



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 6, 2021 – 02:16 PM EST

PDB ID : 7M54
Title : Crystallographic structure of a cubic crystal form of STMV grown from bromide
Authors : McPherson, A.
Deposited on : 2021-03-22
Resolution : 3.80 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

<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	:	2.24
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)	:	2.24

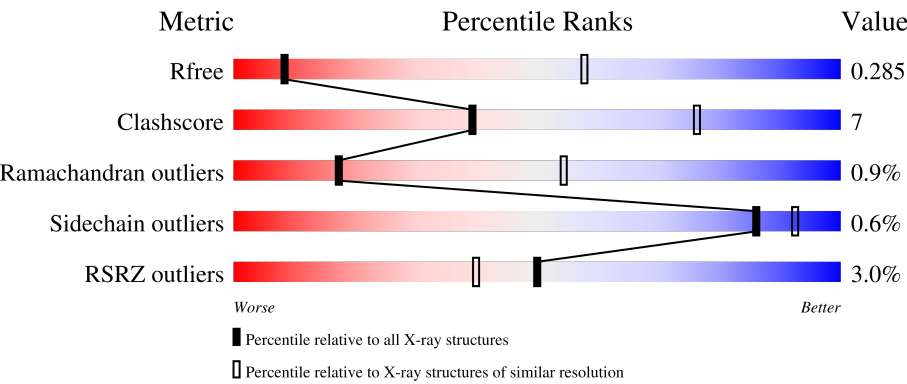
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	B	159	
1	C	159	
1	D	159	
1	E	159	

Continued on next page...

Continued from previous page...

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
3	BR	A	403	-	-	X	-
3	BR	B	202	-	-	X	-
3	BR	B	210	-	-	X	-
3	BR	C	203	-	-	-	X
3	BR	C	205	-	-	X	-
3	BR	D	202	-	-	X	-
3	BR	D	214	-	-	-	X
3	BR	E	201	-	-	X	-
3	BR	E	208	-	-	X	-
3	BR	G	203	-	-	X	-
3	BR	G	204	-	-	X	-
3	BR	G	205	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BR	G	208	-	-	X	-
3	BR	G	211	-	-	X	-
3	BR	GG	304	-	-	X	-
3	BR	GG	312	-	-	X	-
3	BR	HH	201	-	-	X	-
3	BR	HH	210	-	-	X	-
3	BR	I	203	-	-	X	-
3	BR	I	205	-	-	-	X
3	BR	II	205	-	-	X	-
3	BR	II	208	-	-	X	-
3	BR	J	208	-	-	X	-
3	BR	K	206	-	-	X	-
3	BR	KK	202	-	-	X	-
3	BR	KK	214	-	-	X	-
3	BR	KK	218	-	-	-	X
3	BR	L	201	-	-	X	-
3	BR	L	202	-	-	X	-
3	BR	N	202	-	-	X	-
3	BR	N	203	-	-	X	-
3	BR	N	204	-	-	X	-
3	BR	O	203	-	-	X	-
5	CL	F	301	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 47048 atoms, of which 22612 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
1	A	144	Total	C	H	N	O	S	0	13	0
			2267	716	1134	200	210	7			
1	B	144	Total	C	H	N	O	S	0	12	0
			2218	707	1095	199	210	7			
1	C	145	Total	C	H	N	O	S	0	21	0
			2242	712	1107	202	215	6			
1	D	145	Total	C	H	N	O	S	1	20	0
			2256	712	1123	201	214	6			
1	E	154	Total	C	H	N	O	S	2	18	0
			2302	752	1103	215	225	7			
1	F	150	Total	C	H	N	O	S	3	14	0
			2306	737	1129	211	222	7			
1	G	155	Total	C	H	N	O	S	2	15	0
			2341	765	1124	218	227	7			
1	H	157	Total	C	H	N	O	S	0	20	0
			2413	788	1161	225	232	7			
1	I	153	Total	C	H	N	O	S	0	13	0
			2327	751	1129	215	225	7			
1	J	157	Total	C	H	N	O	S	0	15	0
			2383	781	1138	225	232	7			
1	K	154	Total	C	H	N	O	S	1	13	0
			2370	766	1149	219	230	6			
1	L	158	Total	C	H	N	O	S	1	15	0
			2469	802	1194	228	237	8			
1	M	151	Total	C	H	N	O	S	1	9	0
			2373	757	1168	215	226	7			
1	N	144	Total	C	H	N	O	S	1	13	0
			2321	728	1167	201	216	9			
1	O	149	Total	C	H	N	O	S	0	22	0
			2271	725	1114	205	221	6			
1	GG	146	Total	C	H	N	O	S	0	19	0
			2252	713	1117	201	214	7			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	HH	148	Total	C	H	N	O	S	3	16	0
			2308	732	1145	204	220	7			
1	II	151	Total	C	H	N	O	S	1	15	0
			2287	740	1106	211	222	8			
1	JJ	151	Total	C	H	N	O	S	0	16	0
			2266	727	1107	207	219	6			
1	KK	154	Total	C	H	N	O	S	2	13	0
			2296	748	1102	215	225	6			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	G	1	Total	Ca	0	0
			1	1		
2	H	1	Total	Ca	0	0
			1	1		
2	J	1	Total	Ca	0	0
			1	1		
2	GG	1	Total	Ca	0	0
			1	1		
2	JJ	1	Total	Ca	0	0
			1	1		

- Molecule 3 is BROMIDE ION (three-letter code: BR) (formula: Br) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total	Br	0	0
			9	9		
3	B	12	Total	Br	0	0
			12	12		
3	C	3	Total	Br	0	0
			3	3		
3	D	15	Total	Br	0	0
			15	15		
3	E	10	Total	Br	0	0
			10	10		
3	F	7	Total	Br	0	0
			7	7		
3	G	12	Total	Br	0	0
			12	12		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	10	Total 10	Br 10	0	0
3	I	5	Total 5	Br 5	0	0
3	J	7	Total 7	Br 7	0	0
3	K	8	Total 8	Br 8	0	0
3	L	11	Total 11	Br 11	0	0
3	M	5	Total 5	Br 5	0	0
3	N	4	Total 4	Br 4	0	0
3	O	5	Total 5	Br 5	0	0
3	GG	13	Total 13	Br 13	0	0
3	HH	11	Total 11	Br 11	0	0
3	II	9	Total 9	Br 9	0	0
3	JJ	9	Total 9	Br 9	0	0
3	KK	17	Total 17	Br 17	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Mg 1	0	0
4	F	2	Total 2	Mg 2	0	0
4	G	1	Total 1	Mg 1	0	0
4	H	1	Total 1	Mg 1	0	0
4	O	1	Total 1	Mg 1	0	0
4	II	1	Total 1	Mg 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	JJ	1	Total 1	Mg 1	0	0
4	KK	1	Total 1	Mg 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	2	Total 2	Cl 2	0	0
5	F	1	Total 1	Cl 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	18	Total 18	O 18	0	0
6	B	22	Total 22	O 22	0	0
6	C	13	Total 13	O 13	0	0
6	D	30	Total 30	O 30	0	0
6	E	39	Total 39	O 39	0	0
6	F	40	Total 40	O 40	0	0
6	G	52	Total 52	O 52	0	0
6	H	36	Total 36	O 36	0	0
6	I	17	Total 17	O 17	0	0
6	J	43	Total 43	O 43	0	0
6	K	37	Total 37	O 37	0	0
6	L	13	Total 13	O 13	0	0
6	M	22	Total 22	O 22	0	0

Continued on next page...


Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	N	18	Total 18	O 18	0	0
6	O	40	Total 40	O 40	0	0
6	GG	27	Total 27	O 27	0	0
6	HH	40	Total 40	O 40	0	0
6	II	32	Total 32	O 32	0	0
6	JJ	20	Total 20	O 20	0	0
6	KK	21	Total 21	O 21	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.

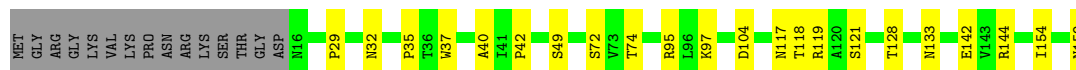
- Molecule 1: Coat protein

Chain A: 




- Molecule 1: Coat protein

Chain B: 




- Molecule 1: Coat protein

Chain C: 




- Molecule 1: Coat protein

Chain D: 

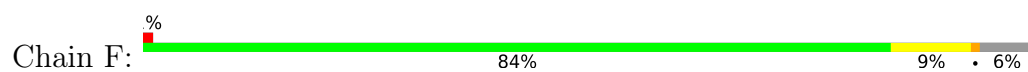


- Molecule 1: Coat protein

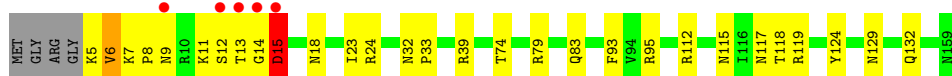
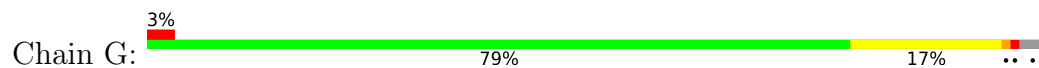
Chain E: 



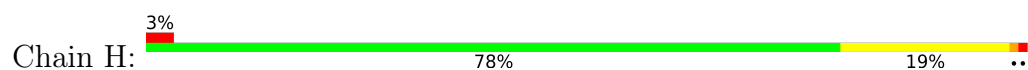
- Molecule 1: Coat protein



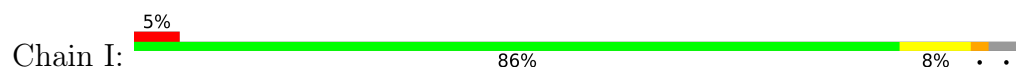
• Molecule 1: Coat protein



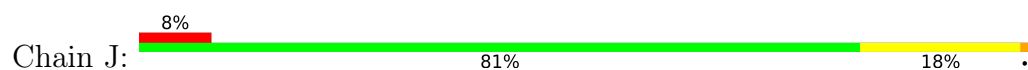
• Molecule 1: Coat protein



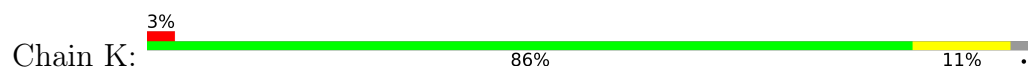
• Molecule 1: Coat protein



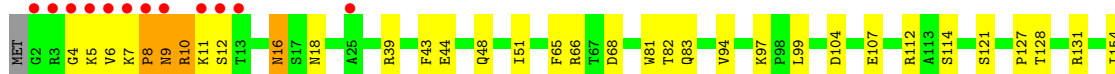
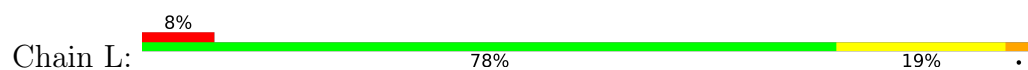
• Molecule 1: Coat protein



• Molecule 1: Coat protein

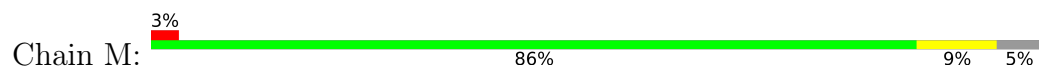


• Molecule 1: Coat protein

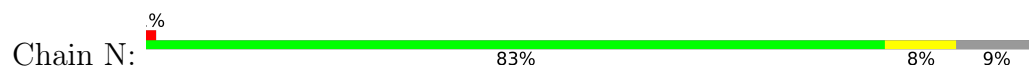




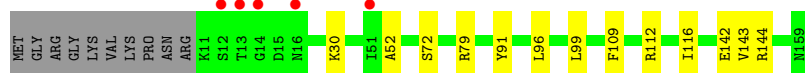
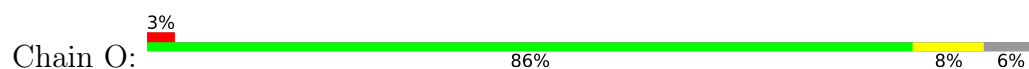
- Molecule 1: Coat protein



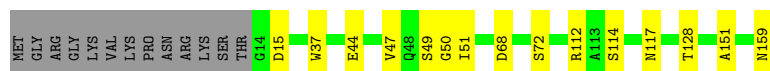
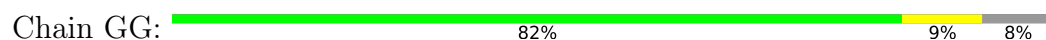
- Molecule 1: Coat protein



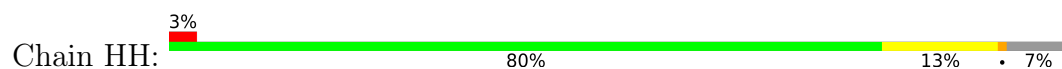
- Molecule 1: Coat protein



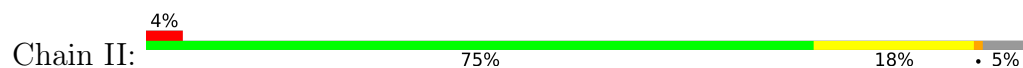
- Molecule 1: Coat protein



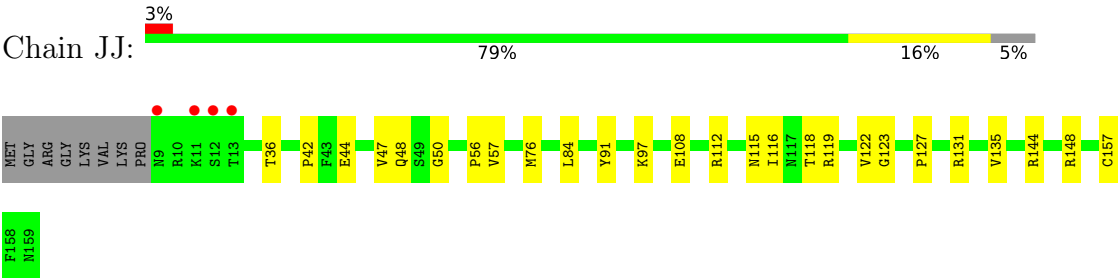
- Molecule 1: Coat protein



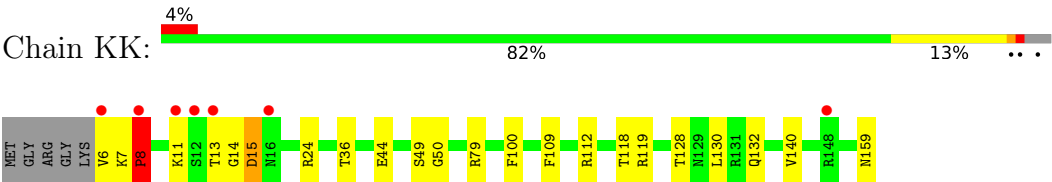
- Molecule 1: Coat protein



- Molecule 1: Coat protein



● Molecule 1: Coat protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 3	Depositor
Cell constants a, b, c, α , β , γ	234.65Å 234.65Å 234.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.91 – 3.80 47.90 – 3.80	Depositor EDS
% Data completeness (in resolution range)	78.8 (56.91-3.80) 62.3 (47.90-3.80)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.213 , 0.285 0.195 , 0.285	Depositor DCC
R_{free} test set	25249 reflections (95.09%)	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 63.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.038 for l,-k,h	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	47048	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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, 0.333 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: CA, MG, CL, BR

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	0.33	0/1166	0.57	0/1587
1	B	0.32	0/1150	0.56	0/1566
1	C	0.30	0/1159	0.55	0/1579
1	D	0.32	0/1185	0.56	0/1615
1	E	0.34	0/1254	0.56	0/1705
1	F	0.32	0/1247	0.55	0/1696
1	G	0.29	0/1279	0.56	0/1739
1	GG	0.32	0/1169	0.56	0/1592
1	H	0.33	0/1320	0.61	1/1794 (0.1%)
1	HH	0.31	0/1227	0.54	0/1672
1	I	0.34	0/1229	0.59	0/1671
1	II	0.31	0/1246	0.56	0/1693
1	J	0.32	0/1305	0.57	0/1771
1	JJ	0.33	0/1183	0.56	0/1611
1	K	0.35	0/1301	0.56	0/1772
1	KK	0.32	0/1246	0.56	0/1695
1	L	0.30	0/1362	0.55	0/1849
1	M	0.30	0/1269	0.56	0/1725
1	N	0.30	0/1230	0.54	0/1675
1	O	0.30	0/1184	0.55	0/1612
All	All	0.32	0/24711	0.56	1/33619 (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	E	0	1
1	G	0	2
1	H	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	1
All	All	0	5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	17	SER	CA-C-N	-6.42	103.08	117.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	12	SER	Peptide
1	G	11	LYS	Peptide
1	G	15	ASP	Peptide
1	H	17	SER	Mainchain
1	I	15	ASP	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	1133	1134	1105	12	0
1	B	1123	1095	1099	15	2
1	C	1135	1107	1063	14	2
1	D	1133	1123	1061	15	1
1	E	1199	1103	1146	18	0
1	F	1177	1129	1107	15	0
1	G	1217	1124	1181	42	0
1	GG	1135	1117	1060	15	2
1	H	1252	1161	1217	23	2
1	HH	1163	1145	1116	18	1
1	I	1198	1129	1167	15	1
1	II	1181	1106	1137	35	0
1	J	1245	1138	1225	25	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	JJ	1159	1107	1112	16	0
1	K	1221	1149	1167	18	0
1	KK	1194	1102	1146	20	0
1	L	1275	1194	1267	28	2
1	M	1205	1168	1196	10	1
1	N	1154	1167	1121	15	1
1	O	1157	1114	1094	11	0
2	A	1	0	0	0	0
2	G	1	0	0	0	0
2	GG	1	0	0	0	0
2	H	1	0	0	0	0
2	J	1	0	0	0	0
2	JJ	1	0	0	0	0
3	A	9	0	0	7	0
3	B	12	0	0	8	0
3	C	3	0	0	3	1
3	D	15	0	0	6	0
3	E	10	0	0	5	0
3	F	7	0	0	1	0
3	G	12	0	0	21	0
3	GG	13	0	0	9	0
3	H	10	0	0	3	0
3	HH	11	0	0	6	0
3	I	5	0	0	7	0
3	II	9	0	0	6	0
3	J	7	0	0	5	0
3	JJ	9	0	0	1	0
3	K	8	0	0	6	0
3	KK	17	0	0	8	0
3	L	11	0	0	8	1
3	M	5	0	0	1	0
3	N	4	0	0	9	0
3	O	5	0	0	2	0
4	B	1	0	0	0	0
4	F	2	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	II	1	0	0	0	0
4	JJ	1	0	0	0	0
4	KK	1	0	0	0	0
4	O	1	0	0	0	0
5	C	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	1	0	0	6	0
6	A	18	0	0	0	0
6	B	22	0	0	1	0
6	C	13	0	0	0	0
6	D	30	0	0	0	0
6	E	39	0	0	0	0
6	F	40	0	0	1	0
6	G	52	0	0	0	0
6	GG	27	0	0	0	0
6	H	36	0	0	2	0
6	HH	40	0	0	0	0
6	I	17	0	0	1	0
6	II	32	0	0	0	0
6	J	43	0	0	0	0
6	JJ	20	0	0	0	0
6	K	37	0	0	0	0
6	KK	21	0	0	0	0
6	L	13	0	0	0	0
6	M	22	0	0	0	0
6	N	18	0	0	1	0
6	O	40	0	0	0	0
All	All	24436	22612	22787	352	9

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 7.

The worst 5 of 352 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:G:32:ASN:CB	3:G:208:BR:BR	2.20	1.44
1:G:32:ASN:HB2	3:G:208:BR:BR	1.72	1.44
1:GG:128:THR:HG22	3:GG:304:BR:BR	1.71	1.44
1:K:49[A]:SER:CB	3:K:206:BR:BR	2.25	1.40
1:B:128:THR:HG22	3:B:202:BR:BR	1.82	1.34

The worst 5 of 9 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GG:68[A]:ASP:OD1	3:C:204:BR:BR[6_566]	2.00	0.20

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:ASN:O	1:H:39:ARG:NH2[12_665]	2.06	0.14
1:L:81:TRP:HE1	1:M:26:GLY:O[6_566]	1.47	0.13
1:C:30:LYS:HZ2	1:HH:121:SER:O[12_665]	1.48	0.12
1:D:104:ASP:O	1:GG:72:SER:OG[12_665]	2.08	0.12

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	145/159 (91%)	133 (92%)	11 (8%)	1 (1%)	22	60
1	B	143/159 (90%)	133 (93%)	7 (5%)	3 (2%)	7	40
1	C	144/159 (91%)	130 (90%)	14 (10%)	0	100	100
1	D	147/159 (92%)	137 (93%)	10 (7%)	0	100	100
1	E	156/159 (98%)	145 (93%)	10 (6%)	1 (1%)	25	62
1	F	155/159 (98%)	137 (88%)	16 (10%)	2 (1%)	12	48
1	G	159/159 (100%)	142 (89%)	16 (10%)	1 (1%)	25	62
1	GG	146/159 (92%)	126 (86%)	20 (14%)	0	100	100
1	H	165/159 (104%)	139 (84%)	22 (13%)	4 (2%)	6	37
1	HH	154/159 (97%)	144 (94%)	9 (6%)	1 (1%)	25	62
1	I	153/159 (96%)	139 (91%)	11 (7%)	3 (2%)	7	41
1	II	155/159 (98%)	137 (88%)	16 (10%)	2 (1%)	12	48
1	J	162/159 (102%)	146 (90%)	15 (9%)	1 (1%)	25	62
1	JJ	149/159 (94%)	135 (91%)	13 (9%)	1 (1%)	22	60
1	K	162/159 (102%)	149 (92%)	13 (8%)	0	100	100
1	KK	155/159 (98%)	132 (85%)	20 (13%)	3 (2%)	8	42
1	L	171/159 (108%)	146 (85%)	22 (13%)	3 (2%)	8	42
1	M	158/159 (99%)	146 (92%)	12 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	154/159 (97%)	136 (88%)	18 (12%)	0	100	100
1	O	148/159 (93%)	137 (93%)	11 (7%)	0	100	100
All	All	3081/3180 (97%)	2769 (90%)	286 (9%)	26 (1%)	17	57

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	6	VAL
1	H	9	ASN
1	I	8	PRO
1	L	8	PRO
1	L	10	ARG

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	131/140 (94%)	130 (99%)	1 (1%)	81	89
1	B	129/140 (92%)	128 (99%)	1 (1%)	81	89
1	C	130/140 (93%)	130 (100%)	0	100	100
1	D	133/140 (95%)	133 (100%)	0	100	100
1	E	141/140 (101%)	140 (99%)	1 (1%)	84	91
1	F	140/140 (100%)	139 (99%)	1 (1%)	84	91
1	G	144/140 (103%)	143 (99%)	1 (1%)	84	91
1	GG	131/140 (94%)	130 (99%)	1 (1%)	81	89
1	H	149/140 (106%)	146 (98%)	3 (2%)	55	75
1	HH	139/140 (99%)	137 (99%)	2 (1%)	67	81
1	I	138/140 (99%)	138 (100%)	0	100	100
1	II	140/140 (100%)	140 (100%)	0	100	100
1	J	146/140 (104%)	145 (99%)	1 (1%)	84	91
1	JJ	131/140 (94%)	131 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	147/140 (105%)	147 (100%)	0	100	100
1	KK	140/140 (100%)	138 (99%)	2 (1%)	67	81
1	L	154/140 (110%)	153 (99%)	1 (1%)	86	92
1	M	142/140 (101%)	142 (100%)	0	100	100
1	N	140/140 (100%)	140 (100%)	0	100	100
1	O	133/140 (95%)	133 (100%)	0	100	100
All	All	2778/2800 (99%)	2763 (100%)	15 (0%)	86	94

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	156	CYS
1	KK	8	PRO
1	J	17	SER
1	KK	132	GLN
1	HH	138	ASP

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

Mol	Chain	Res	Type
1	A	16	ASN
1	G	32	ASN

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

Of 200 ligands modelled in this entry, 200 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

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, 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	144/159 (90%)	-0.30	0	100	100	58, 80, 103, 151	3 (2%)
1	B	144/159 (90%)	-0.24	0	100	100	58, 78, 102, 128	3 (2%)
1	C	145/159 (91%)	-0.30	0	100	100	55, 76, 98, 128	2 (1%)
1	D	145/159 (91%)	-0.14	1 (0%)	87	83	51, 75, 104, 136	6 (4%)
1	E	154/159 (96%)	-0.20	7 (4%)	33	28	54, 77, 128, 194	6 (3%)
1	F	150/159 (94%)	-0.31	1 (0%)	87	83	54, 81, 119, 162	2 (1%)
1	G	155/159 (97%)	0.12	5 (3%)	47	38	57, 83, 127, 173	3 (1%)
1	GG	146/159 (91%)	-0.09	0	100	100	50, 73, 101, 172	5 (3%)
1	H	157/159 (98%)	-0.02	5 (3%)	47	38	55, 84, 134, 175	6 (3%)
1	HH	148/159 (93%)	-0.02	5 (3%)	45	37	57, 77, 114, 195	2 (1%)
1	I	153/159 (96%)	-0.08	8 (5%)	27	24	60, 78, 141, 184	4 (2%)
1	II	151/159 (94%)	-0.04	7 (4%)	32	28	50, 76, 128, 206	5 (3%)
1	J	157/159 (98%)	0.15	12 (7%)	13	11	64, 83, 124, 158	4 (2%)
1	JJ	151/159 (94%)	-0.13	4 (2%)	56	47	47, 72, 132, 191	2 (1%)
1	K	154/159 (96%)	0.13	5 (3%)	47	38	60, 85, 129, 183	3 (1%)
1	KK	154/159 (96%)	-0.05	7 (4%)	33	28	54, 73, 143, 225	2 (1%)
1	L	158/159 (99%)	0.43	12 (7%)	13	11	70, 96, 175, 215	1 (0%)
1	M	151/159 (94%)	0.26	5 (3%)	46	38	65, 98, 144, 215	1 (0%)
1	N	144/159 (90%)	0.17	2 (1%)	75	68	60, 92, 133, 172	0
1	O	149/159 (93%)	0.06	5 (3%)	45	37	66, 87, 142, 200	7 (4%)
All	All	3010/3180 (94%)	-0.03	91 (3%)	50	40	47, 81, 131, 225	67 (2%)

The worst 5 of 91 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	6	VAL	8.7
1	L	8	PRO	7.5
1	HH	12	SER	6.5
1	HH	13	THR	6.1
1	L	4	GLY	6.1

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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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, 95th 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(Å ²)	Q<0.9
3	BR	KK	218	1/1	0.26	0.76	290,290,290,290	1
3	BR	H	208	1/1	0.33	0.38	161,161,161,161	0
3	BR	G	212	1/1	0.44	0.23	119,119,119,119	0
3	BR	JJ	211	1/1	0.45	0.25	164,164,164,164	0
3	BR	O	204	1/1	0.49	0.29	148,148,148,148	0
3	BR	II	204	1/1	0.49	0.29	156,156,156,156	0
3	BR	B	212	1/1	0.61	0.38	150,150,150,150	0
3	BR	A	410	1/1	0.67	0.21	137,137,137,137	0
3	BR	D	205	1/1	0.67	0.28	118,118,118,118	0
3	BR	A	407	1/1	0.69	0.24	135,135,135,135	0
3	BR	J	207	1/1	0.70	0.27	144,144,144,144	0
3	BR	E	207	1/1	0.71	0.16	141,141,141,141	0
3	BR	F	310	1/1	0.72	0.39	189,189,189,189	0
3	BR	E	206	1/1	0.73	0.24	122,122,122,122	0
3	BR	L	206	1/1	0.74	0.20	144,144,144,144	0
3	BR	GG	310	1/1	0.74	0.21	119,119,119,119	0
3	BR	KK	210	1/1	0.74	0.27	130,130,130,130	0
3	BR	II	203	1/1	0.74	0.23	118,118,118,118	0
3	BR	C	203	1/1	0.75	0.43	150,150,150,150	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	BR	D	214	1/1	0.76	0.68	273,273,273,273	1
3	BR	H	210	1/1	0.76	0.24	129,129,129,129	0
3	BR	H	212	1/1	0.76	0.14	129,129,129,129	0
3	BR	E	210	1/1	0.76	0.24	130,130,130,130	0
3	BR	B	206	1/1	0.77	0.23	152,152,152,152	0
3	BR	KK	206	1/1	0.78	0.28	159,159,159,159	0
3	BR	HH	203	1/1	0.78	0.21	122,122,122,122	0
3	BR	I	205	1/1	0.78	0.50	121,121,121,121	0
3	BR	KK	205	1/1	0.79	0.18	117,117,117,117	0
3	BR	II	206	1/1	0.80	0.25	113,113,113,113	0
3	BR	D	209	1/1	0.80	0.18	119,119,119,119	0
3	BR	B	213	1/1	0.80	0.31	178,178,178,178	0
5	CL	C	201	1/1	0.80	0.20	103,103,103,103	0
3	BR	GG	314	1/1	0.81	0.28	154,154,154,154	0
3	BR	M	205	1/1	0.81	0.12	193,193,193,193	1
3	BR	K	204	1/1	0.81	0.22	122,122,122,122	0
3	BR	E	209	1/1	0.81	0.34	147,147,147,147	0
3	BR	GG	311	1/1	0.81	0.14	136,136,136,136	0
3	BR	II	209	1/1	0.81	0.32	141,141,141,141	0
3	BR	D	212	1/1	0.82	0.20	118,118,118,118	0
3	BR	G	209	1/1	0.82	0.31	141,141,141,141	0
3	BR	J	208	1/1	0.82	0.31	235,235,235,235	0
3	BR	K	203	1/1	0.83	0.26	135,135,135,135	0
3	BR	JJ	208	1/1	0.83	0.22	135,135,135,135	0
3	BR	F	304	1/1	0.83	0.12	142,142,142,142	0
3	BR	D	211	1/1	0.83	0.16	128,128,128,128	0
3	BR	D	208	1/1	0.84	0.22	149,149,149,149	0
3	BR	L	204	1/1	0.84	0.17	145,145,145,145	0
2	CA	G	202	1/1	0.84	0.31	74,74,74,74	0
3	BR	JJ	209	1/1	0.84	0.18	117,117,117,117	0
3	BR	L	208	1/1	0.84	0.15	129,129,129,129	0
3	BR	B	210	1/1	0.85	0.26	129,129,129,129	0
3	BR	HH	202	1/1	0.85	0.21	128,128,128,128	0
2	CA	GG	301	1/1	0.85	0.18	104,104,104,104	0
3	BR	F	305	1/1	0.85	0.18	85,85,85,85	0
3	BR	GG	307	1/1	0.85	0.17	124,124,124,124	0
3	BR	C	205	1/1	0.85	0.56	163,163,163,163	0
3	BR	L	207	1/1	0.85	0.20	135,135,135,135	0
3	BR	II	210	1/1	0.85	0.27	120,120,120,120	0
2	CA	J	202	1/1	0.86	0.28	90,90,90,90	0
3	BR	B	203	1/1	0.86	0.22	117,117,117,117	0
3	BR	L	202	1/1	0.86	0.22	177,177,177,177	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MG	F	302	1/1	0.86	0.45	78,78,78,78	0
4	MG	F	303	1/1	0.86	0.75	167,167,167,167	0
4	MG	KK	201	1/1	0.86	0.27	40,40,40,40	0
3	BR	B	205	1/1	0.86	0.17	110,110,110,110	0
3	BR	F	308	1/1	0.87	0.25	130,130,130,130	0
3	BR	F	309	1/1	0.87	0.25	117,117,117,117	0
3	BR	J	203	1/1	0.87	0.17	118,118,118,118	0
3	BR	H	204	1/1	0.87	0.21	178,178,178,178	0
3	BR	E	205	1/1	0.87	0.14	116,116,116,116	0
3	BR	G	207	1/1	0.87	0.10	122,122,122,122	0
3	BR	K	208	1/1	0.88	0.35	128,128,128,128	0
3	BR	L	211	1/1	0.88	0.44	127,127,127,127	0
3	BR	D	215	1/1	0.88	0.15	155,155,155,155	0
3	BR	N	202	1/1	0.88	0.15	158,158,158,158	0
3	BR	N	203	1/1	0.88	0.37	171,171,171,171	0
3	BR	L	203	1/1	0.88	0.15	99,99,99,99	0
3	BR	G	214	1/1	0.88	0.36	147,147,147,147	0
3	BR	I	203	1/1	0.88	0.31	134,134,134,134	0
4	MG	H	203	1/1	0.88	0.99	94,94,94,94	0
3	BR	JJ	206	1/1	0.88	0.12	105,105,105,105	0
3	BR	K	207	1/1	0.88	0.24	109,109,109,109	0
3	BR	A	409	1/1	0.89	0.17	142,142,142,142	0
3	BR	J	204	1/1	0.89	0.18	114,114,114,114	0
3	BR	K	205	1/1	0.89	0.16	111,111,111,111	0
4	MG	G	201	1/1	0.89	0.28	48,48,48,48	0
3	BR	HH	205	1/1	0.89	0.17	133,133,133,133	0
3	BR	O	202	1/1	0.89	0.23	145,145,145,145	0
3	BR	JJ	207	1/1	0.89	0.13	107,107,107,107	0
3	BR	KK	211	1/1	0.90	0.26	130,130,130,130	0
3	BR	KK	214	1/1	0.90	0.10	94,94,94,94	0
3	BR	II	202	1/1	0.90	0.26	113,113,113,113	0
3	BR	G	206	1/1	0.90	0.24	117,117,117,117	0
2	CA	A	401	1/1	0.90	0.33	90,90,90,90	0
3	BR	E	208	1/1	0.90	0.15	104,104,104,104	0
3	BR	H	209	1/1	0.90	0.27	142,142,142,142	0
3	BR	F	307	1/1	0.90	0.11	94,94,94,94	0
3	BR	GG	308	1/1	0.90	0.27	119,119,119,119	0
3	BR	B	207	1/1	0.91	0.14	128,128,128,128	0
3	BR	B	208	1/1	0.91	0.13	97,97,97,97	0
3	BR	GG	306	1/1	0.91	0.10	104,104,104,104	0
3	BR	H	211	1/1	0.91	0.09	132,132,132,132	0
3	BR	II	207	1/1	0.91	0.23	123,123,123,123	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	BR	E	201	1/1	0.91	0.12	74,74,74,74	0
3	BR	E	202	1/1	0.91	0.21	109,109,109,109	0
3	BR	L	210	1/1	0.91	0.24	196,196,196,196	1
3	BR	K	206	1/1	0.91	0.10	116,116,116,116	0
3	BR	E	203	1/1	0.91	0.11	89,89,89,89	0
3	BR	H	207	1/1	0.91	0.10	76,76,76,76	0
3	BR	A	408	1/1	0.91	0.28	112,112,112,112	0
3	BR	M	204	1/1	0.92	0.25	165,165,165,165	1
3	BR	II	205	1/1	0.92	0.16	109,109,109,109	0
3	BR	KK	208	1/1	0.92	0.48	130,130,130,130	0
3	BR	GG	309	1/1	0.92	0.15	95,95,95,95	0
3	BR	L	205	1/1	0.92	0.14	127,127,127,127	0
3	BR	D	210	1/1	0.92	0.20	115,115,115,115	0
3	BR	D	204	1/1	0.92	0.13	106,106,106,106	0
3	BR	G	213	1/1	0.92	0.14	139,139,139,139	0
3	BR	J	205	1/1	0.92	0.14	110,110,110,110	0
3	BR	GG	305	1/1	0.92	0.15	107,107,107,107	0
3	BR	I	204	1/1	0.92	0.12	145,145,145,145	0
3	BR	M	202	1/1	0.92	0.12	106,106,106,106	0
3	BR	KK	204	1/1	0.92	0.13	96,96,96,96	0
3	BR	KK	209	1/1	0.93	0.14	123,123,123,123	0
3	BR	G	203	1/1	0.93	0.15	135,135,135,135	0
2	CA	H	202	1/1	0.93	0.14	53,53,53,53	0
3	BR	KK	212	1/1	0.93	0.12	123,123,123,123	0
3	BR	A	403	1/1	0.93	0.12	96,96,96,96	0
3	BR	KK	215	1/1	0.93	0.23	123,123,123,123	0
3	BR	KK	216	1/1	0.93	0.21	124,124,124,124	0
3	BR	JJ	210	1/1	0.93	0.11	129,129,129,129	0
3	BR	B	211	1/1	0.93	0.23	122,122,122,122	0
3	BR	G	211	1/1	0.93	0.25	125,125,125,125	0
3	BR	HH	204	1/1	0.93	0.28	99,99,99,99	0
3	BR	F	306	1/1	0.93	0.12	99,99,99,99	0
3	BR	KK	207	1/1	0.93	0.11	91,91,91,91	0
3	BR	L	209	1/1	0.93	0.29	142,142,142,142	0
3	BR	M	203	1/1	0.94	0.14	93,93,93,93	0
3	BR	G	210	1/1	0.94	0.07	113,113,113,113	0
3	BR	HH	208	1/1	0.94	0.16	126,126,126,126	0
3	BR	HH	211	1/1	0.94	0.33	130,130,130,130	0
3	BR	H	206	1/1	0.94	0.10	84,84,84,84	0
3	BR	N	201	1/1	0.94	0.24	138,138,138,138	0
3	BR	KK	203	1/1	0.94	0.11	116,116,116,116	0
3	BR	I	202	1/1	0.94	0.17	107,107,107,107	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	BR	B	209	1/1	0.94	0.23	101,101,101,101	0
3	BR	GG	313	1/1	0.94	0.11	118,118,118,118	0
3	BR	D	213	1/1	0.94	0.38	116,116,116,116	1
4	MG	II	201	1/1	0.94	0.19	90,90,90,90	0
3	BR	D	207	1/1	0.94	0.13	115,115,115,115	0
3	BR	A	405	1/1	0.94	0.12	79,79,79,79	0
3	BR	JJ	203	1/1	0.95	0.09	81,81,81,81	0
3	BR	JJ	204	1/1	0.95	0.09	106,106,106,106	0
3	BR	JJ	205	1/1	0.95	0.15	92,92,92,92	0
3	BR	O	206	1/1	0.95	0.28	118,118,118,118	0
3	BR	HH	210	1/1	0.95	0.10	136,136,136,136	0
3	BR	GG	312	1/1	0.95	0.11	123,123,123,123	0
3	BR	C	204	1/1	0.95	0.28	143,143,143,143	0
3	BR	A	404	1/1	0.95	0.09	115,115,115,115	0
3	BR	HH	201	1/1	0.95	0.13	107,107,107,107	0
3	BR	G	204	1/1	0.95	0.16	103,103,103,103	0
3	BR	G	205	1/1	0.95	0.08	95,95,95,95	0
3	BR	K	202	1/1	0.95	0.07	114,114,114,114	0
3	BR	II	208	1/1	0.95	0.12	98,98,98,98	0
3	BR	E	204	1/1	0.95	0.08	101,101,101,101	0
3	BR	HH	207	1/1	0.95	0.21	109,109,109,109	0
5	CL	C	202	1/1	0.95	0.13	35,35,35,35	0
3	BR	KK	217	1/1	0.96	0.20	70,70,70,70	1
3	BR	J	206	1/1	0.96	0.09	100,100,100,100	0
3	BR	O	203	1/1	0.96	0.11	110,110,110,110	0
3	BR	B	204	1/1	0.96	0.10	98,98,98,98	0
3	BR	L	201	1/1	0.96	0.11	101,101,101,101	0
3	BR	GG	303	1/1	0.96	0.08	93,93,93,93	0
4	MG	O	201	1/1	0.96	0.15	55,55,55,55	0
3	BR	KK	213	1/1	0.96	0.24	112,112,112,112	0
3	BR	GG	304	1/1	0.96	0.10	49,49,49,49	1
3	BR	D	206	1/1	0.96	0.10	111,111,111,111	0
3	BR	A	406	1/1	0.96	0.12	90,90,90,90	0
3	BR	D	201	1/1	0.97	0.07	81,81,81,81	0
3	BR	GG	302	1/1	0.97	0.10	84,84,84,84	0
3	BR	D	203	1/1	0.97	0.15	106,106,106,106	0
3	BR	HH	209	1/1	0.97	0.10	113,113,113,113	0
4	MG	JJ	202	1/1	0.97	0.55	85,85,85,85	0
2	CA	JJ	201	1/1	0.97	0.14	50,50,50,50	0
3	BR	A	402	1/1	0.97	0.10	86,86,86,86	0
3	BR	O	205	1/1	0.97	0.24	127,127,127,127	0
5	CL	F	301	1/1	0.97	0.16	86,86,86,86	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	BR	H	205	1/1	0.98	0.14	96,96,96,96	0
3	BR	G	208	1/1	0.98	0.13	154,154,154,154	0
3	BR	H	201	1/1	0.98	0.08	88,88,88,88	0
3	BR	N	204	1/1	0.98	0.14	125,125,125,125	0
3	BR	M	201	1/1	0.98	0.41	114,114,114,114	1
3	BR	B	202	1/1	0.98	0.14	51,51,51,51	1
3	BR	J	201	1/1	0.98	0.06	85,85,85,85	0
3	BR	K	201	1/1	0.98	0.08	91,91,91,91	0
3	BR	I	201	1/1	0.98	0.16	83,83,83,83	1
3	BR	HH	206	1/1	0.98	0.10	104,104,104,104	0
4	MG	B	201	1/1	0.99	0.37	174,174,174,174	0
3	BR	D	202	1/1	0.99	0.10	81,81,81,81	1
3	BR	KK	202	1/1	1.00	0.19	72,72,72,72	1

6.5 Other polymers ⓘ

There are no such residues in this entry.