



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:45 AM GMT

PDB ID : 3PVU
Title : Bovine GRK2 in complex with Gbetagamma subunits and a selective kinase inhibitor (CMPD101)
Authors : Thal, D.M.; Tesmer, J.J.
Deposited on : 2010-12-07
Resolution : 2.48 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

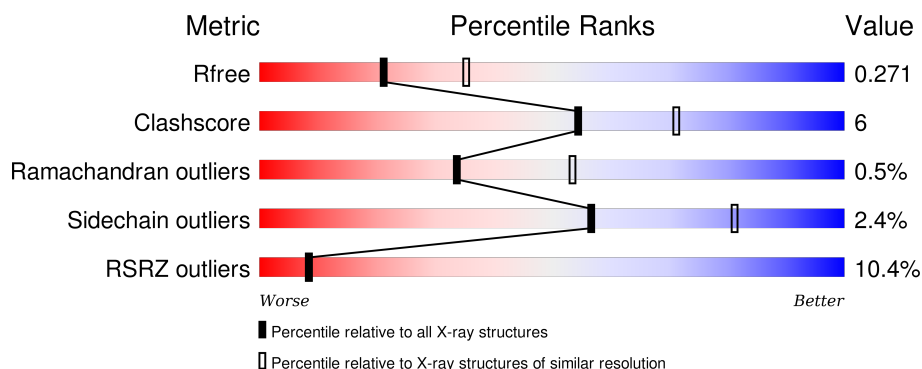
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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}	91344	4309 (2.50-2.46)
Clashscore	102246	5050 (2.50-2.46)
Ramachandran outliers	100387	4961 (2.50-2.46)
Sidechain outliers	100360	4963 (2.50-2.46)
RSRZ outliers	91569	4319 (2.50-2.46)

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 on the lower 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 $\leq 5\%$. 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	695	<div> <div>10%</div> <div>74%</div> <div>13%</div> <div>12%</div> </div>
2	B	340	<div> <div>10%</div> <div>83%</div> <div>15%</div> <div></div> </div>
3	G	74	<div> <div>4%</div> <div>70%</div> <div>12%</div> <div>18%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8132 atoms, of which 0 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 Beta-adrenergic receptor kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	609	Total	C	N	O	S	0	0	0
			4998	3189	870	903	36			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	670	ALA	SER	ENGINEERED MUTATION	UNP P21146
A	690	HIS	-	EXPRESSION TAG	UNP P21146
A	691	HIS	-	EXPRESSION TAG	UNP P21146
A	692	HIS	-	EXPRESSION TAG	UNP P21146
A	693	HIS	-	EXPRESSION TAG	UNP P21146
A	694	HIS	-	EXPRESSION TAG	UNP P21146
A	695	HIS	-	EXPRESSION TAG	UNP P21146

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	339	Total	C	N	O	S	0	0	0
			2607	1607	468	511	21			

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	61	Total	C	N	O	S	0	0	0
			481	305	83	89	4			

There are 6 discrepancies between the modelled and reference sequences:

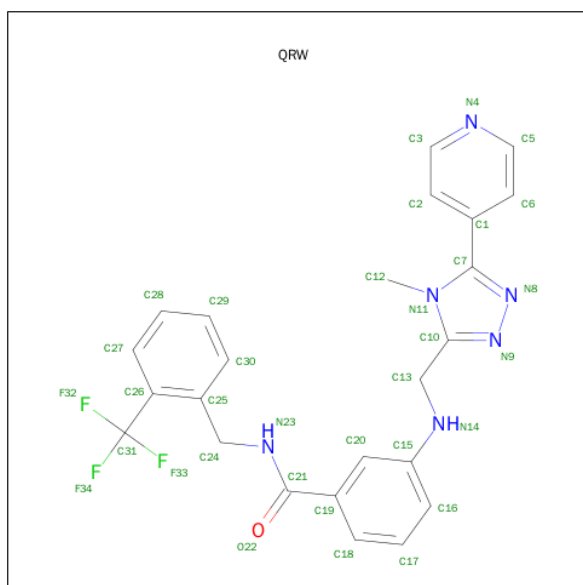
Chain	Residue	Modelled	Actual	Comment	Reference
G	-5	HIS	-	EXPRESSION TAG	UNP P63212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	HIS	-	EXPRESSION TAG	UNP P63212
G	-3	HIS	-	EXPRESSION TAG	UNP P63212
G	-2	HIS	-	EXPRESSION TAG	UNP P63212
G	-1	HIS	-	EXPRESSION TAG	UNP P63212
G	0	HIS	-	EXPRESSION TAG	UNP P63212

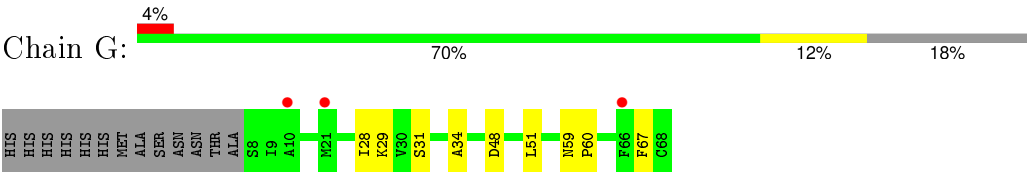
- Molecule 4 is 3-({[4-METHYL-5-(PYRIDIN-4-YL)-4H-1,2,4-TRIAZOL-3-YL]METHYL}AMINO)-N-[2-(TRIFLUOROMETHYL)BENZYL]BENZAMIDE (three-letter code: QRW) (formula: C₂₄H₂₁F₃N₆O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			34	24	3	6	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	8	Total	O	0	0
			8	8		
5	B	4	Total	O	0	0
			4	4		



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	186.50Å 73.50Å 121.99Å 90.00° 115.10° 90.00°	Depositor
Resolution (Å)	30.00 – 2.48 29.48 – 2.48	Depositor EDS
% Data completeness (in resolution range)	96.9 (30.00-2.48) 97.0 (29.48-2.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.226 , 0.274 0.229 , 0.271	Depositor DCC
R_{free} test set	2636 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	73.4	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 51725 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8132	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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: CMT, QRW

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	0.43	0/5111	0.58	0/6866
2	B	0.46	0/2654	0.63	0/3597
3	G	0.45	0/481	0.53	0/646
All	All	0.44	0/8246	0.59	0/11109

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
3	G	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	G	67	PHE	Mainchain

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	4998	0	4991	58	1
2	B	2607	0	2510	43	1
3	G	481	0	493	8	0
4	A	34	0	21	2	0
5	A	8	0	0	1	0
5	B	4	0	0	0	0
All	All	8132	0	8015	103	1

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 6.

All (103) 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)
2:B:86:THR:O	2:B:87:THR:HB	1.68	0.90
1:A:609:VAL:HG22	1:A:622:LEU:HD22	1.65	0.77
2:B:128:THR:HG22	2:B:130:GLU:H	1.51	0.75
2:B:176:GLN:NE2	2:B:179:THR:HG22	2.03	0.74
2:B:176:GLN:HE21	2:B:179:THR:HG22	1.54	0.71
1:A:202:PHE:CD2	4:A:800:QRW:H24	2.24	0.71
1:A:609:VAL:HG22	1:A:622:LEU:CD2	2.24	0.66
1:A:294:MET:HE2	1:A:295:ARG:HA	1.77	0.66
2:B:33:ILE:HD11	3:G:31:SER:HA	1.76	0.65
1:A:399:LYS:HA	1:A:402:ILE:HD12	1.80	0.63
2:B:63:TRP:CZ2	2:B:328:ALA:HB2	2.35	0.62
2:B:47:THR:HG22	2:B:339:TRP:CZ3	2.35	0.62
2:B:286:LEU:HD12	2:B:286:LEU:N	2.15	0.61
2:B:149:CYS:O	2:B:150:ARG:NH1	2.35	0.60
1:A:155:GLN:OE1	1:A:158:ARG:NH1	2.35	0.59
2:B:52:ARG:HD2	2:B:335:PHE:HE1	1.67	0.59
2:B:173:THR:HG22	2:B:175:GLN:HG2	1.84	0.59
1:A:62:LYS:NZ	1:A:519:GLN:OE1	2.35	0.59
1:A:202:PHE:HB2	1:A:222:LEU:HD22	1.87	0.57
2:B:71:VAL:HG23	2:B:105:TYR:CD2	2.40	0.57
1:A:357:MET:HB2	1:A:362:LEU:HD21	1.86	0.57
1:A:245:LEU:O	1:A:311:ARG:HD3	2.05	0.56
2:B:61:MET:HE3	2:B:70:LEU:HD13	1.88	0.54
1:A:308:MET:CE	1:A:336:LEU:HD21	2.39	0.52
1:A:385:LEU:HD13	1:A:421:LEU:HD21	1.91	0.52
1:A:169:ASP:N	1:A:169:ASP:OD1	2.41	0.52
2:B:86:THR:O	2:B:87:THR:CB	2.49	0.51
1:A:237:LEU:HD23	1:A:237:LEU:C	2.30	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:318:LEU:HA	2:B:328:ALA:O	2.10	0.51
2:B:33:ILE:HD12	3:G:34:ALA:HB3	1.91	0.51
1:A:434:ASN:HD22	1:A:434:ASN:H	1.59	0.51
1:A:383:LYS:NZ	5:A:702:HOH:O	2.43	0.50
2:B:37:ILE:O	2:B:301:LYS:NZ	2.44	0.50
1:A:298:ALA:HB2	1:A:381:LEU:CD2	2.42	0.50
1:A:357:MET:CB	1:A:362:LEU:HD21	2.42	0.50
2:B:233:CYS:SG	2:B:277:SER:HA	2.52	0.50
1:A:385:LEU:CD1	1:A:421:LEU:HD21	2.42	0.50
3:G:28:ILE:HG22	3:G:29:LYS:O	2.12	0.50
2:B:70:LEU:HD11	2:B:336:LEU:HD22	1.92	0.49
2:B:281:SER:HB3	3:G:48:ASP:HB2	1.93	0.49
1:A:318:LEU:HD21	1:A:377:LEU:HD13	1.94	0.49
1:A:301:ILE:HD11	1:A:323:ILE:HD13	1.95	0.49
2:B:283:ARG:HB3	3:G:51:LEU:HD11	1.94	0.49
2:B:173:THR:HG22	2:B:175:GLN:CG	2.43	0.49
1:A:227:ILE:HG21	1:A:506:TYR:OH	2.13	0.48
1:A:457:ASP:OD2	1:A:457:ASP:C	2.52	0.48
2:B:51:LEU:HD13	2:B:82:TRP:CD2	2.49	0.48
1:A:565:MET:HE3	1:A:634:CYS:SG	2.54	0.48
2:B:301:LYS:O	2:B:302:ALA:HB3	2.14	0.47
1:A:141:VAL:HG23	1:A:141:VAL:O	2.13	0.47
1:A:40:ARG:NH2	1:A:166:ILE:O	2.45	0.47
2:B:33:ILE:CD1	3:G:34:ALA:HB3	2.44	0.47
2:B:286:LEU:CD2	2:B:327:VAL:HG21	2.44	0.47
1:A:299:ALA:HB1	1:A:461:VAL:HG11	1.97	0.46
1:A:113:ILE:O	1:A:117:LEU:HB2	2.15	0.46
2:B:292:PHE:N	2:B:292:PHE:CD1	2.83	0.46
2:B:30:LEU:HD23	2:B:262:MET:CE	2.46	0.46
1:A:308:MET:HE1	1:A:336:LEU:HD21	1.98	0.46
2:B:318:LEU:HD12	2:B:318:LEU:C	2.37	0.46
2:B:61:MET:HE2	2:B:61:MET:HB2	1.63	0.46
1:A:291:GLU:HG2	1:A:421:LEU:HD22	1.98	0.45
2:B:313:ASN:O	2:B:314:ARG:C	2.55	0.45
2:B:33:ILE:CD1	3:G:31:SER:HA	2.46	0.45
1:A:401:GLU:HA	1:A:404:ARG:HG2	1.99	0.45
1:A:325:LEU:HD12	1:A:331:VAL:HG12	1.99	0.45
2:B:128:THR:O	2:B:130:GLU:N	2.50	0.44
2:B:63:TRP:HZ2	2:B:328:ALA:HB2	1.80	0.44
1:A:273:LEU:HD12	1:A:274:MET:H	1.82	0.44
2:B:205:ASP:O	2:B:206:ALA:HB3	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:MET:CE	1:A:411:VAL:HG22	2.48	0.44
2:B:149:CYS:HB3	2:B:159:THR:HG22	2.00	0.43
1:A:637:ASP:O	1:A:641:VAL:HG23	2.18	0.43
2:B:197:ARG:O	2:B:198:LEU:HD23	2.18	0.43
1:A:298:ALA:HB2	1:A:381:LEU:HD21	2.01	0.43
2:B:71:VAL:CG2	2:B:105:TYR:CD2	3.02	0.43
1:A:651:TYR:C	1:A:651:TYR:CD1	2.92	0.43
1:A:565:MET:CE	1:A:634:CYS:SG	3.06	0.43
1:A:436:ARG:HG2	1:A:439:CYS:SG	2.59	0.43
1:A:421:LEU:HD11	1:A:425:LEU:HD11	1.99	0.42
1:A:243:LEU:HD22	1:A:257:MET:HB2	2.00	0.42
1:A:102:LEU:HA	1:A:141:VAL:HG11	2.01	0.42
1:A:254:ILE:HD11	1:A:307:HIS:HB3	2.01	0.42
2:B:163:ASP:C	2:B:164:THR:HG23	2.39	0.42
2:B:286:LEU:CD1	2:B:286:LEU:N	2.82	0.42
2:B:170:ASP:HB3	2:B:173:THR:HB	2.02	0.42
2:B:91:HIS:CD2	2:B:133:VAL:HG21	2.54	0.42
1:A:418:SER:O	1:A:422:ARG:HG3	2.20	0.42
1:A:636:SER:OG	1:A:639:GLU:OE1	2.24	0.42
1:A:552:ASP:OD2	1:A:554:ALA:HB3	2.20	0.41
2:B:104:ALA:HB2	2:B:149:CYS:O	2.20	0.41
1:A:334:SER:O	1:A:335:ASP:C	2.59	0.41
1:A:263:THR:HB	1:A:264:PRO:HD2	2.01	0.41
3:G:59:ASN:HA	3:G:60:PRO:HD2	1.88	0.41
1:A:411:VAL:HG12	1:A:413:LEU:HD23	2.03	0.41
1:A:96:GLU:HG2	1:A:460:MET:CE	2.50	0.41
1:A:205:VAL:HG11	4:A:800:QRW:C2	2.51	0.41
1:A:294:MET:HE3	1:A:298:ALA:CB	2.51	0.41
1:A:666:ASN:N	1:A:666:ASN:HD22	2.18	0.41
1:A:624:ILE:HG22	1:A:625:ARG:N	2.36	0.41
1:A:324:LEU:O	1:A:331:VAL:HA	2.21	0.40
1:A:392:ARG:NH2	1:A:395:LYS:O	2.54	0.40
1:A:162:PHE:O	1:A:165:PHE:HB3	2.22	0.40
1:A:513:ILE:O	1:A:514:SER:C	2.59	0.40

All (1) 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:A:598:GLN:OE1	2:B:46:ARG:NH2[2_657]	2.19	0.01

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	603/695 (87%)	562 (93%)	38 (6%)	3 (0%)	34	53
2	B	337/340 (99%)	316 (94%)	19 (6%)	2 (1%)	30	48
3	G	59/74 (80%)	56 (95%)	3 (5%)	0	100	100
All	All	999/1109 (90%)	934 (94%)	60 (6%)	5 (0%)	34	53

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	129	ARG
1	A	212	ASP
1	A	327	GLU
1	A	394	HIS
2	B	334	SER

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 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	548/617 (89%)	536 (98%)	12 (2%)	60	83
2	B	282/283 (100%)	273 (97%)	9 (3%)	46	72
3	G	50/61 (82%)	50 (100%)	0	100	100
All	All	880/961 (92%)	859 (98%)	21 (2%)	57	81

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	ASP
1	A	240	ARG
1	A	265	ASP
1	A	284	SER
1	A	294	MET
1	A	396	THR
1	A	399	LYS
1	A	415	ASP
1	A	431	ARG
1	A	434	ASN
1	A	508	ASN
1	A	651	TYR
2	B	47	THR
2	B	52	ARG
2	B	61	MET
2	B	70	LEU
2	B	105	TYR
2	B	234	PHE
2	B	292	PHE
2	B	294	CYS
2	B	340	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	GLN
1	A	310	ASN
1	A	348	HIS
1	A	434	ASN
1	A	459	GLN
1	A	607	GLN
1	A	666	ASN
2	B	6	GLN
2	B	91	HIS
2	B	176	GLN
2	B	239	ASN
2	B	259	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
3	CMT	G	68	3	6,7,7	2.33	1 (16%)	6,8,8	2.08	3 (50%)

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	CMT	G	68	3	-	0/8/8/8	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	68	CMT	OXT-C	5.58	1.47	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	68	CMT	CA-CB-SG	-2.30	109.21	114.48
3	G	68	CMT	C1-OXT-C	2.32	121.44	115.99
3	G	68	CMT	OXT-C-CA	3.50	120.62	111.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

1 ligand is 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	$\# Z > 2$
4	QRW	A	800	-	34,37,37	1.52	3 (8%)	43,52,52	1.39	5 (11%)

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
4	QRW	A	800	-	-	0/22/24/24	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	800	QRW	N9-N8	-6.73	1.24	1.37
4	A	800	QRW	C1-C7	-3.11	1.39	1.47
4	A	800	QRW	C31-C26	2.58	1.56	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	800	QRW	C25-C24-N23	-3.24	106.52	113.08
4	A	800	QRW	C24-C25-C30	-2.84	114.78	121.05
4	A	800	QRW	F34-C31-C26	-2.82	107.71	112.68
4	A	800	QRW	C31-C26-C25	3.11	123.57	120.92
4	A	800	QRW	C7-N8-N9	4.22	110.25	104.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	800	QRW	2	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.

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	609/695 (87%)	0.66	67 (11%) 7 7	63, 90, 132, 182	0
2	B	339/340 (99%)	0.56	35 (10%) 9 9	54, 74, 120, 208	0
3	G	60/74 (81%)	0.23	3 (5%) 32 36	63, 82, 161, 176	0
All	All	1008/1109 (90%)	0.60	105 (10%) 8 8	54, 84, 132, 208	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	202	PHE	6.9
2	B	4	LEU	6.5
2	B	8	ARG	6.5
2	B	130	GLU	5.8
2	B	2	SER	5.7
1	A	201	GLY	5.2
1	A	366	VAL	5.1
1	A	474	ARG	5.1
1	A	549	HIS	4.9
1	A	30	LYS	4.6
1	A	393	GLN	4.6
1	A	397	LYS	4.6
1	A	394	HIS	4.4
1	A	546	GLN	4.4
1	A	365	GLY	4.1
2	B	148	CYS	4.1
1	A	550	GLU	4.1
1	A	618	LYS	4.1
2	B	129	ARG	4.1
2	B	9	GLN	4.0
1	A	364	LYS	3.8
1	A	616	GLU	3.8
1	A	396	THR	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	415	ASP	3.7
1	A	120	CYS	3.6
2	B	60	ALA	3.6
1	A	200	GLY	3.6
1	A	376	SER	3.6
2	B	11	ALA	3.6
2	B	232	ILE	3.5
1	A	318	LEU	3.5
1	A	230	LYS	3.4
1	A	542	THR	3.3
1	A	475	GLY	3.3
1	A	199	ARG	3.3
2	B	149	CYS	3.3
1	A	569	GLY	3.3
2	B	233	CYS	3.3
1	A	229	MET	3.2
1	A	547	LEU	3.2
2	B	6	GLN	3.2
1	A	333	ILE	3.1
2	B	102	THR	3.1
2	B	3	GLU	3.1
1	A	345	LYS	3.0
1	A	551	GLU	3.0
1	A	409	MET	3.0
1	A	334	SER	3.0
1	A	304	GLY	2.9
2	B	7	LEU	2.9
1	A	226	ARG	2.9
2	B	150	ARG	2.9
2	B	276	VAL	2.9
2	B	127	LYS	2.9
2	B	103	CYS	2.8
1	A	440	LEU	2.8
2	B	200	VAL	2.8
1	A	382	PHE	2.8
2	B	128	THR	2.8
2	B	191	SER	2.7
2	B	231	ALA	2.7
1	A	262	HIS	2.6
1	A	95	LEU	2.6
1	A	656	GLN	2.6
1	A	373	ASP	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	277	SER	2.6
1	A	412	GLU	2.6
1	A	367	ALA	2.5
1	A	237	LEU	2.5
1	A	336	LEU	2.5
2	B	197	ARG	2.5
2	B	5	ASP	2.5
1	A	504	GLU	2.4
3	G	21	MET	2.4
2	B	189	SER	2.4
1	A	413	LEU	2.4
2	B	270	ILE	2.4
1	A	270	ILE	2.3
1	A	576	TRP	2.3
1	A	315	TYR	2.3
2	B	132	ASN	2.3
1	A	294	MET	2.3
1	A	625	ARG	2.3
1	A	538	ALA	2.3
1	A	222	LEU	2.2
1	A	301	ILE	2.2
1	A	545	LYS	2.2
2	B	317	CYS	2.2
1	A	539	ARG	2.2
1	A	454	ARG	2.2
1	A	221	CYS	2.2
3	G	66	PHE	2.2
1	A	231	GLN	2.1
3	G	10	ALA	2.1
2	B	61	MET	2.1
1	A	501	SER	2.1
1	A	507	ARG	2.1
1	A	356	TYR	2.1
2	B	201	SER	2.1
2	B	319	GLY	2.1
1	A	255	VAL	2.0
1	A	380	MET	2.0
2	B	188	MET	2.0
1	A	206	TYR	2.0
1	A	505	LEU	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	CMT	G	68	8/8	0.80	0.15	-	85,88,93,95	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	QRW	A	800	34/34	0.82	0.23	-0.23	78,84,99,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.