wwPDB EM Validation Summary Report

Jun 26, 2025 – 12:27 AM JST

PDB ID	:	8XY6 / pdb_00008xy6
EMDB ID	:	EMD-38767
Title	:	ASFV RNAP M1249L C-tail occupied complex3 (MCOC3)
Authors	:	Zhu, G.L.; Zhu, Y.; Zhu, Z.X.; Sun, F.; Zheng, H.X.
Deposited on	:	2024-01-19
Resolution	:	3.00 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp
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.

The following versions of software and data (see references ⓘ) were used in the production of this report:

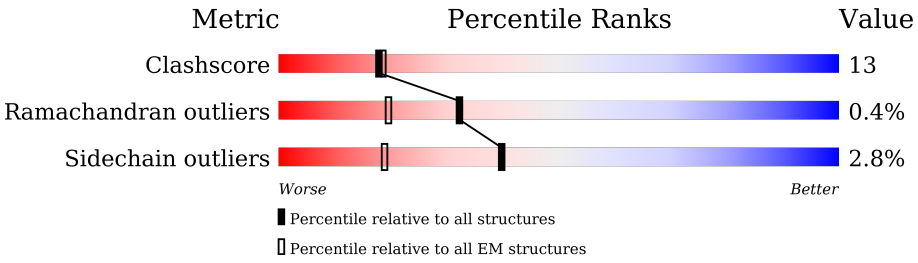
EMDB validation analysis	:	FAILED
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	1441	65% 31% • •
2	B	1235	66% 30% • •
3	C	358	73% 25% •
4	D	205	68% 31%
5	E	130	57% 26% • 16%
6	F	151	44% 17% • 37%
7	G	105	62% 36% •
8	H	80	64% 36%
9	I	577	63% 23% • 14%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 32407 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1410	11216	7120	1949	2085	62	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1200	9492	6003	1662	1777	50	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase RPB3-11 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	358	2907	1885	481	529	12	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase RPB5 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	205	1669	1088	278	295	8	0	0

- Molecule 5 is a protein called C147L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	109	869	554	147	164	4	0	0

- Molecule 6 is a protein called D339L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	95	758	481	130	141	6	0	0

- Molecule 7 is a protein called C122R.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	105	Total	C	N	O	S	0	0
			816	507	141	153	15		

- Molecule 8 is a protein called DNA-directed RNA polymerase RPB10 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	80	Total	C	N	O	S	0	0
			631	411	102	111	7		

- Molecule 9 is a protein called M1249L.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	497	Total	C	N	O	S	0	0
			4042	2605	655	769	13		

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
10	A	2	Total	Zn	0
			2	2	
10	B	1	Total	Zn	0
			1	1	
10	G	2	Total	Zn	0
			2	2	
10	H	1	Total	Zn	0
			1	1	

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

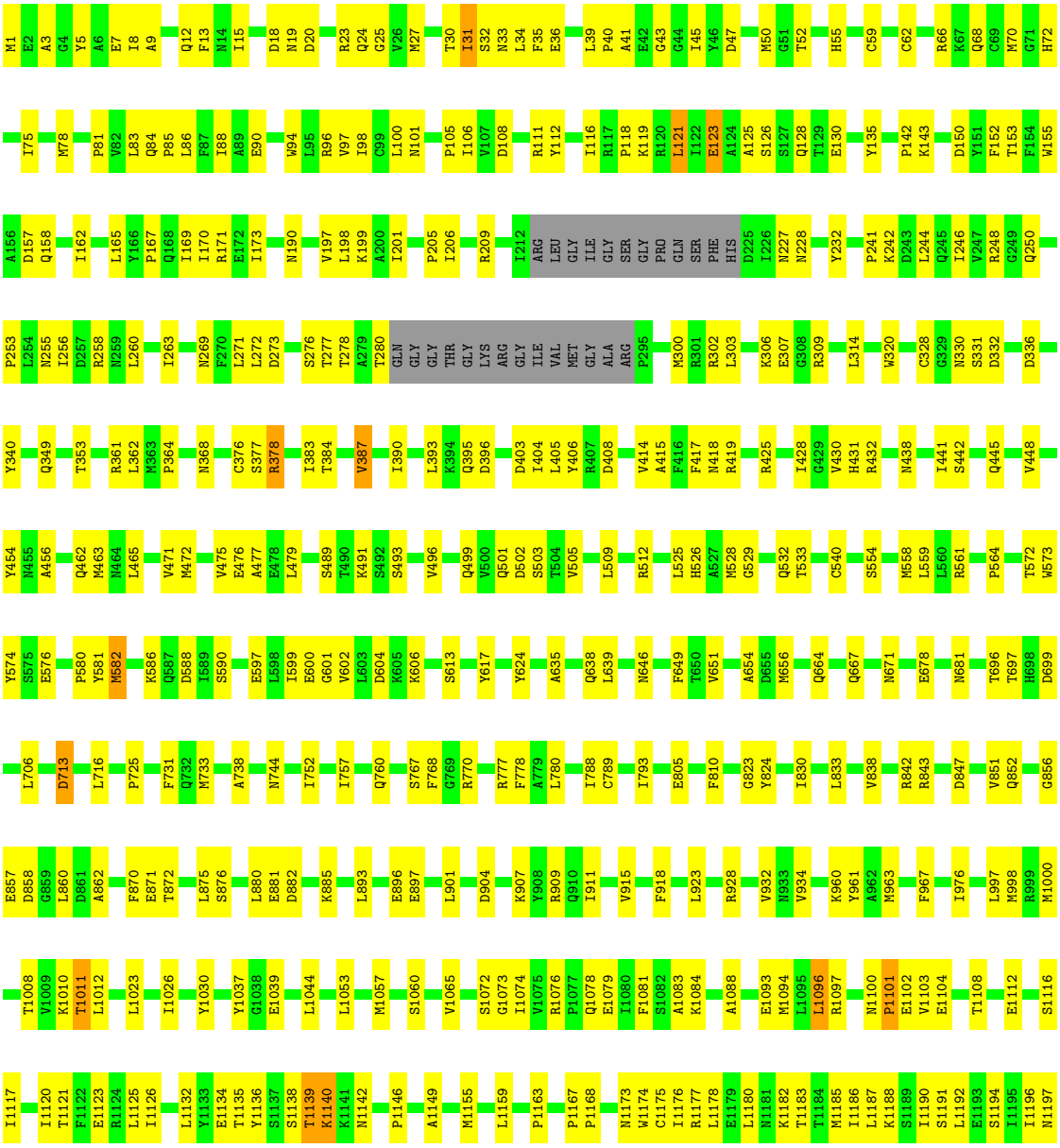
Mol	Chain	Residues	Atoms		AltConf
11	A	1	Total	Mg	0
			1	1	

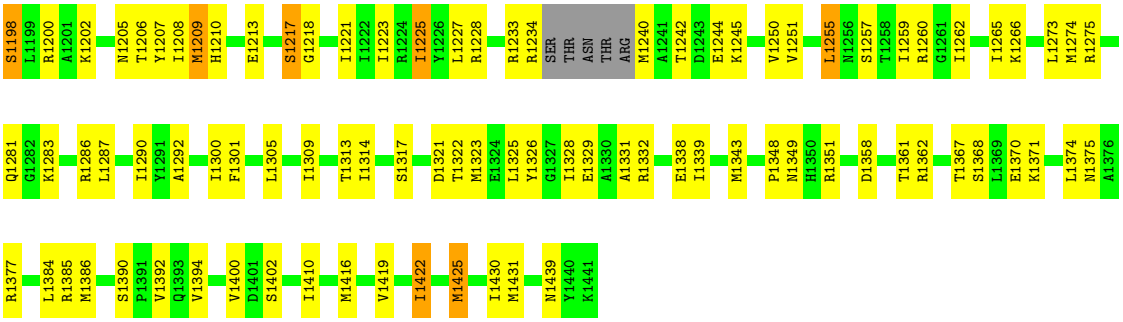
3 Residue-property plots (i)

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. 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. 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: DNA-directed RNA polymerase subunit

Chain A:



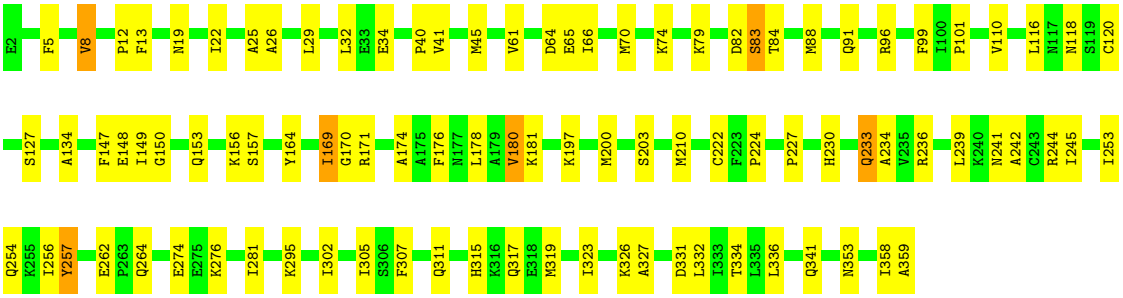


• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain B:

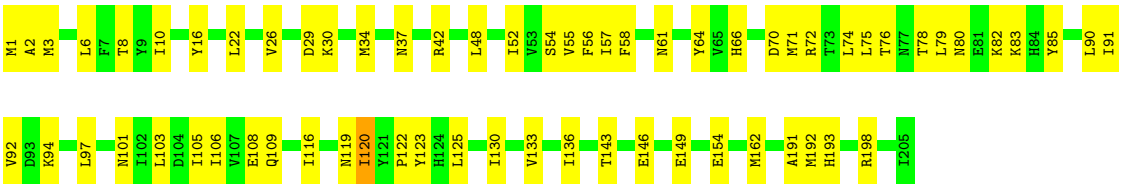
• Molecule 3: DNA-directed RNA polymerase RPB3-11 homolog

Chain C:



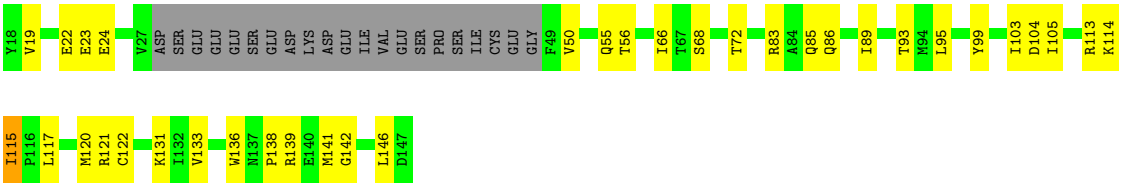
• Molecule 4: DNA-directed RNA polymerase RPB5 homolog

Chain D:



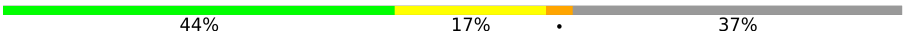
• Molecule 5: C147L

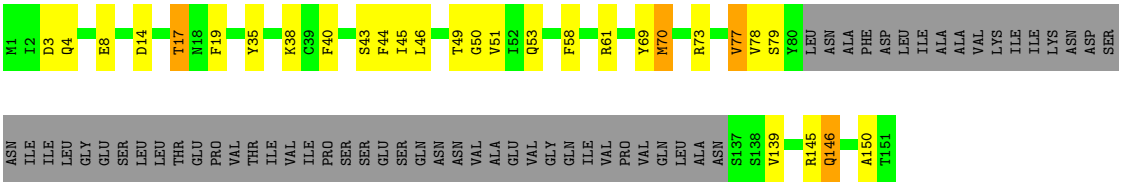
Chain E:



• Molecule 6: D339L

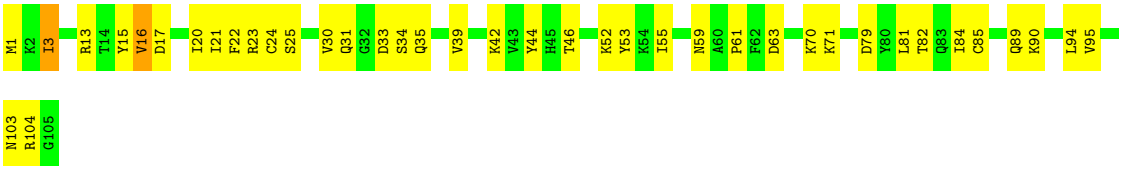
Chain F:





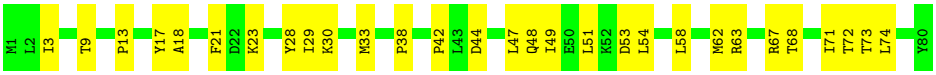
• Molecule 7: C122R

Chain G:



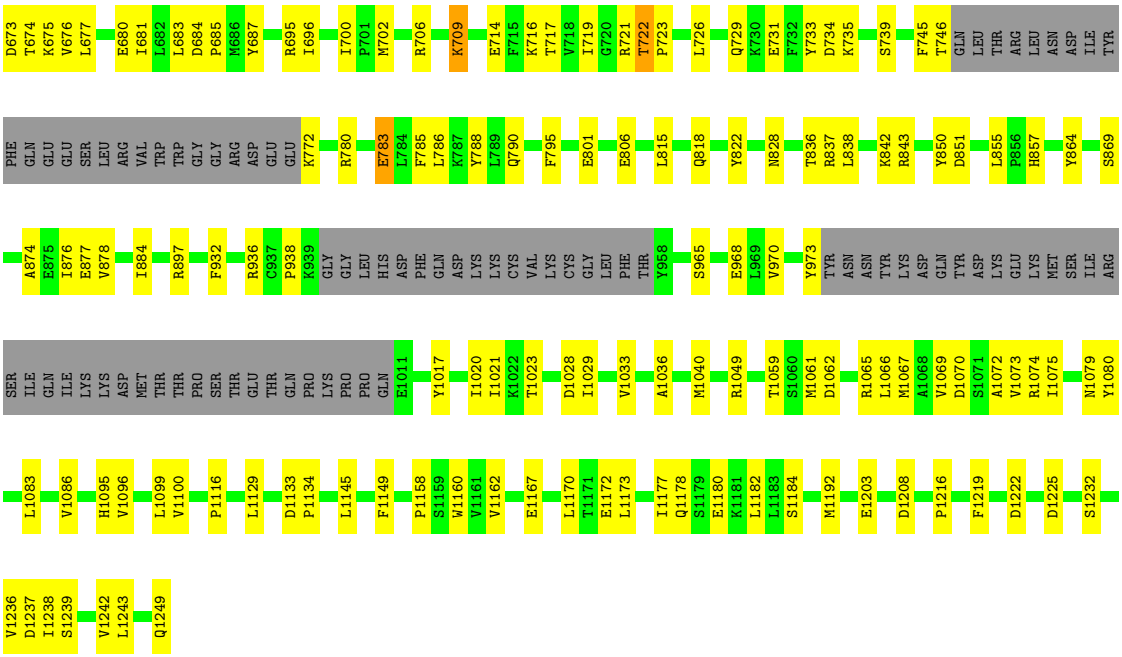
• Molecule 8: DNA-directed RNA polymerase RPB10 homolog

Chain H:



• Molecule 9: M1249L

Chain I:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	60445	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.21	0/11434	0.40	2/15488 (0.0%)
2	B	0.22	0/9680	0.36	0/13094
3	C	0.23	0/2969	0.36	0/4012
4	D	0.19	0/1708	0.44	0/2311
5	E	0.21	0/880	0.40	0/1190
6	F	0.20	0/772	0.44	0/1042
7	G	0.20	0/828	0.41	0/1109
8	H	0.25	0/644	0.38	0/872
9	I	0.17	0/4141	0.36	0/5618
All	All	0.21	0/33056	0.38	2/44736 (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	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1101	PRO	CA-N-CD	-7.76	101.13	112.00
1	A	1163	PRO	CA-N-CD	-6.21	103.30	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1422	ILE	Peptide

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	11216	0	11338	344	0
2	B	9492	0	9449	295	0
3	C	2907	0	2982	70	0
4	D	1669	0	1713	48	0
5	E	869	0	909	28	0
6	F	758	0	751	20	0
7	G	816	0	813	32	0
8	H	631	0	659	27	0
9	I	4042	0	3978	116	0
10	A	2	0	0	0	0
10	B	1	0	0	0	0
10	G	2	0	0	0	0
10	H	1	0	0	0	0
11	A	1	0	0	0	0
All	All	32407	0	32592	851	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 13.

The worst 5 of 851 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)
4:D:1:MET:HE3	4:D:2:ALA:H	1.38	0.87
4:D:10:ILE:HD11	4:D:55:VAL:HG11	1.56	0.87
2:B:98:ARG:NH2	2:B:167:ASN:O	2.10	0.83
2:B:1161:MET:O	2:B:1163:THR:N	2.10	0.83
1:A:1176:ILE:HB	1:A:1225:ILE:HG23	1.65	0.79

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 PDB entries followed by that with respect to all EM entries.

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	1402/1441 (97%)	1328 (95%)	69 (5%)	5 (0%)	30 66
2	B	1186/1235 (96%)	1098 (93%)	83 (7%)	5 (0%)	30 66
3	C	356/358 (99%)	334 (94%)	22 (6%)	0	100 100
4	D	203/205 (99%)	195 (96%)	8 (4%)	0	100 100
5	E	105/130 (81%)	93 (89%)	12 (11%)	0	100 100
6	F	91/151 (60%)	83 (91%)	6 (7%)	2 (2%)	5 27
7	G	103/105 (98%)	96 (93%)	6 (6%)	1 (1%)	13 46
8	H	78/80 (98%)	75 (96%)	3 (4%)	0	100 100
9	I	489/577 (85%)	466 (95%)	21 (4%)	2 (0%)	30 66
All	All	4013/4282 (94%)	3768 (94%)	230 (6%)	15 (0%)	32 66

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	421	SER
2	B	1162	GLN
2	B	1202	ASP
1	A	976	ILE
1	A	1142	ASN

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 PDB entries followed by that with respect to all EM entries.

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	1248/1270 (98%)	1212 (97%)	36 (3%)	37	70
2	B	1042/1074 (97%)	1015 (97%)	27 (3%)	41	72
3	C	327/327 (100%)	320 (98%)	7 (2%)	48	77
4	D	185/185 (100%)	177 (96%)	8 (4%)	25	58
5	E	100/120 (83%)	96 (96%)	4 (4%)	27	61
6	F	86/135 (64%)	82 (95%)	4 (5%)	22	56
7	G	96/96 (100%)	94 (98%)	2 (2%)	48	77
8	H	70/70 (100%)	69 (99%)	1 (1%)	62	83
9	I	447/522 (86%)	435 (97%)	12 (3%)	40	71
All	All	3601/3799 (95%)	3500 (97%)	101 (3%)	40	70

5 of 101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1142	HIS
4	D	48	LEU
9	I	1020	ILE
2	B	1164	ILE
3	C	83	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	364	GLN
9	I	966	GLN
2	B	459	GLN
9	I	1163	ASN
3	C	91	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 7 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.