



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:56 PM BST

PDB ID : 3JAB  
EMDB ID: : EMD-6258  
Title : Domain organization and conformational plasticity of the G protein effector, PDE6  
Authors : Zhang, Z.; He, F.; Constantine, R.; Baker, M.L.; Baehr, W.; Schmid, M.F.; Wensel, T.G.; Agosto, M.A.  
Deposited on : 2015-05-26  
Resolution : 11.00 Å(reported)  
Based on PDB ID : 3IBJ, 3DBA, 3JWR, 12E8

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

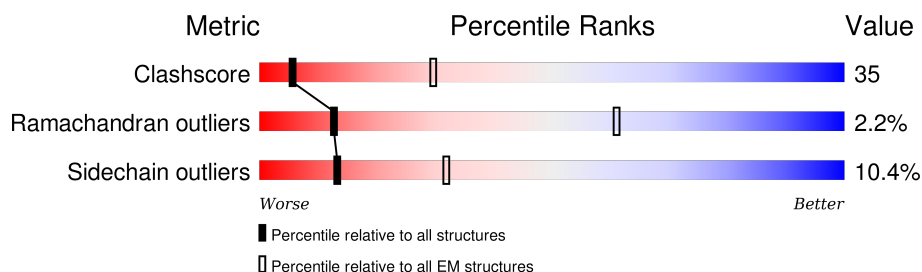
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 11.00 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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  $\geq 3$ , 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	180	67% 26% 5%
1	M	180	67% 26% 5%
2	B	185	21% 43% 19% 13%
2	N	185	19% 44% 19% 13%
3	C	330	57% 38% 5%
3	O	330	57% 38% . .
4	D	18	67% 28% 6%
4	P	18	67% 28% 6%
5	L	214	83% 17%

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Mol	Chain	Length	Quality of chain
5	R	214	 83% 16%
6	H	221	 78% 19% •
6	Q	221	 78% 19% •

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17620 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 GafA domain of cone phosphodiesterase 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	171	Total	C	N	O	S	0	0
			1368	874	230	256	8		
1	M	171	Total	C	N	O	S	0	0
			1368	874	230	256	8		

- Molecule 2 is a protein called GafB domain of phosphodiesterase 2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	161	Total	C	N	O	S	0	0
			1267	805	215	240	7		
2	N	161	Total	C	N	O	S	0	0
			1267	805	215	240	7		

- Molecule 3 is a protein called phosphodiesterase 5/6 chimera catalytic domain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	328	Total	C	N	O	S	0	0
			2671	1700	465	487	19		
3	O	328	Total	C	N	O	S	0	0
			2671	1700	465	487	19		

- Molecule 4 is a protein called phosphodiesterase 6 gamma subunit inhibitory peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	17	Total	C	N	O	0	0
			141	92	23	26		
4	P	17	Total	C	N	O	0	0
			141	92	23	26		

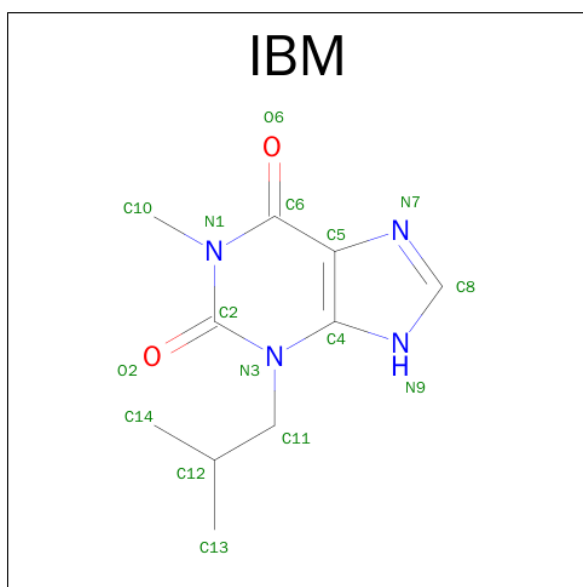
- Molecule 5 is a protein called IgG1-kappa 2E8 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	214	Total	C	N	O	S	0	0
			1649	1020	277	342	10		
5	R	214	Total	C	N	O	S	0	0
			1649	1020	277	342	10		

- Molecule 6 is a protein called IgG1-kappa 2E8 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	221	Total	C	N	O	S	0	0
			1682	1064	276	336	6		
6	Q	221	Total	C	N	O	S	0	0
			1682	1064	276	336	6		

- Molecule 7 is 3-ISOBUTYL-1-METHYLNANTHINE (three-letter code: IBM) (formula:  $C_{10}H_{14}N_4O_2$ ).

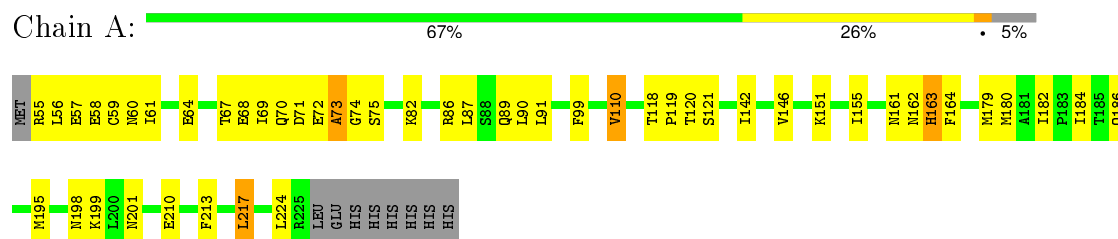


Mol	Chain	Residues	Atoms				AltConf
7	C	1	Total	C	N	O	0
			32	20	8	4	
7	C	1	Total	C	N	O	0
			32	20	8	4	
7	O	1	Total	C	N	O	0
			32	20	8	4	
7	O	1	Total	C	N	O	0
			32	20	8	4	

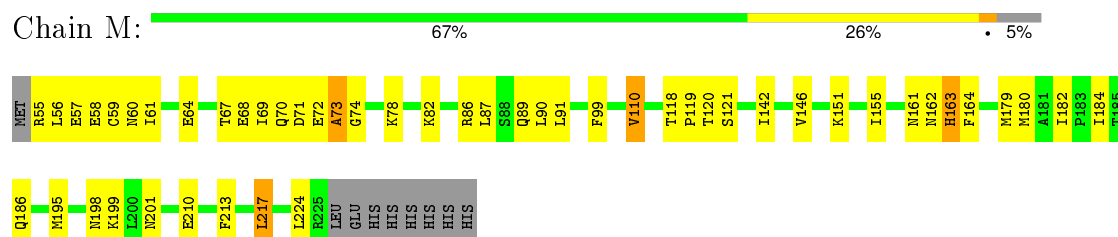
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

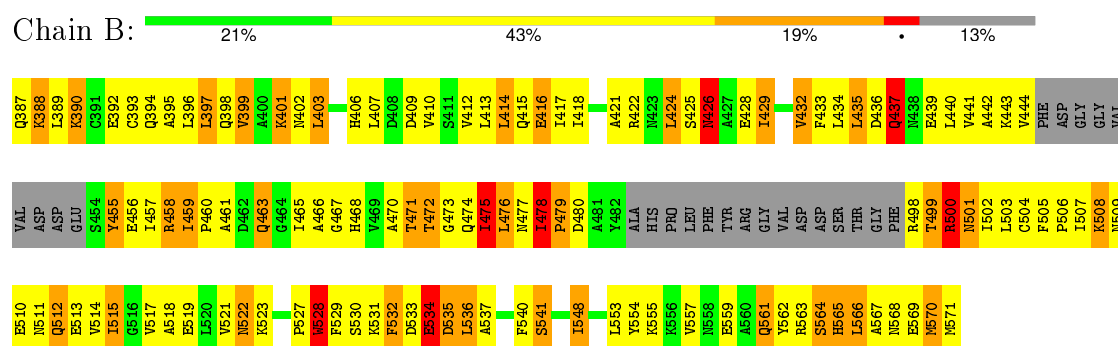
- Molecule 1: GafA domain of cone phosphodiesterase 6C



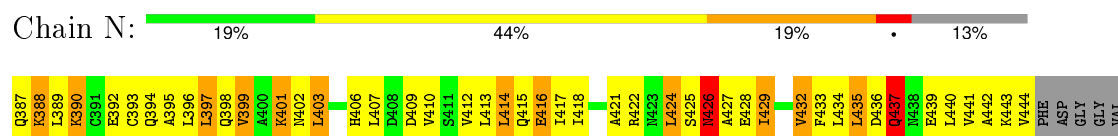
- Molecule 1: GafA domain of cone phosphodiesterase 6C

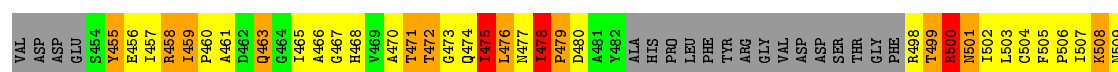


- Molecule 2: GafB domain of phosphodiesterase 2A



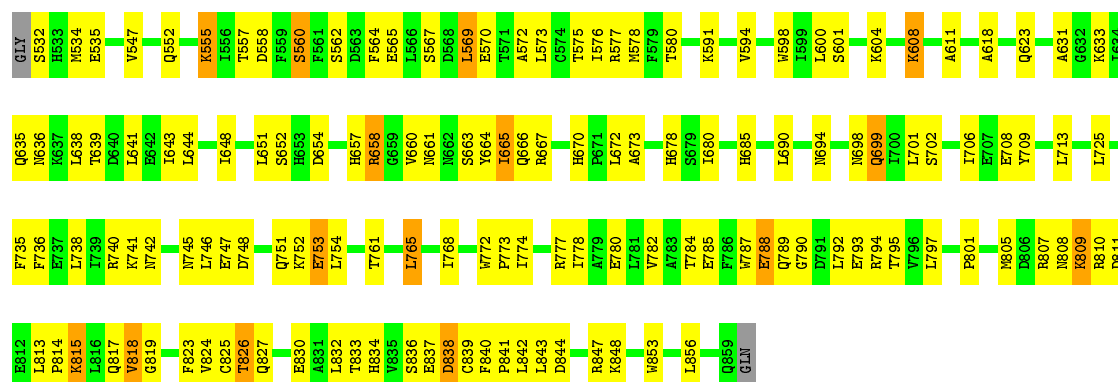
- Molecule 2: GafB domain of phosphodiesterase 2A





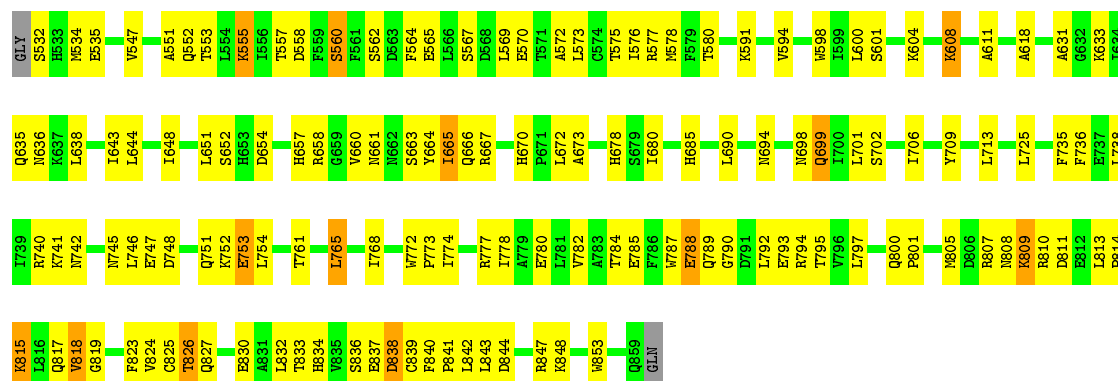
### • Molecule 3: phosphodiesterase 5/6 chimera catalytic domain

Chain C: 57% 38% 5%



### • Molecule 3: phosphodiesterase 5/6 chimera catalytic domain

Chain O: 57% 38% 5%



### • Molecule 4: phosphodiesterase 6 gamma subunit inhibitory peptide

Chain D: 67% 28% 6%

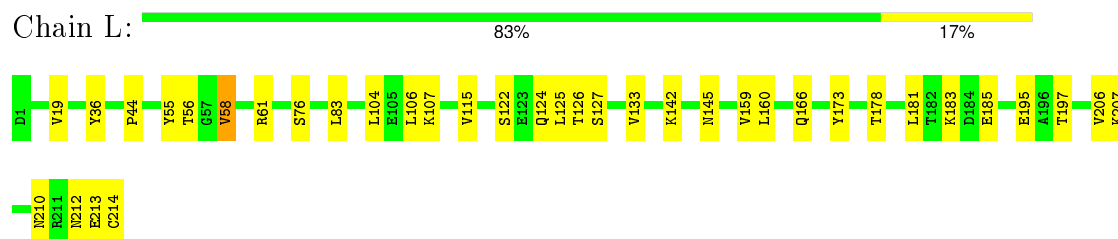


### • Molecule 4: phosphodiesterase 6 gamma subunit inhibitory peptide

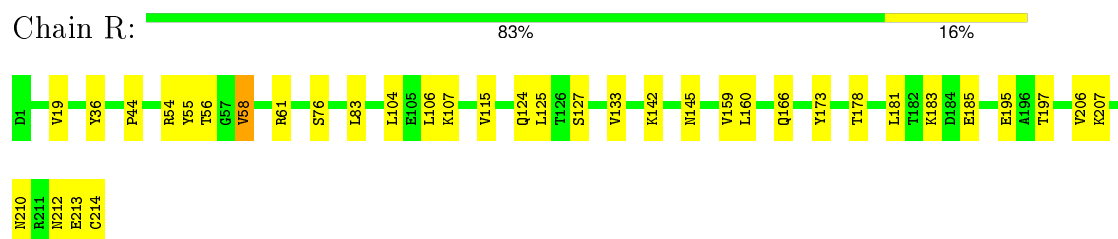
Chain P: 67% 28% 6%



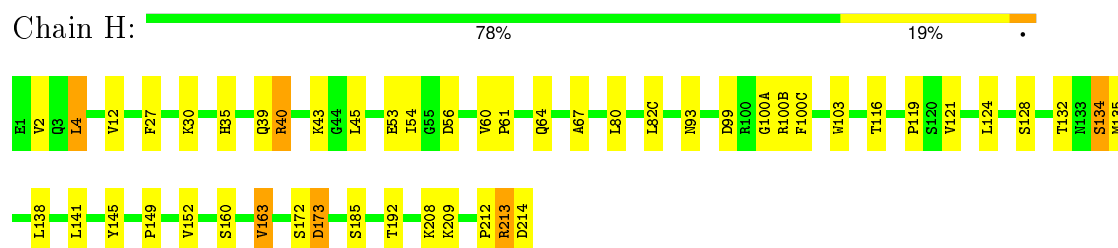
- Molecule 5: IgG1-kappa 2E8 light chain



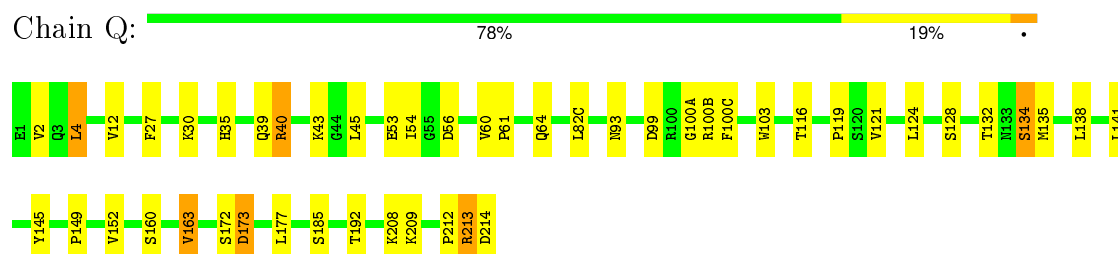
- Molecule 5: IgG1-kappa 2E8 light chain



- Molecule 6: IgG1-kappa 2E8 heavy chain



- Molecule 6: IgG1-kappa 2E8 heavy chain





## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	12373	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	EMAN ctfit	Depositor
Microscope	JEOL 2010F	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	15	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	60000	Depositor
Image detector	GATAN UltraScan 4000 (4k 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: IBM

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	0.47	0/1391	0.60	0/1877
1	M	0.47	0/1391	0.60	0/1877
2	B	0.65	0/1285	0.87	2/1738 (0.1%)
2	N	0.65	0/1285	0.87	2/1738 (0.1%)
3	C	0.39	0/2726	0.53	0/3685
3	O	0.39	0/2726	0.53	0/3685
4	D	0.35	0/144	0.60	0/194
4	P	0.35	0/144	0.60	0/194
5	L	0.53	0/1682	0.73	0/2278
5	R	0.53	0/1682	0.73	0/2278
6	H	0.50	0/1728	0.78	0/2366
6	Q	0.50	0/1728	0.78	0/2366
All	All	0.49	0/17912	0.69	4/24276 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	478	ILE	C-N-CD	-6.88	105.47	120.60
2	B	478	ILE	C-N-CD	-6.88	105.47	120.60
2	B	403	LEU	CA-CB-CG	5.56	128.08	115.30
2	N	403	LEU	CA-CB-CG	5.54	128.05	115.30

There are no chirality outliers.

There are no planarity outliers.

## 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	1368	0	1390	273	0
1	M	1368	0	1393	275	0
2	B	1267	0	1270	276	0
2	N	1267	0	1272	305	0
3	C	2671	0	2668	252	0
3	O	2671	0	2668	246	0
4	D	141	0	131	7	0
4	P	141	0	131	7	0
5	L	1649	0	1578	15	0
5	R	1649	0	1578	15	0
6	H	1682	0	1625	57	0
6	Q	1682	0	1625	55	0
7	C	32	0	28	4	0
7	O	32	0	28	4	0
All	All	17620	0	17385	1227	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 35.

The worst 5 of 1227 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)
3:C:633:LYS:HB2	3:O:840:PHE:CE2	1.21	1.69
3:C:840:PHE:CE2	3:O:633:LYS:HB2	1.21	1.63
2:B:554:TYR:HE1	2:N:554:TYR:CE1	1.04	1.62
2:B:554:TYR:CE1	2:N:554:TYR:HE1	1.05	1.61
3:C:633:LYS:CB	3:O:840:PHE:HE2	1.10	1.60

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	169/180 (94%)	157 (93%)	7 (4%)	5 (3%)	5	42
1	M	169/180 (94%)	157 (93%)	7 (4%)	5 (3%)	5	42
2	B	155/185 (84%)	126 (81%)	18 (12%)	11 (7%)	1	22
2	N	155/185 (84%)	126 (81%)	18 (12%)	11 (7%)	1	22
3	C	326/330 (99%)	295 (90%)	30 (9%)	1 (0%)	46	83
3	O	326/330 (99%)	295 (90%)	30 (9%)	1 (0%)	46	83
4	D	15/18 (83%)	15 (100%)	0	0	100	100
4	P	15/18 (83%)	15 (100%)	0	0	100	100
5	L	212/214 (99%)	208 (98%)	4 (2%)	0	100	100
5	R	212/214 (99%)	208 (98%)	4 (2%)	0	100	100
6	H	219/221 (99%)	209 (95%)	3 (1%)	7 (3%)	5	41
6	Q	219/221 (99%)	209 (95%)	3 (1%)	7 (3%)	5	41
All	All	2192/2296 (96%)	2020 (92%)	124 (6%)	48 (2%)	13	49

5 of 48 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	475	ILE
2	B	499	THR
2	B	500	ARG
2	B	508	LYS
2	B	512	GLN

### 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	155/164 (94%)	150 (97%)	5 (3%)	46	76
1	M	155/164 (94%)	150 (97%)	5 (3%)	46	76
2	B	140/159 (88%)	95 (68%)	45 (32%)	0	2
2	N	140/159 (88%)	95 (68%)	45 (32%)	0	2
3	C	294/295 (100%)	265 (90%)	29 (10%)	10	39
3	O	294/295 (100%)	265 (90%)	29 (10%)	10	39
4	D	14/15 (93%)	14 (100%)	0	100	100
4	P	14/15 (93%)	14 (100%)	0	100	100
5	L	189/189 (100%)	176 (93%)	13 (7%)	19	56
5	R	189/189 (100%)	176 (93%)	13 (7%)	19	56
6	H	189/189 (100%)	179 (95%)	10 (5%)	28	64
6	Q	189/189 (100%)	179 (95%)	10 (5%)	28	64
All	All	1962/2022 (97%)	1758 (90%)	204 (10%)	13	36

5 of 204 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	N	553	LEU
3	C	694	ASN
5	R	145	ASN
2	N	557	VAL
3	C	557	THR

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

Mol	Chain	Res	Type
2	N	511	ASN
3	C	834	HIS
5	R	212	ASN
3	C	808	ASN
3	O	694	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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	$\# Z  > 2$
7	IBM	C	901	-	8,17,17	2.41	3 (37%)	8,25,25	1.58	1 (12%)
7	IBM	C	902	-	8,17,17	1.99	3 (37%)	8,25,25	1.83	1 (12%)
7	IBM	O	901	-	8,17,17	2.41	3 (37%)	8,25,25	1.58	1 (12%)
7	IBM	O	902	-	8,17,17	1.99	3 (37%)	8,25,25	1.83	1 (12%)

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
7	IBM	C	901	-	-	0/4/4/4	0/2/2/2
7	IBM	C	902	-	-	0/4/4/4	0/2/2/2
7	IBM	O	901	-	-	0/4/4/4	0/2/2/2
7	IBM	O	902	-	-	0/4/4/4	0/2/2/2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	901	IBM	C4-N3	-5.14	1.33	1.39
7	O	901	IBM	C4-N3	-5.14	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	902	IBM	C4-N3	-3.35	1.35	1.39
7	O	902	IBM	C4-N3	-3.35	1.35	1.39
7	C	902	IBM	C6-N1	-2.04	1.35	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	902	IBM	C6-C5-C4	-4.82	116.48	119.93
7	O	902	IBM	C6-C5-C4	-4.82	116.48	119.93
7	C	901	IBM	C6-C5-C4	-4.11	116.99	119.93
7	O	901	IBM	C6-C5-C4	-4.11	116.99	119.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	901	IBM	1	0
7	C	902	IBM	3	0
7	O	901	IBM	1	0
7	O	902	IBM	3	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.