



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Jun 18, 2018 – 03:40 PM EDT

PDB ID : 5WP9
EMDB ID: : EMD-8874
Title : Structural Basis of Mitochondrial Receptor Binding and Constriction by
Dynamin-Related Protein 1
Authors : Kalia, R.; Wang, R.Y.R.; Yusuf, A.; Thomas, P.V.; Agard, D.A.; Shaw, J.M.;
Frost, A.
Deposited on : 2017-08-03
Resolution : 4.22 Å(reported)

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB 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.

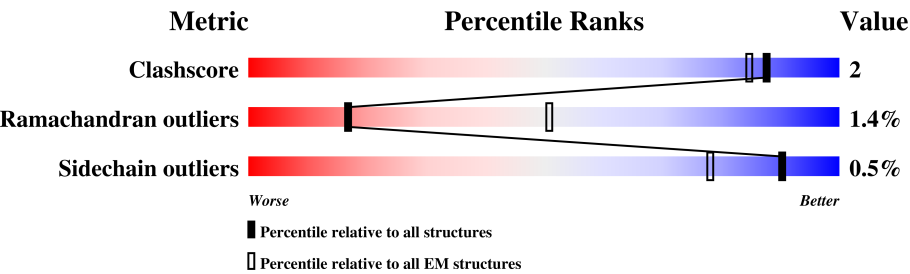
MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031172

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 4.22 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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

Mol	Chain	Length	Quality of chain
1	A	710	
1	C	710	
1	E	710	
1	G	710	
1	I	710	
1	K	710	
1	M	710	
1	O	710	
2	B	329	

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Mol	Chain	Length	Quality of chain
2	D	329	<div><div></div><div>95%</div><div>5%</div></div>
2	F	329	<div><div></div><div>95%</div><div>5%</div></div>
2	H	329	<div><div></div><div>95%</div><div>5%</div></div>
2	J	329	<div><div></div><div>95%</div><div>5%</div></div>
2	L	329	<div><div></div><div>95%</div><div>5%</div></div>
2	N	329	<div><div></div><div>95%</div><div>5%</div></div>
2	P	329	<div><div></div><div>95%</div><div>5%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 117048 atoms, of which 59080 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 Dynamin-1-like protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	590	Total	C	H	N	O	S	0	0
			9471	2946	4806	817	882	20		
1	C	590	Total	C	H	N	O	S	0	0
			9471	2946	4806	817	882	20		
1	E	590	Total	C	H	N	O	S	0	0
			9471	2946	4806	817	882	20		
1	G	590	Total	C	H	N	O	S	0	0
			9471	2946	4806	817	882	20		
1	I	590	Total	C	H	N	O	S	0	0
			9471	2946	4806	817	882	20		
1	K	590	Total	C	H	N	O	S	0	0
			9471	2946	4806	817	882	20		
1	M	590	Total	C	H	N	O	S	0	0
			9471	2946	4806	817	882	20		
1	O	590	Total	C	H	N	O	S	0	0
			9471	2946	4806	817	882	20		

- Molecule 2 is a protein called Mitochondrial dynamics protein MID49.

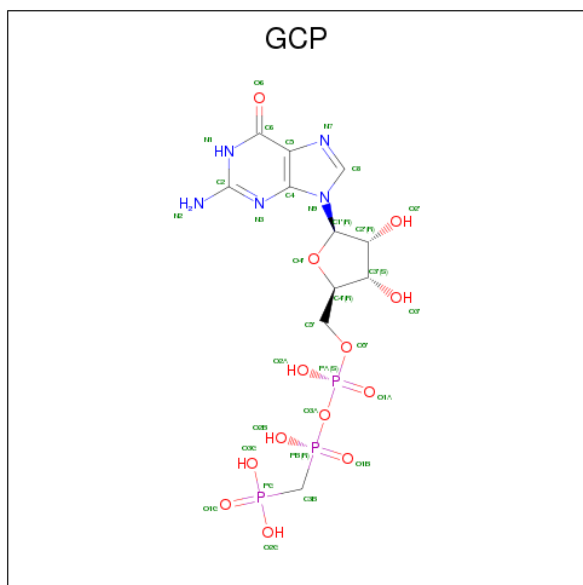
Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	329	Total	C	H	N	O	S	0	0
			5127	1630	2579	445	465	8		
2	D	329	Total	C	H	N	O	S	0	0
			5127	1630	2579	445	465	8		
2	F	329	Total	C	H	N	O	S	0	0
			5127	1630	2579	445	465	8		
2	H	329	Total	C	H	N	O	S	0	0
			5127	1630	2579	445	465	8		
2	J	329	Total	C	H	N	O	S	0	0
			5127	1630	2579	445	465	8		
2	L	329	Total	C	H	N	O	S	0	0
			5127	1630	2579	445	465	8		
2	N	329	Total	C	H	N	O	S	0	0
			5127	1630	2579	445	465	8		

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Mol	Chain	Residues	Atoms						AltConf	Trace
2	P	329	Total	C	H	N	O	S	0	0
			5127	1630	2579	445	465	8		

- Molecule 3 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			32	11	5	13	3	
3	C	1	Total	C	N	O	P	0
			32	11	5	13	3	
3	E	1	Total	C	N	O	P	0
			32	11	5	13	3	
3	G	1	Total	C	N	O	P	0
			32	11	5	13	3	
3	I	1	Total	C	N	O	P	0
			32	11	5	13	3	
3	K	1	Total	C	N	O	P	0
			32	11	5	13	3	
3	M	1	Total	C	N	O	P	0
			32	11	5	13	3	
3	O	1	Total	C	N	O	P	0
			32	11	5	13	3	

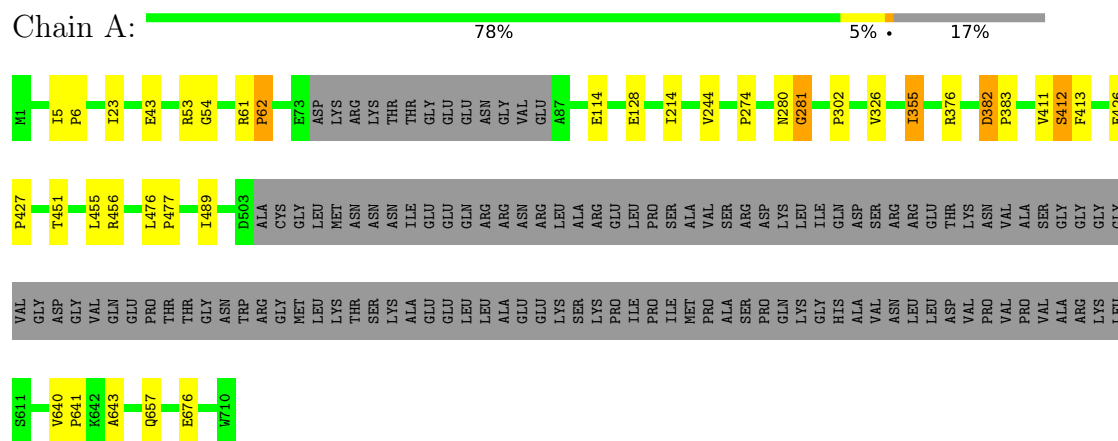
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	G	1	Total 1	Mg 1	0
4	K	1	Total 1	Mg 1	0
4	E	1	Total 1	Mg 1	0
4	I	1	Total 1	Mg 1	0
4	C	1	Total 1	Mg 1	0
4	A	1	Total 1	Mg 1	0
4	O	1	Total 1	Mg 1	0
4	M	1	Total 1	Mg 1	0

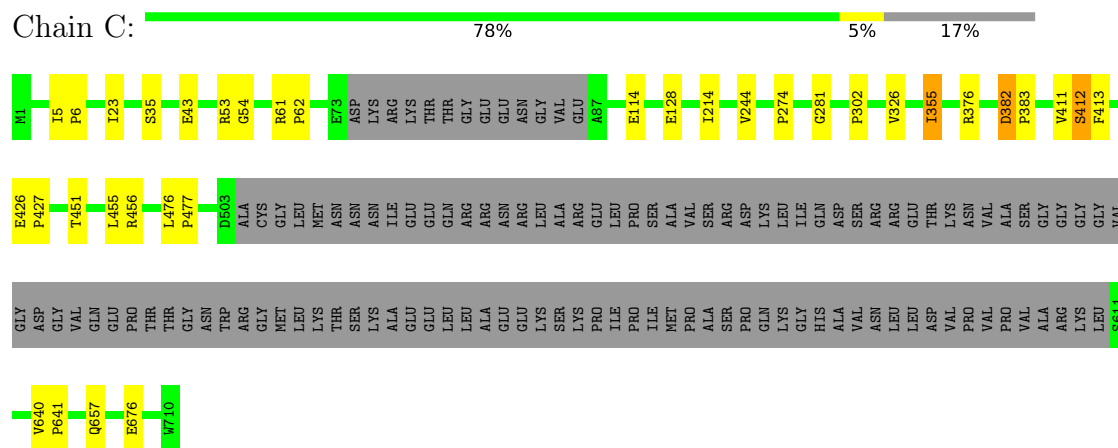
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

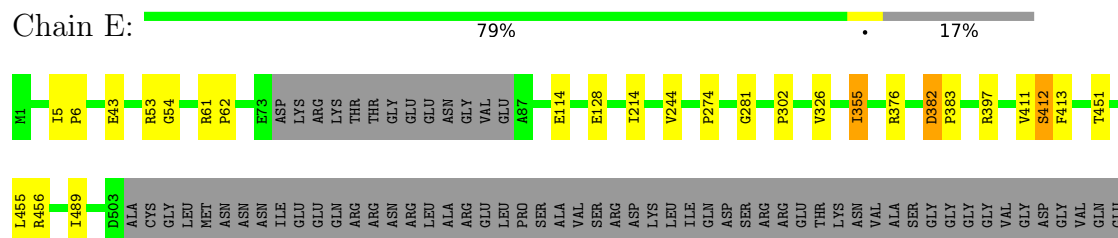
- Molecule 1: Dynamin-1-like protein

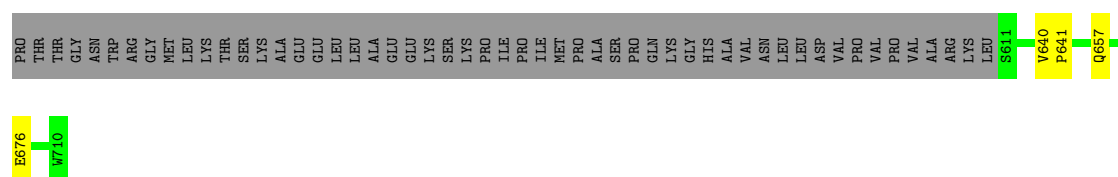


- Molecule 1: Dynamin-1-like protein

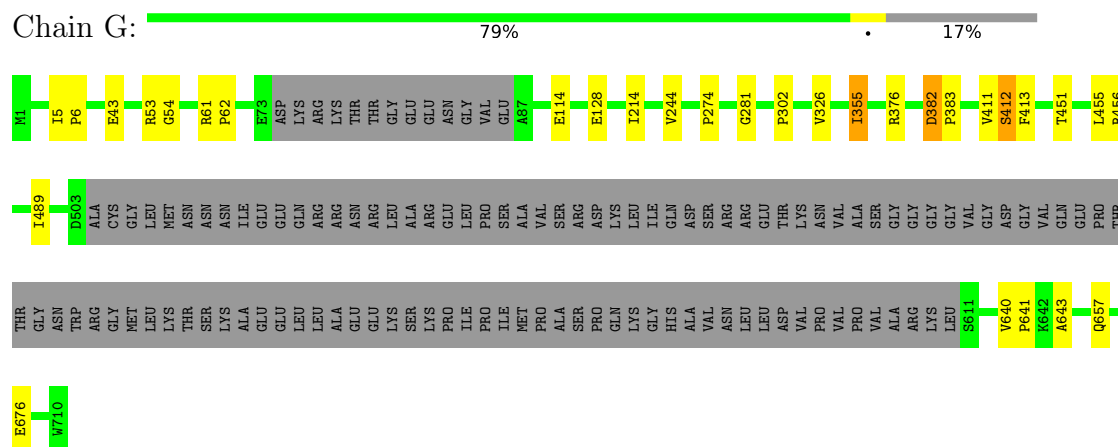


- Molecule 1: Dynamin-1-like protein

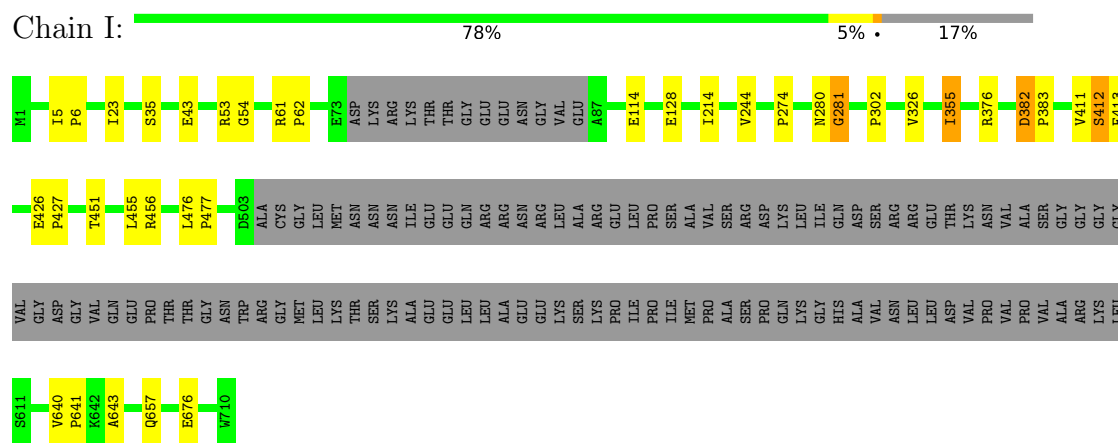




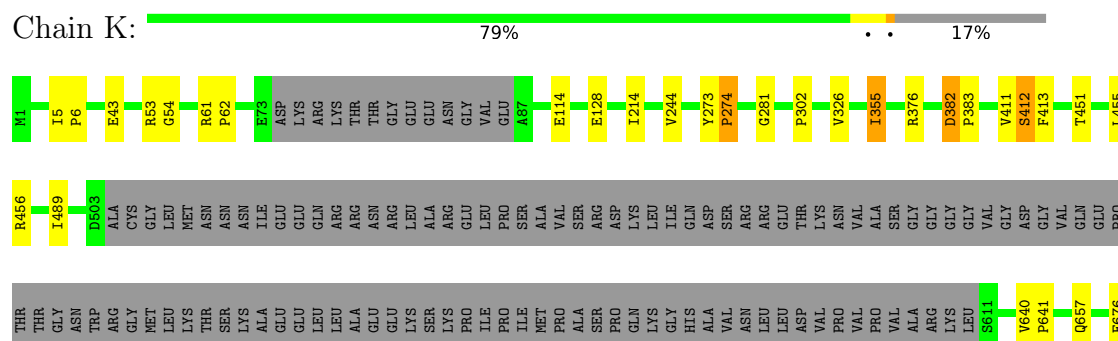
- Molecule 1: Dynamin-1-like protein



- Molecule 1: Dynamin-1-like protein



- Molecule 1: Dynamin-1-like protein





- Molecule 2: Mitochondrial dynamics protein MID49

Chain H: 95% 5%



- Molecule 2: Mitochondrial dynamics protein MID49

Chain J: 95% 5%



- Molecule 2: Mitochondrial dynamics protein MID49

Chain L: 95% 5%



- Molecule 2: Mitochondrial dynamics protein MID49

Chain N: 95% 5%



- Molecule 2: Mitochondrial dynamics protein MID49

Chain P: 95% 5%



4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-0.8°, rise=54.8 Å, axial sym=C1	Depositor
Number of segments used	412684	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	31000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

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: GCP, 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 >2	RMSZ	# Z >2
1	A	0.72	0/4733	0.51	0/6408
1	C	0.72	0/4733	0.51	0/6408
1	E	0.72	0/4733	0.51	0/6408
1	G	0.72	0/4733	0.51	0/6408
1	I	0.72	0/4733	0.51	0/6408
1	K	0.72	0/4733	0.51	0/6408
1	M	0.72	0/4733	0.51	0/6408
1	O	0.72	0/4733	0.51	0/6408
2	B	0.73	0/2601	0.50	0/3543
2	D	0.73	0/2601	0.50	0/3543
2	F	0.73	0/2601	0.50	0/3543
2	H	0.73	0/2601	0.50	0/3543
2	J	0.73	0/2601	0.50	0/3543
2	L	0.73	0/2601	0.50	0/3543
2	N	0.73	0/2601	0.50	0/3543
2	P	0.73	0/2601	0.50	0/3543
All	All	0.72	0/58672	0.51	0/79608

There are no bond length outliers.

There are no bond angle outliers.

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	4665	4806	4804	28	0
1	C	4665	4806	4804	25	0
1	E	4665	4806	4804	23	0
1	G	4665	4806	4804	23	0
1	I	4665	4806	4804	27	0
1	K	4665	4806	4804	23	0
1	M	4665	4806	4804	23	0
1	O	4665	4806	4804	21	0
2	B	2548	2579	2578	9	0
2	D	2548	2579	2578	8	0
2	F	2548	2579	2578	7	0
2	H	2548	2579	2578	7	0
2	J	2548	2579	2578	8	0
2	L	2548	2579	2578	9	0
2	N	2548	2579	2578	7	0
2	P	2548	2579	2578	8	0
3	A	32	0	14	1	0
3	C	32	0	14	2	0
3	E	32	0	14	1	0
3	G	32	0	14	1	0
3	I	32	0	14	2	0
3	K	32	0	14	1	0
3	M	32	0	14	2	0
3	O	32	0	14	1	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
4	M	1	0	0	0	0
4	O	1	0	0	0	0
All	All	57968	59080	59168	246	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 2.

The worst 5 of 246 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:657:GLN:N	1:I:657:GLN:OE1	2.13	0.81
1:A:657:GLN:OE1	1:A:657:GLN:N	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:657:GLN:OE1	1:C:657:GLN:N	2.13	0.80
1:E:657:GLN:OE1	1:E:657:GLN:N	2.13	0.80
1:G:657:GLN:OE1	1:G:657:GLN:N	2.13	0.80

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	584/710 (82%)	548 (94%)	29 (5%)	7 (1%)	14	55
1	C	584/710 (82%)	548 (94%)	29 (5%)	7 (1%)	14	55
1	E	584/710 (82%)	548 (94%)	29 (5%)	7 (1%)	14	55
1	G	584/710 (82%)	548 (94%)	29 (5%)	7 (1%)	14	55
1	I	584/710 (82%)	548 (94%)	29 (5%)	7 (1%)	14	55
1	K	584/710 (82%)	548 (94%)	29 (5%)	7 (1%)	14	55
1	M	584/710 (82%)	548 (94%)	29 (5%)	7 (1%)	14	55
1	O	584/710 (82%)	548 (94%)	29 (5%)	7 (1%)	14	55
2	B	327/329 (99%)	300 (92%)	21 (6%)	6 (2%)	9	47
2	D	327/329 (99%)	300 (92%)	21 (6%)	6 (2%)	9	47
2	F	327/329 (99%)	300 (92%)	21 (6%)	6 (2%)	9	47
2	H	327/329 (99%)	300 (92%)	21 (6%)	6 (2%)	9	47
2	J	327/329 (99%)	301 (92%)	20 (6%)	6 (2%)	9	47
2	L	327/329 (99%)	301 (92%)	20 (6%)	6 (2%)	9	47
2	N	327/329 (99%)	300 (92%)	21 (6%)	6 (2%)	9	47
2	P	327/329 (99%)	300 (92%)	21 (6%)	6 (2%)	9	47
All	All	7288/8312 (88%)	6786 (93%)	398 (6%)	104 (1%)	17	51

5 of 104 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	382	ASP
1	A	412	SER
2	B	292	VAL
1	C	382	ASP
1	C	412	SER

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 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	528/627 (84%)	526 (100%)	2 (0%)	92	95
1	C	528/627 (84%)	526 (100%)	2 (0%)	92	95
1	E	528/627 (84%)	526 (100%)	2 (0%)	92	95
1	G	528/627 (84%)	526 (100%)	2 (0%)	92	95
1	I	528/627 (84%)	526 (100%)	2 (0%)	92	95
1	K	528/627 (84%)	526 (100%)	2 (0%)	92	95
1	M	528/627 (84%)	526 (100%)	2 (0%)	92	95
1	O	528/627 (84%)	526 (100%)	2 (0%)	92	95
2	B	268/268 (100%)	266 (99%)	2 (1%)	85	92
2	D	268/268 (100%)	266 (99%)	2 (1%)	85	92
2	F	268/268 (100%)	266 (99%)	2 (1%)	85	92
2	H	268/268 (100%)	266 (99%)	2 (1%)	85	92
2	J	268/268 (100%)	266 (99%)	2 (1%)	85	92
2	L	268/268 (100%)	266 (99%)	2 (1%)	85	92
2	N	268/268 (100%)	266 (99%)	2 (1%)	85	92
2	P	268/268 (100%)	266 (99%)	2 (1%)	85	92
All	All	6368/7160 (89%)	6336 (100%)	32 (0%)	90	94

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	269	PRO
1	I	302	PRO
1	O	302	PRO
1	I	53	ARG
2	J	269	PRO

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

Mol	Chain	Res	Type
2	D	294	HIS
2	L	294	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GCP	A	801	4	25,34,34	2.84	6 (24%)	31,54,54	1.35	4 (12%)
3	GCP	C	801	4	25,34,34	2.85	6 (24%)	31,54,54	1.35	4 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GCP	E	801	4	25,34,34	2.83	6 (24%)	31,54,54	1.31	3 (9%)
3	GCP	G	801	4	25,34,34	2.83	6 (24%)	31,54,54	1.31	3 (9%)
3	GCP	I	801	4	25,34,34	2.84	6 (24%)	31,54,54	1.35	4 (12%)
3	GCP	K	801	4	25,34,34	2.83	6 (24%)	31,54,54	1.31	3 (9%)
3	GCP	M	801	4	25,34,34	2.85	6 (24%)	31,54,54	1.35	4 (12%)
3	GCP	O	801	4	25,34,34	2.83	6 (24%)	31,54,54	1.31	3 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GCP	A	801	4	-	0/18/38/38	0/3/3/3
3	GCP	C	801	4	-	0/18/38/38	0/3/3/3
3	GCP	E	801	4	-	0/18/38/38	0/3/3/3
3	GCP	G	801	4	-	0/18/38/38	0/3/3/3
3	GCP	I	801	4	-	0/18/38/38	0/3/3/3
3	GCP	K	801	4	-	0/18/38/38	0/3/3/3
3	GCP	M	801	4	-	0/18/38/38	0/3/3/3
3	GCP	O	801	4	-	0/18/38/38	0/3/3/3

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	801	GCP	C4-N9	-12.10	1.31	1.47
3	M	801	GCP	C4-N9	-12.06	1.31	1.47
3	O	801	GCP	C4-N9	-12.06	1.31	1.47
3	A	801	GCP	C4-N9	-12.06	1.31	1.47
3	K	801	GCP	C4-N9	-12.05	1.31	1.47

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	801	GCP	O1G-PG-C3B	-3.23	104.04	111.25
3	M	801	GCP	O1G-PG-C3B	-3.23	104.05	111.25
3	I	801	GCP	O1G-PG-C3B	-3.22	104.07	111.25
3	A	801	GCP	O1G-PG-C3B	-3.21	104.09	111.25
3	G	801	GCP	O1G-PG-C3B	-2.94	104.70	111.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	GCP	1	0
3	C	801	GCP	2	0
3	E	801	GCP	1	0
3	G	801	GCP	1	0
3	I	801	GCP	2	0
3	K	801	GCP	1	0
3	M	801	GCP	2	0
3	O	801	GCP	1	0

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.