,48,48	0
2	BR	F	607	1/1	0.99	0.07	45,45,45,45	0
2	BR	F	609	1/1	0.99	0.05	61,61,61,61	0
2	BR	G	505	1/1	0.99	0.06	45,45,45,45	0
2	BR	G	506	1/1	0.99	0.04	40,40,40,40	0
2	BR	G	507	1/1	0.99	0.05	47,47,47,47	0
2	BR	G	509	1/1	0.99	0.04	50,50,50,50	0
2	BR	H	207	1/1	0.99	0.06	46,46,46,46	0
2	BR	H	209	1/1	0.99	0.03	48,48,48,48	0
2	BR	H	210	1/1	0.99	0.05	54,54,54,54	0
2	BR	H	211	1/1	0.99	0.03	59,59,59,59	0
2	BR	H	212	1/1	0.99	0.01	65,65,65,65	0
2	BR	H	213	1/1	0.99	0.03	54,54,54,54	0
2	BR	I	208	1/1	0.99	0.06	53,53,53,53	0
2	BR	I	209	1/1	0.99	0.05	78,78,78,78	0
2	BR	J	201	1/1	0.99	0.06	49,49,49,49	0
2	BR	J	202	1/1	0.99	0.06	43,43,43,43	0
2	BR	J	203	1/1	0.99	0.05	47,47,47,47	0
2	BR	J	204	1/1	0.99	0.05	48,48,48,48	0
2	BR	J	208	1/1	0.99	0.07	52,52,52,52	0
2	BR	J	209	1/1	0.99	0.03	61,61,61,61	0
2	BR	K	204	1/1	0.99	0.06	46,46,46,46	0
2	BR	K	206	1/1	0.99	0.07	46,46,46,46	0
2	BR	B	207	1/1	0.99	0.02	47,47,47,47	0
2	BR	L	1004	1/1	0.99	0.04	41,41,41,41	0
2	BR	L	1005	1/1	0.99	0.03	49,49,49,49	0
2	BR	L	1006	1/1	0.99	0.04	40,40,40,40	0
2	BR	L	1007	1/1	0.99	0.04	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BR	M	501	1/1	0.99	0.06	39,39,39,39	0
2	BR	B	208	1/1	0.99	0.07	43,43,43,43	0
2	BR	M	507	1/1	0.99	0.03	38,38,38,38	0
2	BR	M	508	1/1	0.99	0.03	52,52,52,52	0
2	BR	A	703	1/1	0.99	0.09	39,39,39,39	0
2	BR	N	1306	1/1	0.99	0.05	44,44,44,44	0
2	BR	N	1307	1/1	0.99	0.04	54,54,54,54	0
2	BR	C	301	1/1	0.99	0.24	106,106,106,106	0
2	BR	N	1313	1/1	0.99	0.03	53,53,53,53	0
2	BR	O	503	1/1	0.99	0.04	49,49,49,49	0
2	BR	A	705	1/1	0.99	0.06	29,29,29,29	0
2	BR	O	506	1/1	0.99	0.06	44,44,44,44	0
2	BR	O	508	1/1	0.99	0.02	51,51,51,51	0
2	BR	O	510	1/1	0.99	0.04	54,54,54,54	0
2	BR	O	511	1/1	0.99	0.10	91,91,91,91	0
2	BR	GG	205	1/1	0.99	0.05	35,35,35,35	0
2	BR	GG	207	1/1	0.99	0.06	44,44,44,44	0
2	BR	A	707	1/1	0.99	0.06	64,64,64,64	0
2	BR	C	309	1/1	0.99	0.07	56,56,56,56	0
2	BR	C	310	1/1	0.99	0.04	57,57,57,57	0
2	BR	HH	207	1/1	0.99	0.03	57,57,57,57	0
2	BR	II	205	1/1	0.99	0.04	50,50,50,50	0
2	BR	JJ	202	1/1	0.99	0.04	41,41,41,41	0
2	BR	JJ	204	1/1	0.99	0.05	49,49,49,49	0
2	BR	C	311	1/1	0.99	0.03	46,46,46,46	0
2	BR	KK	203	1/1	0.99	0.04	62,62,62,62	0
2	BR	KK	206	1/1	0.99	0.06	45,45,45,45	0
2	BR	KK	207	1/1	0.99	0.05	41,41,41,41	0
2	BR	KK	209	1/1	0.99	0.03	57,57,57,57	0
3	MG	D	302	1/1	0.99	0.05	34,34,34,34	0
2	BR	C	312	1/1	0.99	0.03	64,64,64,64	0
3	MG	G	502	1/1	0.99	0.06	27,27,27,27	0
2	BR	C	313	1/1	0.99	0.03	60,60,60,60	0
3	MG	K	201	1/1	0.99	0.05	21,21,21,21	0
3	MG	O	502	1/1	0.99	0.05	21,21,21,21	0
2	BR	F	604	1/1	1.00	0.03	44,44,44,44	0
2	BR	J	210	1/1	1.00	0.06	50,50,50,50	0
2	BR	K	202	1/1	1.00	0.05	42,42,42,42	0
2	BR	K	203	1/1	1.00	0.05	46,46,46,46	0
2	BR	F	605	1/1	1.00	0.06	45,45,45,45	0
2	BR	K	205	1/1	1.00	0.07	47,47,47,47	0
2	BR	B	210	1/1	1.00	0.04	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BR	K	207	1/1	1.00	0.04	48,48,48,48	0
2	BR	L	1001	1/1	1.00	0.07	22,22,22,22	0
2	BR	D	303	1/1	1.00	0.07	45,45,45,45	0
2	BR	L	1003	1/1	1.00	0.05	41,41,41,41	0
2	BR	F	608	1/1	1.00	0.04	52,52,52,52	0
2	BR	D	304	1/1	1.00	0.06	47,47,47,47	0
2	BR	G	501	1/1	1.00	0.09	26,26,26,26	0
2	BR	G	503	1/1	1.00	0.06	44,44,44,44	0
2	BR	L	1008	1/1	1.00	0.04	41,41,41,41	0
2	BR	G	504	1/1	1.00	0.06	38,38,38,38	0
2	BR	M	502	1/1	1.00	0.04	38,38,38,38	0
2	BR	B	201	1/1	1.00	0.08	30,30,30,30	0
2	BR	M	504	1/1	1.00	0.03	40,40,40,40	0
2	BR	M	505	1/1	1.00	0.02	41,41,41,41	0
2	BR	M	506	1/1	1.00	0.01	45,45,45,45	0
2	BR	A	701	1/1	1.00	0.05	25,25,25,25	0
2	BR	B	203	1/1	1.00	0.08	40,40,40,40	0
2	BR	N	1301	1/1	1.00	0.08	22,22,22,22	0
2	BR	G	508	1/1	1.00	0.02	44,44,44,44	0
2	BR	N	1303	1/1	1.00	0.04	28,28,28,28	1
2	BR	N	1304	1/1	1.00	0.06	36,36,36,36	0
2	BR	N	1305	1/1	1.00	0.07	38,38,38,38	0
2	BR	D	308	1/1	1.00	0.03	38,38,38,38	0
2	BR	H	201	1/1	1.00	0.05	45,45,45,45	0
2	BR	N	1308	1/1	1.00	0.04	42,42,42,42	0
2	BR	H	203	1/1	1.00	0.03	58,58,58,58	0
2	BR	N	1310	1/1	1.00	0.04	51,51,51,51	0
2	BR	N	1311	1/1	1.00	0.05	48,48,48,48	0
2	BR	N	1312	1/1	1.00	0.03	43,43,43,43	0
2	BR	H	204	1/1	1.00	0.08	39,39,39,39	0
2	BR	O	501	1/1	1.00	0.07	35,35,35,35	0
2	BR	H	205	1/1	1.00	0.05	41,41,41,41	0
2	BR	O	504	1/1	1.00	0.06	43,43,43,43	0
2	BR	H	206	1/1	1.00	0.02	43,43,43,43	0
2	BR	D	309	1/1	1.00	0.09	47,47,47,47	0
2	BR	O	507	1/1	1.00	0.04	45,45,45,45	0
2	BR	H	208	1/1	1.00	0.03	39,39,39,39	0
2	BR	O	509	1/1	1.00	0.04	46,46,46,46	0
2	BR	E	401	1/1	1.00	0.10	28,28,28,28	0
2	BR	C	303	1/1	1.00	0.08	41,41,41,41	0
2	BR	GG	201	1/1	1.00	0.09	43,43,43,43	0
2	BR	GG	202	1/1	1.00	0.08	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BR	GG	203	1/1	1.00	0.09	83,83,83,83	0
2	BR	GG	204	1/1	1.00	0.05	50,50,50,50	0
2	BR	C	304	1/1	1.00	0.04	46,46,46,46	0
2	BR	GG	206	1/1	1.00	0.05	45,45,45,45	0
2	BR	C	305	1/1	1.00	0.06	48,48,48,48	0
2	BR	GG	208	1/1	1.00	0.05	38,38,38,38	0
2	BR	GG	209	1/1	1.00	0.05	47,47,47,47	0
2	BR	GG	210	1/1	1.00	0.03	41,41,41,41	0
2	BR	GG	211	1/1	1.00	0.02	42,42,42,42	0
2	BR	GG	212	1/1	1.00	0.06	48,48,48,48	0
2	BR	C	306	1/1	1.00	0.05	39,39,39,39	0
2	BR	GG	214	1/1	1.00	0.04	43,43,43,43	0
2	BR	I	201	1/1	1.00	0.06	43,43,43,43	0
2	BR	GG	216	1/1	1.00	0.05	28,28,28,28	1
2	BR	GG	217	1/1	1.00	0.03	79,79,79,79	1
2	BR	GG	218	1/1	1.00	0.02	45,45,45,45	0
2	BR	HH	201	1/1	1.00	0.06	44,44,44,44	0
2	BR	I	202	1/1	1.00	0.06	44,44,44,44	0
2	BR	HH	203	1/1	1.00	0.04	40,40,40,40	0
2	BR	HH	204	1/1	1.00	0.06	51,51,51,51	0
2	BR	HH	205	1/1	1.00	0.07	45,45,45,45	0
2	BR	HH	206	1/1	1.00	0.04	45,45,45,45	0
2	BR	I	203	1/1	1.00	0.05	42,42,42,42	0
2	BR	II	202	1/1	1.00	0.09	40,40,40,40	0
2	BR	II	203	1/1	1.00	0.08	35,35,35,35	0
2	BR	II	204	1/1	1.00	0.06	34,34,34,34	0
2	BR	I	204	1/1	1.00	0.06	44,44,44,44	0
2	BR	II	206	1/1	1.00	0.04	38,38,38,38	0
2	BR	II	207	1/1	1.00	0.05	45,45,45,45	0
2	BR	II	208	1/1	1.00	0.03	49,49,49,49	0
2	BR	II	209	1/1	1.00	0.03	45,45,45,45	0
2	BR	II	210	1/1	1.00	0.03	50,50,50,50	0
2	BR	JJ	201	1/1	1.00	0.04	36,36,36,36	0
2	BR	I	205	1/1	1.00	0.06	38,38,38,38	0
2	BR	JJ	203	1/1	1.00	0.04	37,37,37,37	0
2	BR	I	206	1/1	1.00	0.05	42,42,42,42	0
2	BR	JJ	205	1/1	1.00	0.04	48,48,48,48	0
2	BR	KK	201	1/1	1.00	0.05	37,37,37,37	0
2	BR	I	207	1/1	1.00	0.03	53,53,53,53	0
2	BR	C	307	1/1	1.00	0.05	74,74,74,74	0
2	BR	KK	204	1/1	1.00	0.02	55,55,55,55	0
2	BR	KK	205	1/1	1.00	0.02	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BR	B	204	1/1	1.00	0.05	52,52,52,52	0
2	BR	B	205	1/1	1.00	0.04	43,43,43,43	0
2	BR	KK	208	1/1	1.00	0.02	43,43,43,43	0
2	BR	A	708	1/1	1.00	0.07	46,46,46,46	0
3	MG	A	706	1/1	1.00	0.07	23,23,23,23	0
2	BR	A	704	1/1	1.00	0.06	52,52,52,52	0
2	BR	A	702	1/1	1.00	0.06	26,26,26,26	0
2	BR	J	205	1/1	1.00	0.05	41,41,41,41	0
2	BR	J	206	1/1	1.00	0.04	41,41,41,41	0
2	BR	J	207	1/1	1.00	0.04	47,47,47,47	0
2	BR	B	209	1/1	1.00	0.03	47,47,47,47	0
3	MG	II	201	1/1	1.00	0.07	16,16,16,16	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.