



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 01:38 pm BST

PDB ID : 3PVW
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

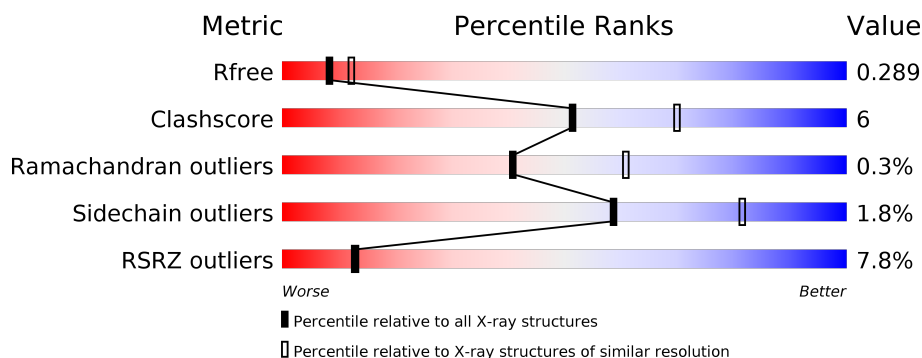
1 Overall quality at a glance

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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 on 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	<div> <div>8%</div> <div> <div></div> <div>78%</div> <div>10%</div> <div>12%</div> </div> </div>
2	B	340	<div> <div>7%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>••</div> </div> </div>
3	G	74	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>5%</div> <div>•</div> <div>18%</div> </div> </div>

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
			Total	C	N	O	S			
1	A	613	5029	3210	875	908	36	0	0	0

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
			Total	C	N	O	S			
2	B	338	2598	1603	466	508	21	0	0	0

- 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
			Total	C	N	O	S			
3	G	61	481	305	83	89	4	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

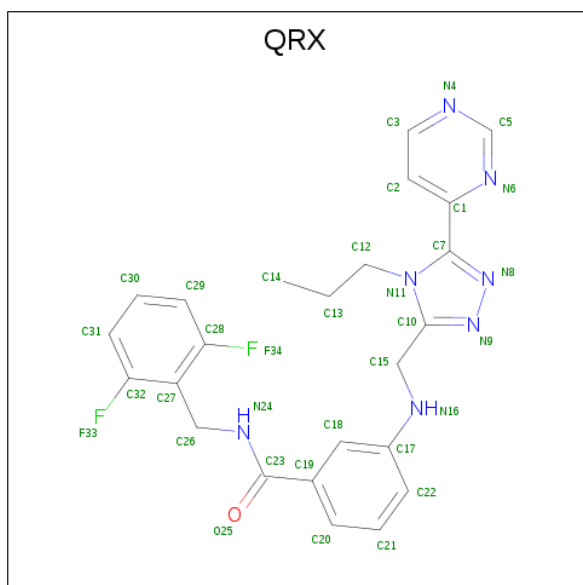
Chain	Residue	Modelled	Actual	Comment	Reference
G	-5	HIS	-	EXPRESSION TAG	UNP P63212

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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 (three-letter code: QRX) (formula: C₂₄H₂₃F₂N₇O).



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

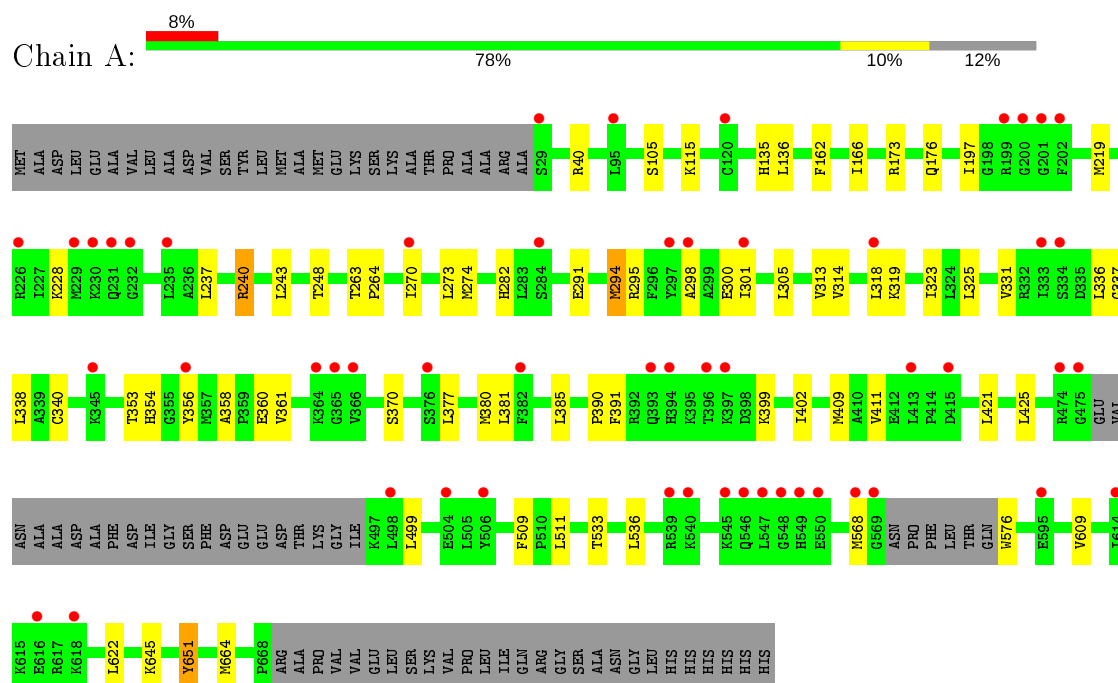
- Molecule 5 is water.

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

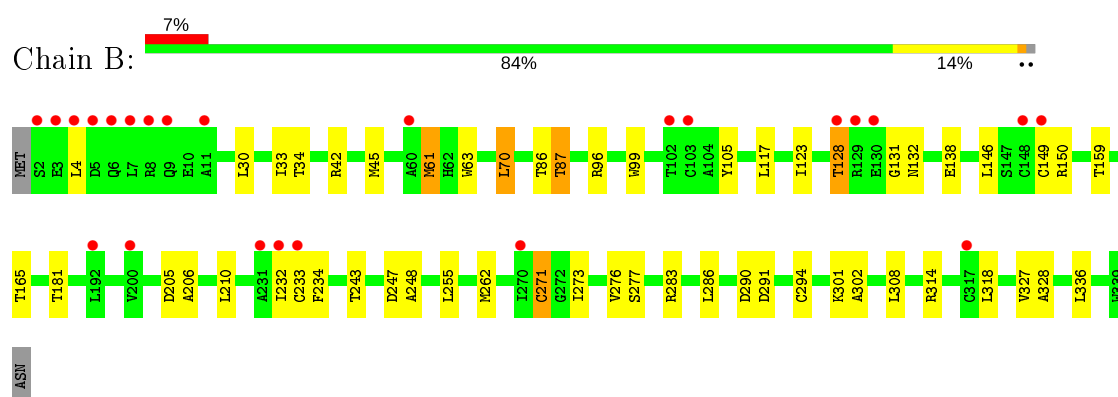
3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Beta-adrenergic receptor kinase 1

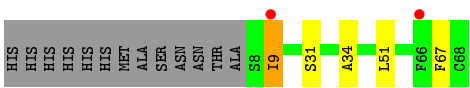


- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1



- Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2





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 29.56 – 2.49	Depositor EDS
% Data completeness (in resolution range)	93.7 (30.00-2.49) 93.7 (29.56-2.49)	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 , 42.2	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	0.44	0/5142	0.58	0/6907
2	B	0.46	0/2645	0.61	0/3586
3	G	0.46	0/481	0.54	0/646
All	All	0.45	0/8268	0.59	0/11139

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	5029	0	5031	53	0
2	B	2598	0	2504	36	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	91	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 6.

All (91) 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:298:ALA:HB2	1.54	0.89
4:A:800:QRX:C13	4:A:800:QRX:H2	2.15	0.76
1:A:294:MET:HE2	1:A:295:ARG:HA	1.69	0.73
4:A:800:QRX:H13	4:A:800:QRX:H2	1.71	0.73
2:B:33:ILE:HD11	3:G:31:SER:HA	1.74	0.69
2:B:165:THR:HG22	2:B:181:THR:HG22	1.76	0.67
1:A:243:LEU:HD23	1:A:336:LEU:HD12	1.76	0.66
2:B:33:ILE:CD1	3:G:34:ALA:HB3	2.29	0.62
1:A:282:HIS:CD2	1:A:325:LEU:HD22	2.36	0.60
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
1:A:391:PHE:CD1	1:A:409:MET:HE1	2.37	0.59
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:45:MET:HE3	2:B:308:LEU:HD21	1.84	0.57
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:294:MET:CE	1:A:298:ALA:HB2	2.30	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
2:B:96:ARG:NH1	2:B:138:GLU:OE2	2.39	0.56
4:A:800:QRX:C14	4:A:800:QRX:H2	2.36	0.55
1:A:338:LEU:CD1	4:A:800:QRX:H30	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:MET:HE3	1:A:298:ALA:CB	2.34	0.54
2:B:45:MET:CE	2:B:308:LEU:HD21	2.37	0.54
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
4:A:800:QRX:H14B	4:A:800:QRX:H2	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: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
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:HD12	2:B:273:ILE:N	2.28	0.49
1:A:664:MET:HE3	2:B:117:LEU:HD11	1.95	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
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
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:294:MET:CE	1:A:298:ALA:CB	2.91	0.47
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
2:B:233:CYS:SG	2:B:277:SER:HA	2.56	0.46
1:A:294:MET:CE	1:A:381:LEU:HD13	2.46	0.45
1:A:40:ARG:NH2	1:A:166:ILE:O	2.48	0.45
2:B:271:CYS:SG	2:B:291:ASP:HB3	2.57	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
2:B:61:MET:HE2	2:B:61:MET:HB2	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:GLY:HA3	4:A:800:QRX:H29	1.98	0.44
1:A:294:MET:HE1	1:A:381:LEU:HD13	1.99	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
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: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
1:A:664:MET:CE	2:B:117:LEU:HD11	2.49	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:409:MET:HE3	1:A:411:VAL:CB	2.50	0.41
1:A:273:LEU:HD12	1:A:274:MET:H	1.86	0.41
1:A:409:MET:HE3	1:A:411:VAL:HG23	2.03	0.41
1:A:240:ARG:HG3	1:A:509:PHE:CE1	2.56	0.41
2:B:123:ILE:N	2:B:123:ILE:HD12	2.35	0.41
1:A:356:TYR:CD2	1:A:356:TYR:N	2.89	0.41
1:A:237:LEU:HD23	1:A:237:LEU:C	2.41	0.41
1:A:243:LEU:HD23	1:A:336:LEU:CD1	2.48	0.40
1:A:651:TYR:C	1:A:651:TYR:CD1	2.94	0.40
1:A:533:THR:HA	1:A:536:LEU:HD12	2.03	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%)	25	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	59/74 (80%)	54 (92%)	4 (7%)	1 (2%)	9	16
All	All	1002/1109 (90%)	935 (93%)	64 (6%)	3 (0%)	41	61

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 ⓘ

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%)	544 (99%)	8 (1%)	67	86
2	B	281/283 (99%)	273 (97%)	8 (3%)	43	70
3	G	50/61 (82%)	50 (100%)	0	100	100
All	All	883/961 (92%)	867 (98%)	16 (2%)	59	81

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	LYS
1	A	135	HIS
1	A	240	ARG
1	A	248	THR
1	A	294	MET
1	A	353	THR
1	A	645	LYS
1	A	651	TYR
2	B	61	MET
2	B	70	LEU
2	B	87	THR
2	B	105	TYR

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Mol	Chain	Res	Type
2	B	128	THR
2	B	234	PHE
2	B	271	CYS
2	B	294	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	GLN
1	A	231	GLN
1	A	310	ASN
1	A	459	GLN
1	A	613	GLN
1	A	656	GLN
2	B	6	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	2.20	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	5.67	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	3.65	120.86	111.52
3	G	68	CMT	C1-OXT-C	3.02	122.77	115.94
3	G	68	CMT	OXT-C-O	-2.07	119.79	123.84

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

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	QRX	A	800	-	34,37,37	1.55	3 (8%)	40,50,50	1.73	8 (20%)

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	-	-	3/19/21/21	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	QRX	N9-N8	-6.92	1.24	1.37
4	A	800	QRX	C1-C7	-3.80	1.40	1.47
4	A	800	QRX	C19-C23	2.40	1.55	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	800	QRX	N4-C5-N6	-5.65	121.49	127.70
4	A	800	QRX	C5-N6-C1	4.44	121.75	115.74
4	A	800	QRX	C3-N4-C5	3.22	120.25	115.00
4	A	800	QRX	C2-C1-N6	-3.22	117.47	122.26
4	A	800	QRX	C2-C3-N4	-2.15	119.87	123.62
4	A	800	QRX	C32-C27-C28	2.14	117.50	114.51
4	A	800	QRX	C3-C2-C1	2.06	119.17	117.22
4	A	800	QRX	C10-N9-N8	2.05	109.81	105.96

There are no chirality outliers.

All (3) torsion outliers are listed below:

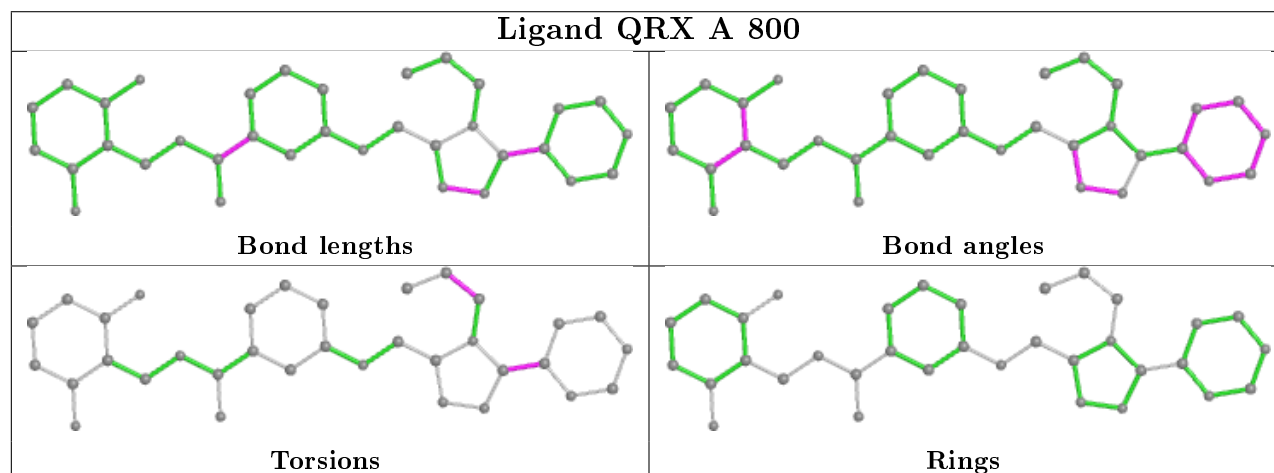
Mol	Chain	Res	Type	Atoms
4	A	800	QRX	N6-C1-C7-N8
4	A	800	QRX	N11-C12-C13-C14
4	A	800	QRX	C2-C1-C7-N8

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	53 (8%)	10 10	53, 79, 119, 183	0
2	B	338/340 (99%)	0.38	24 (7%)	16 16	45, 65, 106, 195	0
3	G	60/74 (81%)	0.19	2 (3%)	46 50	54, 73, 148, 162	0
All	All	1011/1109 (91%)	0.44	79 (7%)	13 13	45, 74, 119, 195	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	569	GLY	7.8
1	A	232	GLY	6.2
2	B	4	LEU	5.8
1	A	202	PHE	5.4
1	A	475	GLY	5.1
1	A	474	ARG	5.0
2	B	129	ARG	4.9
1	A	547	LEU	4.9
1	A	546	GLN	4.7
2	B	8	ARG	4.7
1	A	396	THR	4.7
1	A	29	SER	4.6
2	B	11	ALA	4.6
2	B	2	SER	4.5
2	B	130	GLU	4.3
2	B	9	GLN	4.3
1	A	549	HIS	4.0
1	A	397	LYS	3.9
1	A	616	GLU	3.9
1	A	498	LEU	3.7
2	B	7	LEU	3.7
1	A	364	LYS	3.6
1	A	230	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	229	MET	3.5
2	B	3	GLU	3.5
1	A	376	SER	3.4
2	B	149	CYS	3.4
1	A	318	LEU	3.4
1	A	393	GLN	3.3
1	A	334	SER	3.3
1	A	366	VAL	3.3
1	A	618	LYS	3.3
2	B	5	ASP	3.2
1	A	201	GLY	3.1
1	A	365	GLY	3.1
1	A	415	ASP	3.0
1	A	595	GLU	2.9
1	A	506	TYR	2.9
1	A	301	ILE	2.8
1	A	297	TYR	2.8
2	B	148	CYS	2.7
1	A	394	HIS	2.7
1	A	539	ARG	2.7
1	A	284	SER	2.7
1	A	540	LYS	2.7
2	B	103	CYS	2.7
1	A	545	LYS	2.7
1	A	345	LYS	2.6
1	A	333	ILE	2.6
1	A	550	GLU	2.6
1	A	568	MET	2.6
2	B	231	ALA	2.5
2	B	6	GLN	2.5
1	A	199	ARG	2.5
2	B	60	ALA	2.5
2	B	102	THR	2.5
2	B	128	THR	2.5
1	A	270	ILE	2.4
1	A	120	CYS	2.4
1	A	200	GLY	2.3
1	A	226	ARG	2.3
1	A	548	GLY	2.3
1	A	413	LEU	2.3
2	B	270	ILE	2.3
1	A	95	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	232	ILE	2.2
3	G	66	PHE	2.2
1	A	504	GLU	2.2
2	B	233	CYS	2.2
2	B	317	CYS	2.1
3	G	9	ILE	2.1
1	A	382	PHE	2.1
2	B	192	LEU	2.1
1	A	614	ILE	2.1
1	A	298	ALA	2.1
1	A	231	GLN	2.0
2	B	200	VAL	2.0
1	A	235	LEU	2.0
1	A	356	TYR	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(\AA^2)	Q<0.9
3	CMT	G	68	8/8	0.83	0.12	76,77,82,87	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

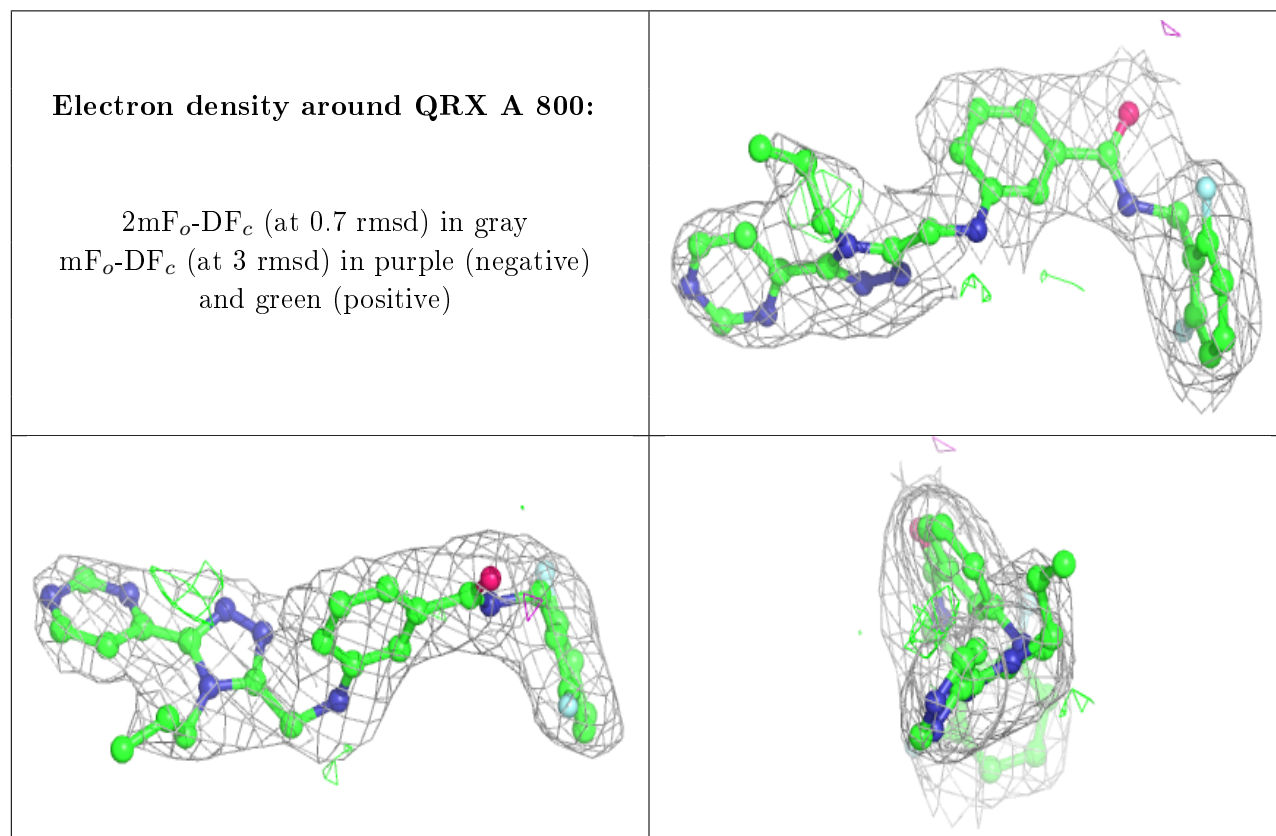
6.4 Ligands [i](#)

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. 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(\AA^2)	Q<0.9
4	QRX	A	800	34/34	0.92	0.17	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.