



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:59 PM BST

PDB ID : 3JBQ
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 : 2015-09-17
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

A user guide is available at

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

MolProbity : 4.02b-467
Mogul : unknown
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

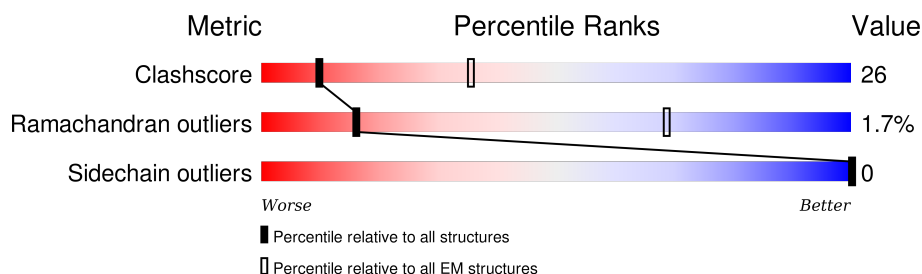
1 Overall quality at a glance

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 ≥ 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	L	214	44% 56%
1	l	214	100%
2	H	220	35% 60% ..
2	h	220	96% ..
3	B	330	44% 55% .
3	F	330	41% 58% ..
4	D	18	50% 44% 6%
4	X	18	28% 67% 6%
5	C	185	45% 42% . 13%

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Mol	Chain	Length	Quality of chain
5	G	185	<div><div></div><div>46%</div><div>41%</div><div>•</div><div>13%</div></div>
6	1	186	<div><div></div><div>40%</div><div>49%</div><div>•</div><div>8%</div></div>
6	2	186	<div><div></div><div>39%</div><div>52%</div><div>•</div><div>8%</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17450 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 IgG1-kappa 2E8 light chain.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	214	Total	C	N	O	S	0	0
			1629	1030	266	327	6		
2	h	214	Total	C	N	O	S	0	0
			1629	1030	266	327	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	328	Total	C	N	O	S	0	0
			2671	1700	465	487	19		
3	F	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	X	17	Total	C	N	O	0	0
			141	92	23	26		

- Molecule 5 is a protein called GafB domain of phosphodiesterase 2A.

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

- Molecule 6 is a protein called GafA domain of cone phosphodiesterase 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1	171	Total	C	N	O	S	0	0
			1368	874	230	256	8		
6	2	171	Total	C	N	O	S	0	0
			1368	874	230	256	8		

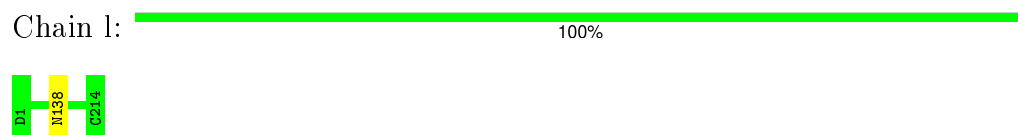
3 Residue-property plots

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.

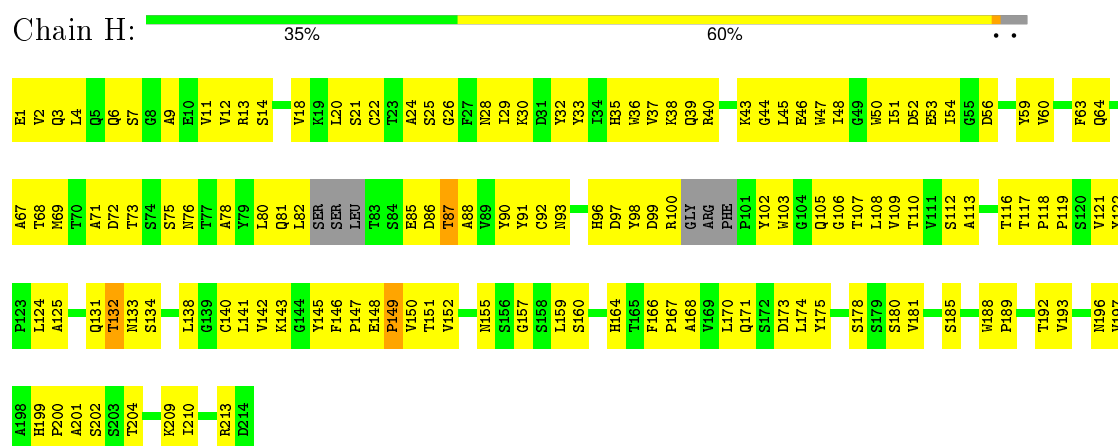
- Molecule 1: IgG1-kappa 2E8 light chain



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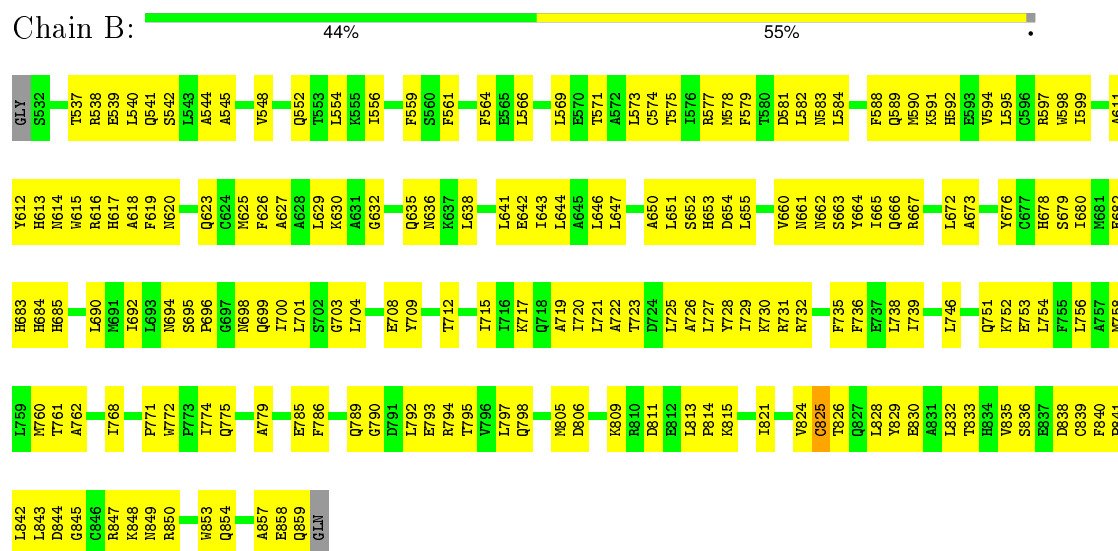
- Molecule 2: IgG1-kappa 2E8 heavy chain



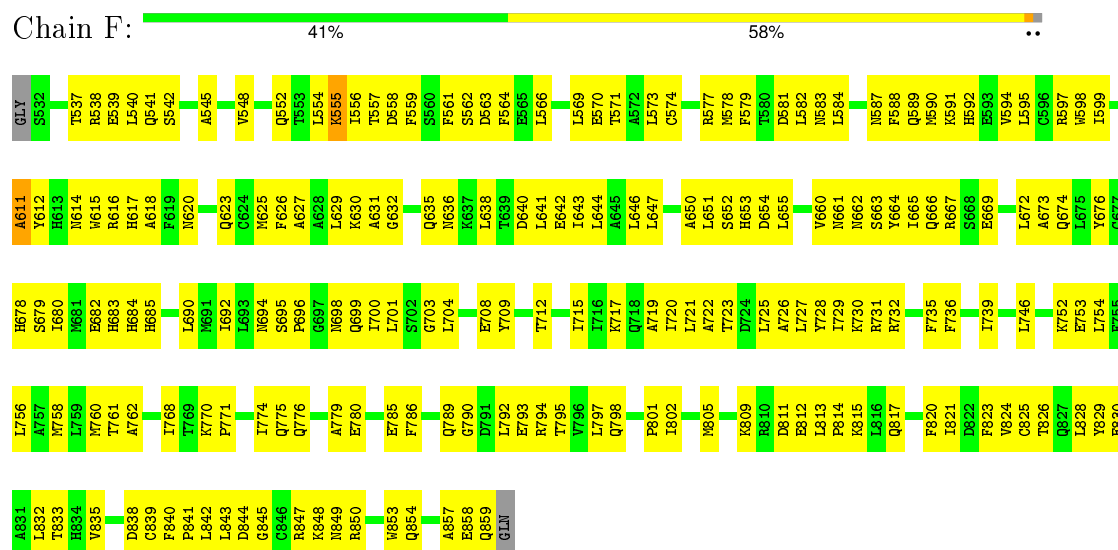
- Molecule 2: IgG1-kappa 2E8 heavy chain



- Molecule 3: phosphodiesterase 5/6 chimera catalytic domain



- Molecule 3: phosphodiesterase 5/6 chimera catalytic domain

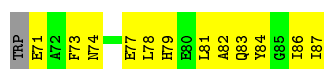


- Molecule 4: phosphodiesterase 6 gamma subunit inhibitory peptide



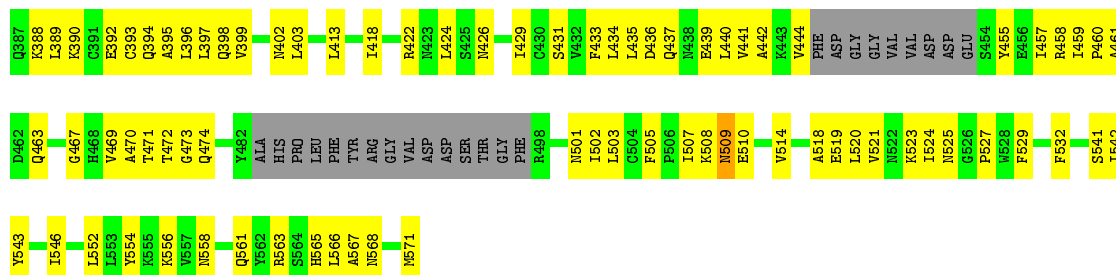
- Molecule 4: phosphodiesterase 6 gamma subunit inhibitory peptide





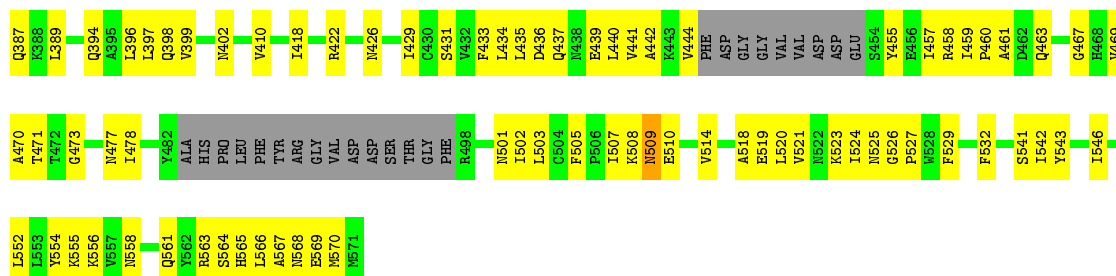
- Molecule 5: GafB domain of phosphodiesterase 2A

Chain C: 45% 42% 13%



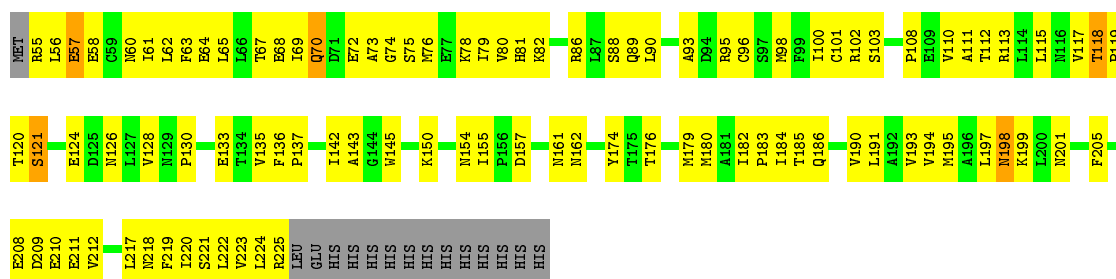
- Molecule 5: GafB domain of phosphodiesterase 2A

Chain G: 46% 41% 13%



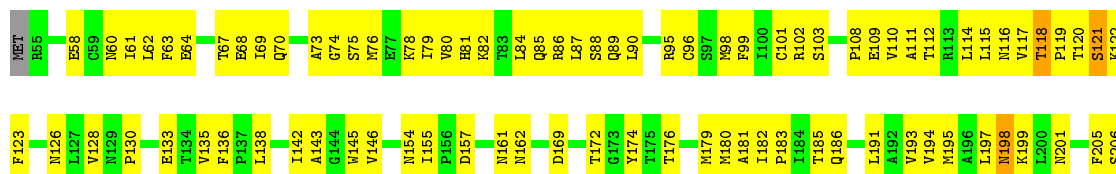
- Molecule 6: GafA domain of cone phosphodiesterase 6C

Chain 1: 40% 49% 8%



- Molecule 6: GafA domain of cone phosphodiesterase 6C

Chain 2: 39% 52% 8%



E207	E208	D209	E210	E211	V212	E215	Y216	L217	N218	F219	I220	S221	I222	V223	L224	R225	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS
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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	by particle using 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 [i](#)

5.1 Standard geometry [i](#)

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	L	0.24	0/1682	0.47	0/2278
1	l	0.24	0/1682	0.47	0/2278
2	H	0.25	0/1671	0.52	0/2285
2	h	0.26	0/1671	0.53	0/2285
3	B	0.26	0/2726	0.50	0/3685
3	F	0.26	0/2726	0.50	0/3685
4	D	0.24	0/144	0.44	0/194
4	X	0.24	0/144	0.47	0/194
5	C	0.24	0/1285	0.47	0/1738
5	G	0.24	0/1285	0.47	0/1738
6	1	0.28	0/1391	0.56	0/1877
6	2	0.28	0/1391	0.56	0/1877
All	All	0.26	0/17798	0.50	0/24114

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	L	1649	0	1578	115	0
1	l	1649	0	1578	0	0
2	H	1629	0	1571	131	0
2	h	1629	0	1571	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2671	0	2671	171	0
3	F	2671	0	2671	185	0
4	D	141	0	131	13	0
4	X	141	0	131	18	0
5	C	1267	0	1273	75	0
5	G	1267	0	1273	67	0
6	1	1368	0	1396	99	0
6	2	1368	0	1396	104	0
All	All	17450	0	17240	888	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 26.

The worst 5 of 888 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)
6:1:81:HIS:NE2	6:1:121:SER:O	2.04	0.89
6:1:208:GLU:HB2	6:2:201:ASN:HA	1.54	0.88
1:L:8:GLN:NE2	1:L:11:MET:SD	2.50	0.85
6:2:81:HIS:NE2	6:2:121:SER:O	2.10	0.84
5:C:390:LYS:HG3	6:1:70:GLN:HG2	1.60	0.83

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	L	212/214 (99%)	189 (89%)	22 (10%)	1 (0%)	34 77
1	l	212/214 (99%)	191 (90%)	20 (9%)	1 (0%)	34 77
2	H	208/220 (94%)	190 (91%)	14 (7%)	4 (2%)	10 52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	h	208/220 (94%)	190 (91%)	16 (8%)	2 (1%)	19	65
3	B	326/330 (99%)	301 (92%)	21 (6%)	4 (1%)	16	61
3	F	326/330 (99%)	301 (92%)	20 (6%)	5 (2%)	13	57
4	D	15/18 (83%)	14 (93%)	1 (7%)	0	100	100
4	X	15/18 (83%)	15 (100%)	0	0	100	100
5	C	155/185 (84%)	142 (92%)	9 (6%)	4 (3%)	7	45
5	G	155/185 (84%)	141 (91%)	8 (5%)	6 (4%)	4	36
6	1	169/186 (91%)	148 (88%)	15 (9%)	6 (4%)	4	38
6	2	169/186 (91%)	151 (89%)	14 (8%)	4 (2%)	7	47
All	All	2170/2306 (94%)	1973 (91%)	160 (7%)	37 (2%)	16	55

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	149	PRO
5	C	508	LYS
5	G	508	LYS
5	G	509	ASN
2	h	149	PRO

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	L	189/189 (100%)	189 (100%)	0	100	100
1	l	189/189 (100%)	189 (100%)	0	100	100
2	H	183/188 (97%)	183 (100%)	0	100	100
2	h	183/188 (97%)	183 (100%)	0	100	100
3	B	294/295 (100%)	294 (100%)	0	100	100
3	F	294/295 (100%)	294 (100%)	0	100	100
4	D	14/15 (93%)	14 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	X	14/15 (93%)	14 (100%)	0	100	100
5	C	140/159 (88%)	140 (100%)	0	100	100
5	G	140/159 (88%)	140 (100%)	0	100	100
6	1	155/170 (91%)	155 (100%)	0	100	100
6	2	155/170 (91%)	155 (100%)	0	100	100
All	All	1950/2032 (96%)	1950 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
5	C	511	ASN
3	F	678	HIS
2	h	96	HIS
5	C	568	ASN
3	F	552	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.