



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:13 AM EDT

PDB ID : 3PVW / pdb_00003pvw
Title : Bovine GRK2 in complex with Gbetagamma subunits and a selective kinase inhibitor (CMPD103A)
Authors : Thal, D.M.; Tesmer, J.J.
Deposited on : 2010-12-07
Resolution : 2.49 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

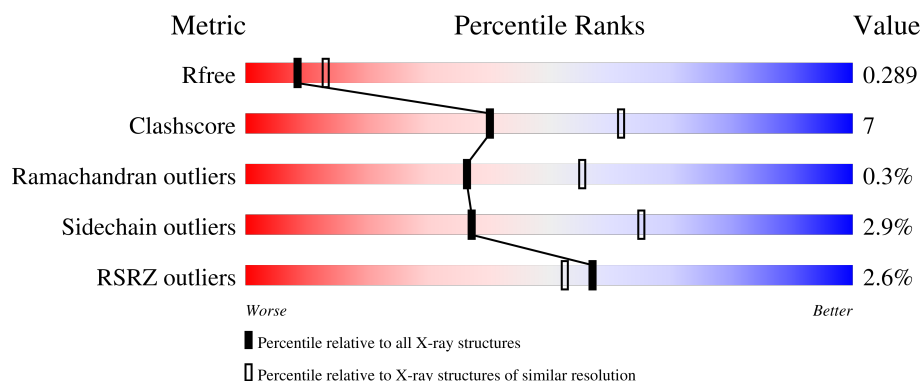
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 of the lower 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 $\leq 5\%$. 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	 3% 76% 11% 12%
2	B	340	 % 81% 16% 3%
3	G	74	 3% 73% 8% 18%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8165 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	613	Total	C	N	O	S	0	0	0
			5029	3210	875	908	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	338	Total	C	N	O	S	0	0	0
			2598	1603	466	508	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:

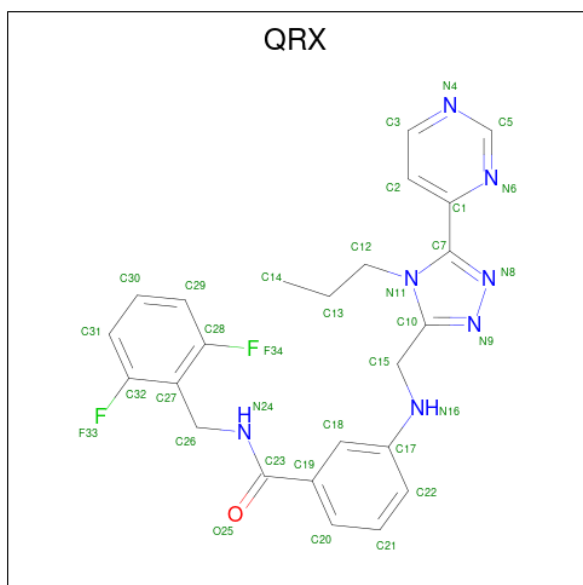
Chain	Residue	Modelled	Actual	Comment	Reference
G	-5	HIS	-	expression tag	UNP P63212

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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 N-(2,6-difluorobenzyl)-3-({[4-propyl-5-(pyrimidin-4-yl)-4H-1,2,4-triazol-3-yl]methyl}amino)benzamide (CCD ID: QRX) (formula: C₂₄H₂₃F₂N₇O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			34	24	2	7	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	12	Total	O	0	0
			12	12		
5	B	10	Total	O	0	0
			10	10		
5	G	1	Total	O	0	0
			1	1		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	187.56Å 74.23Å 123.35Å 90.00° 115.65° 90.00°	Depositor
Resolution (Å)	30.00 – 2.49 30.00 – 2.49	Depositor EDS
% Data completeness (in resolution range)	93.7 (30.00-2.49) 93.6 (30.00-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.237 , 0.285 0.241 , 0.289	Depositor DCC
R_{free} test set	2550 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	61.9	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8165	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: QRX, CMT

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	0.55	0/5142	0.80	2/6907 (0.0%)
2	B	0.59	0/2645	0.75	1/3586 (0.0%)
3	G	0.54	0/481	0.75	0/646
All	All	0.56	0/8268	0.78	3/11139 (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
3	G	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	71	VAL	CB-CA-C	-6.26	102.15	110.98
1	A	354	HIS	N-CA-C	5.66	117.53	111.36
1	A	96	GLU	N-CA-C	5.11	116.85	111.28

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 ⓘ

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	5029	0	5031	61	0
2	B	2598	0	2504	44	0
3	G	481	0	493	6	0
4	A	34	0	23	8	0
5	A	12	0	0	0	0
5	B	10	0	0	0	0
5	G	1	0	0	0	0
All	All	8165	0	8051	106	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 7.

All (106) 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:A:609:VAL:HG22	1:A:622:LEU:HD22	1.39	1.04
2:B:86:THR:O	2:B:87:THR:HB	1.69	0.92
1:A:294:MET:HE3	1:A:381:LEU:HD13	1.62	0.81
4:A:800:QRX:C13	4:A:800:QRX:H2	2.15	0.76
4:A:800:QRX:H2	4:A:800:QRX:H13	1.71	0.73
1:A:294:MET:HE3	1:A:298:ALA:HB2	1.72	0.70
2:B:33:ILE:HD11	3:G:31:SER:HA	1.74	0.69
2:B:45:MET:HE3	2:B:308:LEU:HD21	1.74	0.69
1:A:391:PHE:CD1	1:A:409:MET:HE2	2.28	0.68
2:B:165:THR:HG22	2:B:181:THR:HG22	1.76	0.67
1:A:391:PHE:CE1	1:A:409:MET:HE2	2.29	0.67
1:A:243:LEU:HD23	1:A:336:LEU:HD12	1.76	0.66
1:A:357:MET:HE3	1:A:362:LEU:HD21	1.79	0.65
2:B:61:MET:HE2	2:B:62:HIS:N	2.13	0.64
1:A:664:MET:HE1	2:B:117:LEU:HD11	1.81	0.62
1:A:294:MET:HE2	1:A:295:ARG:HA	1.82	0.62
2:B:33:ILE:CD1	3:G:34:ALA:HB3	2.29	0.62
1:A:294:MET:CE	1:A:298:ALA:HB2	2.30	0.61
1:A:409:MET:HE3	1:A:411:VAL:HA	1.81	0.60
1:A:282:HIS:CD2	1:A:325:LEU:HD22	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:233:CYS:HB2	2:B:276:VAL:HG23	1.83	0.60
1:A:325:LEU:HD12	1:A:331:VAL:HG12	1.83	0.60
2:B:30:LEU:O	2:B:34:THR:HG23	2.02	0.59
2:B:128:THR:HB	2:B:132:ASN:O	2.03	0.59
2:B:149:CYS:O	2:B:150:ARG:NH1	2.36	0.59
2:B:290:ASP:OD2	2:B:314:ARG:NE	2.35	0.57
1:A:338:LEU:HD13	4:A:800:QRX:H30	1.87	0.57
1:A:385:LEU:HD13	1:A:421:LEU:HD21	1.85	0.57
1:A:197:ILE:HG22	4:A:800:QRX:H14	1.87	0.57
1:A:399:LYS:HA	1:A:402:ILE:HD12	1.87	0.56
1:A:354:HIS:HA	1:A:357:MET:HE2	1.87	0.56
2:B:96:ARG:NH1	2:B:138:GLU:OE2	2.39	0.56
1:A:565:MET:HE3	1:A:634:CYS:SG	2.46	0.56
4:A:800:QRX:H2	4:A:800:QRX:C14	2.36	0.55
1:A:338:LEU:CD1	4:A:800:QRX:H30	2.37	0.55
2:B:86:THR:O	2:B:87:THR:CB	2.49	0.54
1:A:105:SER:HB2	1:A:136:LEU:HD21	1.88	0.54
2:B:4:LEU:HD21	3:G:9:ILE:HA	1.90	0.53
2:B:33:ILE:HD13	3:G:34:ALA:HB3	1.89	0.53
2:B:45:MET:CE	2:B:308:LEU:HD21	2.37	0.53
4:A:800:QRX:H2	4:A:800:QRX:H14B	1.91	0.52
1:A:568:MET:SD	1:A:576:TRP:N	2.82	0.52
1:A:533:THR:HG22	1:A:536:LEU:HD12	1.91	0.52
1:A:96:GLU:OE1	1:A:460:MET:HE1	2.10	0.52
1:A:319:LYS:HA	1:A:380:MET:HG3	1.92	0.51
1:A:305:LEU:HD11	1:A:318:LEU:HD22	1.93	0.51
1:A:300:GLU:OE1	1:A:331:VAL:HG22	2.10	0.50
1:A:409:MET:HE3	1:A:411:VAL:CA	2.41	0.50
2:B:247:ASP:O	2:B:248:ALA:HB3	2.11	0.50
1:A:314:VAL:HG13	1:A:370:SER:HA	1.95	0.49
2:B:318:LEU:HA	2:B:328:ALA:O	2.12	0.49
2:B:273:ILE:N	2:B:273:ILE:HD12	2.28	0.49
2:B:70:LEU:HD11	2:B:336:LEU:HD22	1.94	0.48
2:B:99:TRP:HB3	2:B:117:LEU:HD12	1.95	0.48
2:B:262:MET:SD	2:B:302:ALA:HB2	2.53	0.48
1:A:243:LEU:CD2	1:A:336:LEU:HD12	2.43	0.48
1:A:313:VAL:HA	1:A:340:CYS:O	2.14	0.48
1:A:263:THR:HB	1:A:264:PRO:HD2	1.96	0.48
1:A:294:MET:CE	1:A:298:ALA:CB	2.91	0.48
2:B:33:ILE:HD12	3:G:34:ALA:HB3	1.95	0.48
1:A:173:ARG:HA	1:A:176:GLN:OE1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:GLU:CG	1:A:421:LEU:HD22	2.44	0.47
1:A:301:ILE:HD11	1:A:323:ILE:HD13	1.96	0.47
2:B:232:ILE:HG13	2:B:243:THR:HG22	1.95	0.47
1:A:409:MET:HE3	1:A:411:VAL:CB	2.45	0.46
1:A:421:LEU:HD11	1:A:425:LEU:HD11	1.97	0.46
1:A:240:ARG:NH1	1:A:511:LEU:HD22	2.30	0.46
1:A:318:LEU:HD21	1:A:377:LEU:HD13	1.97	0.46
2:B:210:LEU:HD22	2:B:255:LEU:HD22	1.96	0.46
1:A:228:LYS:HD2	1:A:499:LEU:HD12	1.98	0.46
1:A:409:MET:HE3	1:A:411:VAL:HB	1.98	0.46
2:B:233:CYS:SG	2:B:277:SER:HA	2.56	0.46
1:A:40:ARG:NH2	1:A:166:ILE:O	2.48	0.45
1:A:237:LEU:C	1:A:237:LEU:HD23	2.41	0.45
1:A:651:TYR:CD1	1:A:651:TYR:C	2.94	0.45
2:B:271:CYS:SG	2:B:291:ASP:HB3	2.57	0.45
2:B:163:ASP:O	2:B:164:THR:OG1	2.30	0.45
1:A:390:PRO:HB3	1:A:411:VAL:HG21	1.99	0.45
1:A:219:MET:HG3	1:A:270:ILE:HD13	1.99	0.44
1:A:337:GLY:HA3	4:A:800:QRX:H29	1.98	0.44
2:B:63:TRP:CZ2	2:B:328:ALA:HB2	2.53	0.43
1:A:358:ALA:HB1	1:A:360:GLU:OE1	2.19	0.43
1:A:664:MET:HE1	2:B:117:LEU:CD1	2.45	0.43
2:B:205:ASP:O	2:B:206:ALA:HB3	2.19	0.43
2:B:301:LYS:O	2:B:302:ALA:HB3	2.18	0.43
1:A:513:ILE:O	1:A:514:SER:C	2.62	0.43
2:B:61:MET:HE3	2:B:70:LEU:HD13	2.01	0.42
1:A:358:ALA:HB3	1:A:361:VAL:HG23	2.01	0.42
1:A:162:PHE:CZ	1:A:166:ILE:HD11	2.54	0.42
2:B:122:SER:C	2:B:123:ILE:HD12	2.44	0.42
2:B:286:LEU:HD22	2:B:327:VAL:HG11	2.02	0.42
1:A:354:HIS:CG	1:A:399:LYS:HB3	2.54	0.42
2:B:283:ARG:HB3	3:G:51:LEU:HD11	2.02	0.42
2:B:146:LEU:HD11	2:B:159:THR:HB	2.02	0.41
1:A:380:MET:HE2	1:A:381:LEU:HD23	2.02	0.41
1:A:273:LEU:HD12	1:A:274:MET:H	1.86	0.41
1:A:240:ARG:HG3	1:A:509:PHE:CE1	2.56	0.41
2:B:123:ILE:HD12	2:B:123:ILE:N	2.35	0.41
1:A:356:TYR:CD2	1:A:356:TYR:N	2.89	0.41
2:B:291:ASP:OD1	2:B:291:ASP:C	2.64	0.41
2:B:313:ASN:O	2:B:314:ARG:C	2.62	0.41
1:A:664:MET:CE	2:B:117:LEU:HD11	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:76:ASP:C	2:B:76:ASP:OD2	2.63	0.41
1:A:243:LEU:HD23	1:A:336:LEU:CD1	2.48	0.40
1:A:533:THR:HA	1:A:536:LEU:HD12	2.03	0.40
2:B:128:THR:HG22	2:B:130:GLU:C	2.47	0.40

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 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	607/695 (87%)	574 (95%)	33 (5%)	0	100	100
2	B	336/340 (99%)	307 (91%)	27 (8%)	2 (1%)	21	38
3	G	59/74 (80%)	54 (92%)	4 (7%)	1 (2%)	7	13
All	All	1002/1109 (90%)	935 (93%)	64 (6%)	3 (0%)	36	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	131	GLY
2	B	42	ARG
3	G	9	ILE

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	552/617 (90%)	536 (97%)	16 (3%)	37	65
2	B	281/283 (99%)	272 (97%)	9 (3%)	34	62
3	G	50/61 (82%)	49 (98%)	1 (2%)	48	75
All	All	883/961 (92%)	857 (97%)	26 (3%)	37	65

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ILE
1	A	52	GLU
1	A	58	ILE
1	A	76	LEU
1	A	115	LYS
1	A	204	GLU
1	A	240	ARG
1	A	248	THR
1	A	294	MET
1	A	314	VAL
1	A	353	THR
1	A	360	GLU
1	A	539	ARG
1	A	567	LYS
1	A	645	LYS
1	A	651	TYR
2	B	61	MET
2	B	70	LEU
2	B	71	VAL
2	B	87	THR
2	B	128	THR
2	B	173	THR
2	B	234	PHE
2	B	271	CYS
2	B	294	CYS
3	G	28	ILE

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

Mol	Chain	Res	Type
1	A	135	HIS
1	A	140	GLN
1	A	194	HIS

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Mol	Chain	Res	Type
1	A	310	ASN
1	A	613	GLN
1	A	656	GLN
2	B	6	GLN
2	B	13	GLN
2	B	156	GLN
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	7,7,7	2.18	1 (14%)	6,8,8	2.23	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	-	4/8/8/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	68	CMT	OXT-C	5.61	1.47	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	68	CMT	OXT-C-CA	3.68	120.86	111.50
3	G	68	CMT	C1-OXT-C	3.02	122.77	115.92
3	G	68	CMT	OXT-C-O	-2.08	119.79	123.85

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	68	CMT	O-C-OXT-C1
3	G	68	CMT	CA-C-OXT-C1
3	G	68	CMT	O-C-CA-N
3	G	68	CMT	OXT-C-CA-N

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	QRX	A	800	-	37,37,37	2.03	6 (16%)	48,50,50	2.87	13 (27%)

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	QRX	A	800	-	-	5/21/21/21	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	800	QRX	N9-N8	-7.31	1.24	1.39
4	A	800	QRX	C15-C10	5.53	1.53	1.49
4	A	800	QRX	C1-C7	-5.19	1.40	1.47
4	A	800	QRX	C10-N11	-3.21	1.32	1.37
4	A	800	QRX	C7-N11	-2.70	1.33	1.38
4	A	800	QRX	C19-C23	2.27	1.55	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	800	QRX	N11-C7-N8	-12.77	105.20	110.32
4	A	800	QRX	C5-N6-C1	10.55	121.75	115.81
4	A	800	QRX	C2-C1-N6	-3.91	117.47	122.74
4	A	800	QRX	C3-C2-C1	3.49	119.17	117.02
4	A	800	QRX	N4-C5-N6	-3.44	121.49	127.33
4	A	800	QRX	N11-C10-N9	-3.20	106.13	110.42
4	A	800	QRX	C2-C1-C7	3.14	123.73	119.40
4	A	800	QRX	C12-N11-C10	-2.88	124.20	128.04
4	A	800	QRX	C3-N4-C5	2.45	120.25	115.35
4	A	800	QRX	C32-C27-C28	2.19	117.50	114.54
4	A	800	QRX	C2-C3-N4	-2.19	119.87	123.60
4	A	800	QRX	C7-N8-N9	2.06	110.34	107.75
4	A	800	QRX	C10-N9-N8	2.02	109.81	107.59

There are no chirality outliers.

All (5) torsion outliers are listed below:

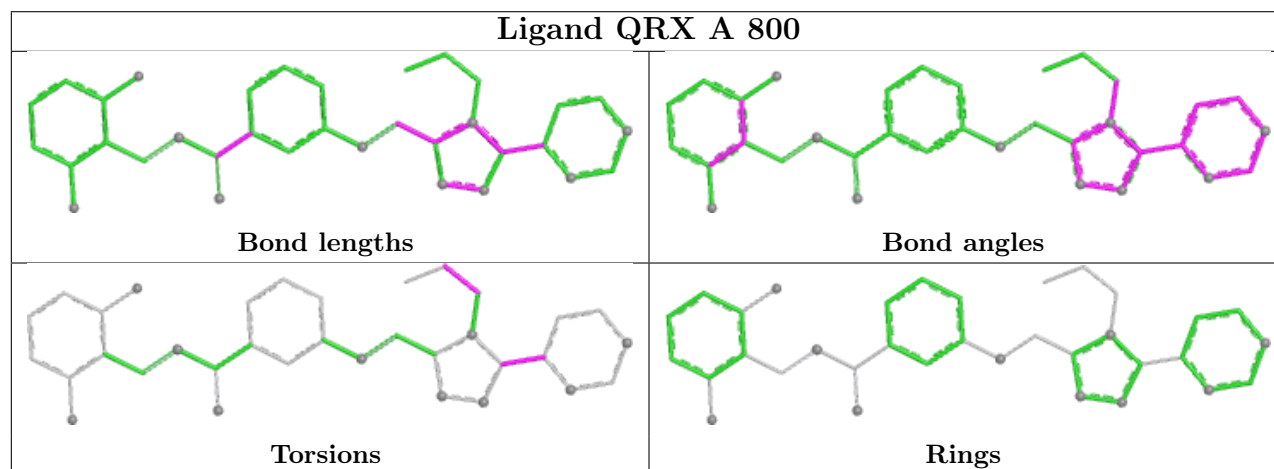
Mol	Chain	Res	Type	Atoms
4	A	800	QRX	N11-C12-C13-C14
4	A	800	QRX	C2-C1-C7-N11
4	A	800	QRX	C2-C1-C7-N8
4	A	800	QRX	N6-C1-C7-N11
4	A	800	QRX	N6-C1-C7-N8

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	800	QRX	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	613/695 (88%)	0.49	20 (3%) 49 45	53, 79, 119, 183	0
2	B	338/340 (99%)	0.09	4 (1%) 76 73	44, 65, 106, 195	0
3	G	60/74 (81%)	0.47	2 (3%) 49 45	54, 73, 148, 162	0
All	All	1011/1109 (91%)	0.35	26 (2%) 57 52	44, 74, 119, 195	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	9	ILE	4.2
1	A	440	LEU	3.7
1	A	202	PHE	3.5
1	A	668	PRO	3.1
1	A	498	LEU	3.0
1	A	382	PHE	2.9
1	A	374	TRP	2.9
1	A	205	VAL	2.8
1	A	232	GLY	2.8
1	A	568	MET	2.6
1	A	410	ALA	2.5
1	A	268	SER	2.5
2	B	2	SER	2.4
2	B	4	LEU	2.3
1	A	408	THR	2.3
2	B	40	VAL	2.3
3	G	66	PHE	2.3
1	A	499	LEU	2.2
1	A	334	SER	2.2
1	A	393	GLN	2.2
1	A	595	GLU	2.1
1	A	345	LYS	2.1
1	A	497	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	397	LYS	2.1
2	B	7	LEU	2.0
1	A	269	PHE	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. 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	B-factors(Å ²)	Q<0.9
3	CMT	G	68	8/8	0.73	0.14	76,77,82,87	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

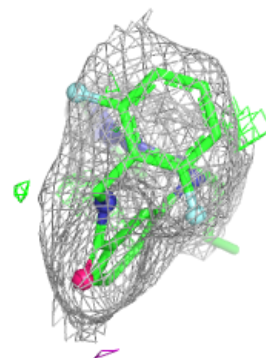
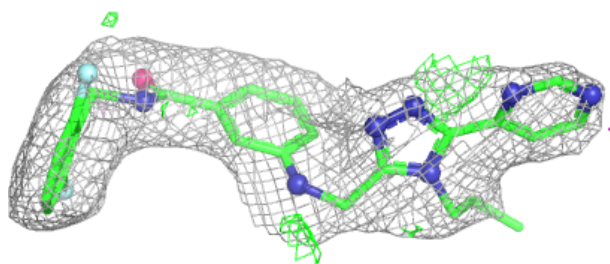
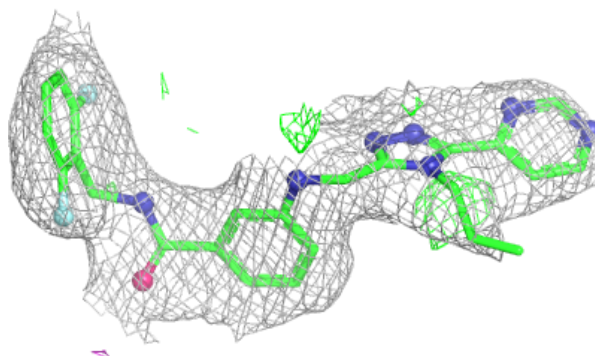
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	QRX	A	800	34/34	0.90	0.11	74,77,84,86	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around QRX A 800:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.