



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:57 PM UTC

PDB ID : 3PSC / pdb\_00003psc  
Title : Bovine GRK2 in complex with Gbetagamma subunits  
Authors : Thal, D.M.; Tesmer, J.J.  
Deposited on : 2010-12-01  
Resolution : 2.67 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](mailto: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>.

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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  
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

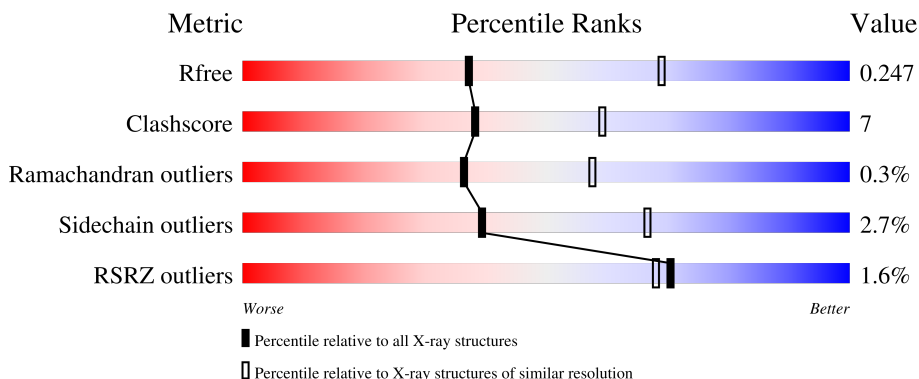
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

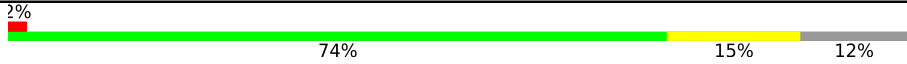


The reported resolution of this entry is 2.67 Å.

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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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  $\geq 3$ , 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	 2% 74% 15% 12%
2	B	340	 82% 16%
3	G	74	 4% 73% 9% 18%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8133 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	614	5037	3216	876	909	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	339	2607	1607	468	511	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 water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total O 4 4	0	0
4	B	3	Total O 3 3	0	0
4	G	1	Total O 1 1	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	187.93Å 73.15Å 122.78Å 90.00° 115.42° 90.00°	Depositor
Resolution (Å)	30.00 – 2.67 30.00 – 2.67	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-2.67) 99.5 (30.00-2.67)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.12 (at 2.68Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.223 , 0.257 0.220 , 0.247	Depositor DCC
$R_{free}$ test set	2165 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.0	Xtrriage
Anisotropy	0.046	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 53.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8133	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	93.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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	0.57	0/5150	0.79	0/6918
2	B	0.65	0/2654	0.79	0/3597
3	G	0.58	0/481	0.78	0/646
All	All	0.60	0/8285	0.79	0/11161

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	5037	0	5042	67	0
2	B	2607	0	2510	45	0
3	G	481	0	493	7	0
4	A	4	0	0	1	0
4	B	3	0	0	0	0
4	G	1	0	0	0	0
All	All	8133	0	8045	111	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 (111) 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:294:MET:CE	1:A:381:LEU:HD13	1.72	1.18
1:A:294:MET:HE3	1:A:381:LEU:HD13	1.42	1.02
2:B:33:ILE:HD12	3:G:34:ALA:HB3	1.44	0.94
2:B:86:THR:O	2:B:87:THR:HB	1.69	0.92
1:A:380:MET:HE2	1:A:381:LEU:HD23	1.51	0.92
1:A:294:MET:HE2	1:A:298:ALA:HB2	1.57	0.86
2:B:340:ASN:HD21	3:G:59:ASN:HD21	1.26	0.83
2:B:45:MET:HE3	2:B:308:LEU:HD21	1.58	0.82
1:A:294:MET:HE2	1:A:381:LEU:HD13	1.71	0.72
1:A:63:LEU:HD22	1:A:526:PHE:CE1	2.26	0.70
1:A:294:MET:HE3	1:A:381:LEU:CD1	2.21	0.70
1:A:609:VAL:HG22	1:A:622:LEU:HD22	1.76	0.66
1:A:338:LEU:HD23	1:A:351:VAL:HG13	1.76	0.66
1:A:294:MET:HE3	1:A:381:LEU:HB3	1.79	0.65
2:B:128:THR:HG22	2:B:130:GLU:H	1.62	0.65
2:B:61:MET:CE	2:B:70:LEU:HD13	2.27	0.64
1:A:257:MET:HE3	1:A:513:ILE:HD11	1.80	0.64
2:B:30:LEU:HD23	2:B:262:MET:HE2	1.79	0.64
1:A:301:ILE:HD11	1:A:323:ILE:HD13	1.82	0.61
1:A:62:LYS:NZ	1:A:519:GLN:OE1	2.34	0.61
1:A:105:SER:HB2	1:A:136:LEU:HD21	1.83	0.60
1:A:357:MET:HE3	1:A:362:LEU:HD21	1.83	0.59
1:A:412:GLU:C	1:A:413:LEU:HD23	2.26	0.59
2:B:33:ILE:HD11	3:G:31:SER:HA	1.85	0.59
1:A:300:GLU:OE1	1:A:331:VAL:HG22	2.03	0.58
1:A:246:VAL:HG11	1:A:254:ILE:HG21	1.85	0.58
1:A:354:HIS:HA	1:A:357:MET:HE2	1.84	0.58
1:A:565:MET:HE3	1:A:634:CYS:SG	2.43	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:MET:HE3	2:B:101:MET:CG	2.34	0.57
1:A:114:MET:HE3	1:A:114:MET:HA	1.86	0.57
2:B:71:VAL:HG23	2:B:105:TYR:CD2	2.39	0.57
2:B:233:CYS:HB2	2:B:276:VAL:HG23	1.87	0.56
2:B:71:VAL:CG2	2:B:105:TYR:CD2	2.87	0.56
1:A:40:ARG:NH2	1:A:166:ILE:O	2.36	0.56
2:B:33:ILE:CD1	3:G:34:ALA:HB3	2.29	0.55
1:A:314:VAL:HG22	1:A:370:SER:HA	1.89	0.55
2:B:58:ILE:HD13	2:B:336:LEU:CD1	2.37	0.55
1:A:664:MET:HE3	2:B:101:MET:HG3	1.89	0.54
2:B:232:ILE:HG13	2:B:243:THR:HG22	1.88	0.54
1:A:413:LEU:HD12	1:A:422:ARG:HG3	1.89	0.54
2:B:273:ILE:N	2:B:273:ILE:HD12	2.24	0.53
1:A:427:GLY:HA3	1:A:437:LEU:HD12	1.91	0.53
1:A:334:SER:O	1:A:336:LEU:HD12	2.09	0.53
2:B:163:ASP:C	2:B:164:THR:HG23	2.34	0.53
1:A:391:PHE:CD1	1:A:406:THR:HA	2.44	0.53
1:A:529:ILE:O	1:A:533:THR:HG23	2.09	0.52
2:B:61:MET:HE3	2:B:70:LEU:HD13	1.91	0.52
1:A:314:VAL:HG23	1:A:342:PHE:CD2	2.46	0.50
1:A:601:LEU:HD21	1:A:624:ILE:HD11	1.93	0.50
2:B:33:ILE:HD12	3:G:34:ALA:CB	2.30	0.50
2:B:205:ASP:O	2:B:206:ALA:HB3	2.11	0.50
2:B:301:LYS:O	2:B:302:ALA:HB3	2.12	0.50
1:A:173:ARG:HA	1:A:176:GLN:OE1	2.12	0.49
1:A:273:LEU:HD12	1:A:274:MET:H	1.78	0.48
1:A:357:MET:HE3	1:A:362:LEU:CD2	2.43	0.48
2:B:340:ASN:HD21	3:G:59:ASN:ND2	2.04	0.48
2:B:247:ASP:O	2:B:248:ALA:HB3	2.14	0.47
1:A:111:THR:O	1:A:115:LYS:HB3	2.14	0.47
2:B:262:MET:SD	2:B:302:ALA:HB2	2.54	0.47
1:A:155:GLN:OE1	1:A:158:ARG:NH2	2.46	0.46
1:A:390:PRO:CB	1:A:411:VAL:HG21	2.45	0.46
1:A:301:ILE:CD1	1:A:323:ILE:HD13	2.44	0.46
2:B:128:THR:HG22	2:B:130:GLU:N	2.29	0.46
1:A:533:THR:HA	1:A:536:LEU:HD12	1.96	0.46
2:B:63:TRP:CD2	2:B:321:THR:HG22	2.51	0.46
1:A:243:LEU:HB3	1:A:257:MET:HE2	1.97	0.46
1:A:197:ILE:O	1:A:197:ILE:HG22	2.16	0.46
2:B:179:THR:HG22	2:B:181:THR:HG23	1.97	0.46
1:A:113:ILE:O	1:A:117:LEU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:LEU:HD13	2:B:82:TRP:CD2	2.52	0.45
1:A:219:MET:HE2	1:A:270:ILE:HD11	1.99	0.45
2:B:79:LEU:HD11	2:B:114:CYS:HB3	1.98	0.45
1:A:246:VAL:CG1	1:A:254:ILE:HG21	2.47	0.45
1:A:600:LEU:C	1:A:600:LEU:HD12	2.42	0.45
2:B:163:ASP:O	2:B:164:THR:HG23	2.16	0.45
1:A:397:LYS:O	1:A:399:LYS:N	2.50	0.44
2:B:128:THR:C	2:B:130:GLU:H	2.24	0.44
1:A:274:MET:HE2	1:A:332:ARG:HB2	1.99	0.44
2:B:58:ILE:HD13	2:B:336:LEU:HD11	1.99	0.44
1:A:319:LYS:HA	1:A:380:MET:HG3	1.99	0.44
1:A:380:MET:HE2	1:A:381:LEU:CD2	2.36	0.44
2:B:63:TRP:CZ2	2:B:328:ALA:HB2	2.53	0.43
1:A:390:PRO:HB3	1:A:411:VAL:HG21	2.00	0.43
2:B:70:LEU:HD11	2:B:336:LEU:HD22	2.00	0.43
1:A:472:PRO:HA	1:A:473:PRO:HD3	1.84	0.43
1:A:509:PHE:N	1:A:510:PRO:CD	2.82	0.43
2:B:210:LEU:HD22	2:B:255:LEU:HD22	2.00	0.42
2:B:262:MET:HG2	2:B:264:TYR:CZ	2.54	0.42
1:A:467:PRO:HA	1:A:468:PRO:HD3	1.93	0.42
1:A:507:ARG:C	1:A:509:PHE:H	2.27	0.42
1:A:565:MET:CE	1:A:634:CYS:SG	3.08	0.42
2:B:249:THR:HG22	2:B:265:SER:HB3	2.01	0.42
2:B:291:ASP:OD1	2:B:291:ASP:C	2.63	0.42
1:A:464:GLN:NE2	4:A:692:HOH:O	2.53	0.41
1:A:651:TYR:CD1	1:A:651:TYR:C	2.97	0.41
2:B:58:ILE:HD13	2:B:336:LEU:HD12	2.02	0.41
1:A:314:VAL:HG21	1:A:369:ASP:C	2.46	0.41
2:B:165:THR:HG22	2:B:181:THR:HG22	2.03	0.41
1:A:380:MET:CE	1:A:381:LEU:HD23	2.36	0.41
2:B:58:ILE:CD1	2:B:336:LEU:HD12	2.51	0.41
1:A:544:ASN:HB3	1:A:549:HIS:CB	2.50	0.40
2:B:231:ALA:CB	2:B:275:SER:HA	2.51	0.40
1:A:391:PHE:CE1	1:A:406:THR:HA	2.55	0.40
1:A:242:MET:HE1	1:A:341:ASP:HB2	2.03	0.40
1:A:274:MET:SD	1:A:332:ARG:HD2	2.61	0.40
1:A:314:VAL:HG23	1:A:342:PHE:CE2	2.57	0.40
1:A:334:SER:O	1:A:335:ASP:C	2.64	0.40
2:B:73:ALA:HB2	2:B:103:CYS:HB3	2.02	0.40
2:B:170:ASP:HB3	2:B:173:THR:HB	2.04	0.40
3:G:28:ILE:HG22	3:G:29:LYS:N	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:ARG:HA	1:A:474:ARG:CZ	2.51	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	608/695 (88%)	573 (94%)	33 (5%)	2 (0%)	36	57
2	B	337/340 (99%)	312 (93%)	24 (7%)	1 (0%)	36	57
3	G	59/74 (80%)	56 (95%)	3 (5%)	0	100	100
All	All	1004/1109 (90%)	941 (94%)	60 (6%)	3 (0%)	36	57

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	398	ASP
2	B	53	GLY
1	A	508	ASN

### 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	553/617 (90%)	539 (98%)	14 (2%)	42	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	282/283 (100%)	272 (96%)	10 (4%)	32	58
3	G	50/61 (82%)	50 (100%)	0	100	100
All	All	885/961 (92%)	861 (97%)	24 (3%)	39	67

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	SER
1	A	150	ILE
1	A	192	SER
1	A	204	GLU
1	A	240	ARG
1	A	244	SER
1	A	262	HIS
1	A	263	THR
1	A	284	SER
1	A	290	SER
1	A	396	THR
1	A	543	LYS
1	A	635	ASP
1	A	666	ASN
2	B	40	VAL
2	B	52	ARG
2	B	70	LEU
2	B	71	VAL
2	B	87	THR
2	B	122	SER
2	B	177	THR
2	B	292	PHE
2	B	318	LEU
2	B	340	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	262	HIS
1	A	310	ASN
1	A	363	GLN
1	A	434	ASN
1	A	459	GLN

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Mol	Chain	Res	Type
1	A	503	GLN
2	B	6	GLN
2	B	91	HIS
2	B	132	ASN
2	B	176	GLN
2	B	239	ASN
2	B	259	GLN
3	G	59	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	2.12	1 (14%)	6,8,8	2.36	4 (66%)

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	5.46	1.46	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	68	CMT	OXT-C-CA	3.80	121.15	111.50
3	G	68	CMT	C1-OXT-C	2.84	122.35	115.92
3	G	68	CMT	CA-CB-SG	-2.38	109.31	114.40
3	G	68	CMT	OXT-C-O	-2.23	119.51	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](#)

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 [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	614/695 (88%)	0.26	12 (1%) 65 61	61, 94, 148, 200	0
2	B	339/340 (99%)	-0.09	1 (0%) 90 89	50, 76, 126, 231	0
3	G	60/74 (81%)	0.13	3 (5%) 34 30	61, 85, 178, 194	0
All	All	1013/1109 (91%)	0.13	16 (1%) 70 68	50, 88, 148, 231	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	496	ILE	5.3
1	A	440	LEU	3.6
1	A	242	MET	3.4
1	A	569	GLY	3.1
3	G	28	ILE	2.9
2	B	7	LEU	2.9
1	A	402	ILE	2.8
3	G	10	ALA	2.7
1	A	222	LEU	2.7
1	A	400	HIS	2.5
3	G	9	ILE	2.3
1	A	506	TYR	2.2
1	A	137	VAL	2.2
1	A	435	ARG	2.1
1	A	460	MET	2.0
1	A	499	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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	CMT	G	68	8/8	0.72	0.14	90,92,98,102	0

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.