Full wwPDB X-ray Structure Validation Report (i)

May 2, 2016 – 01:43 PM EDT

PDB ID	:	5HE0
Title	:	Bovine GRK2 in complex with Gbetagamma subunits and CCG215022
Authors	:	Cato, M.C.; Waninger-Saroni, J.; Tesmer, J.J.G.
Deposited on	:	2016-01-05
Resolution	:	2.56 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

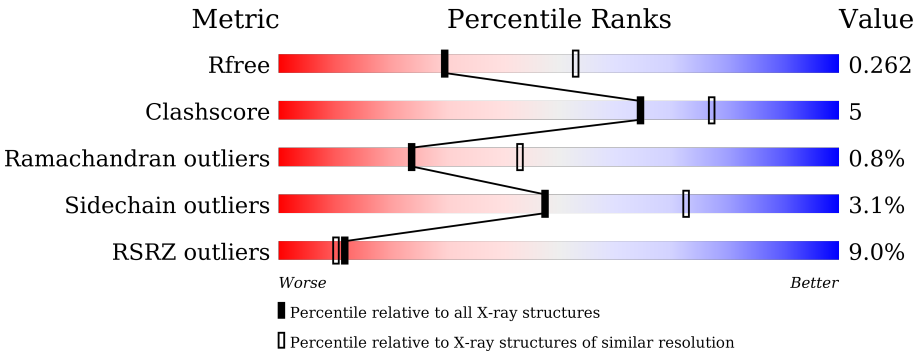
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027457
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	3324 (2.60-2.52)
Clashscore	102246	3729 (2.60-2.52)
Ramachandran outliers	100387	3673 (2.60-2.52)
Sidechain outliers	100360	3673 (2.60-2.52)
RSRZ outliers	91569	3333 (2.60-2.52)

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 <=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	641	10% 81% 14%
2	B	339	6% 85% 14%
3	G	71	8% 72% 11% 15%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8248 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	621	Total	C	N	O	S	0	0	0
			5094	3254	886	918	36			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	670	ALA	SER	engineered mutation	UNP P21146

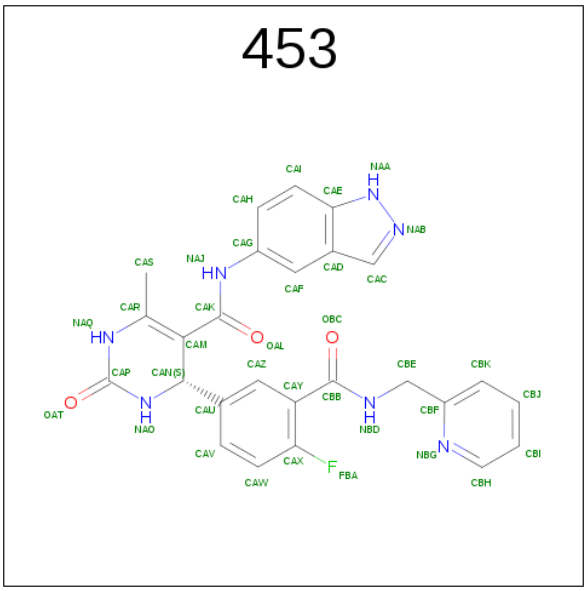
- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	339	Total	C	N	O	S	0	2	0
			2619	1613	470	513	23			

- 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	60	Total	C	N	O	S	0	0	0
			462	288	82	89	3			

- Molecule 4 is (4S)-4-{4-fluoro-3-[(pyridin-2-ylmethyl)carbamoyl]phenyl}-N-(1H-indazol-5-yl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxamide (three-letter code: 453) (formula: $C_{26}H_{22}FN_7O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C F N O 37 26 1 7 3	0	0

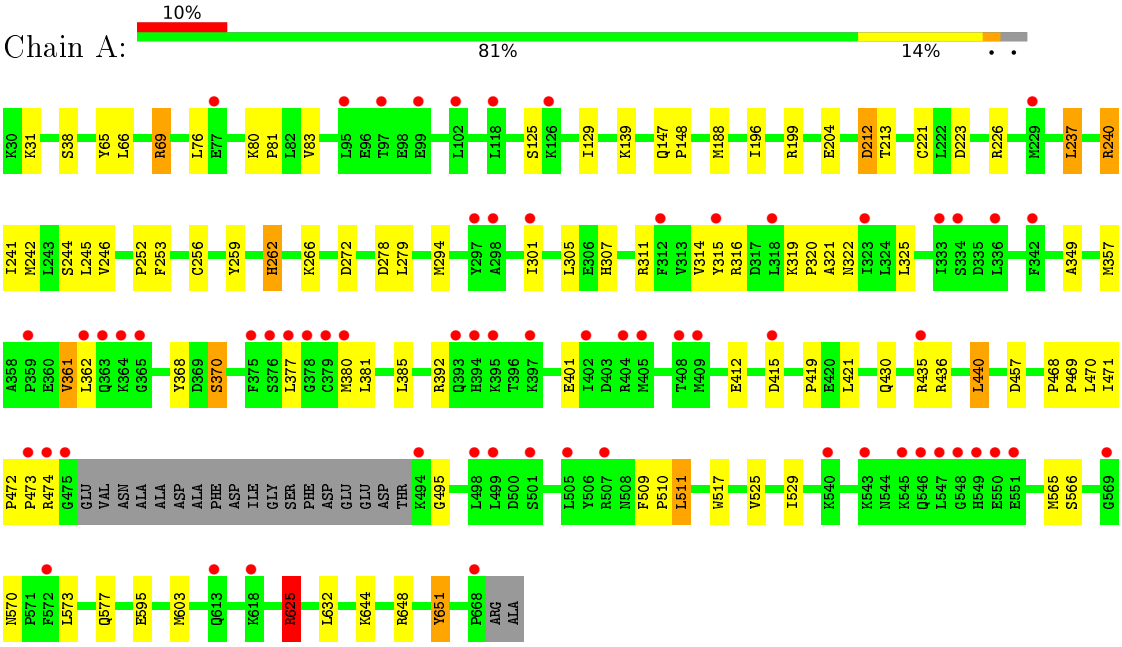
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	17	Total O 17 17	0	0
5	B	19	Total O 19 19	0	0

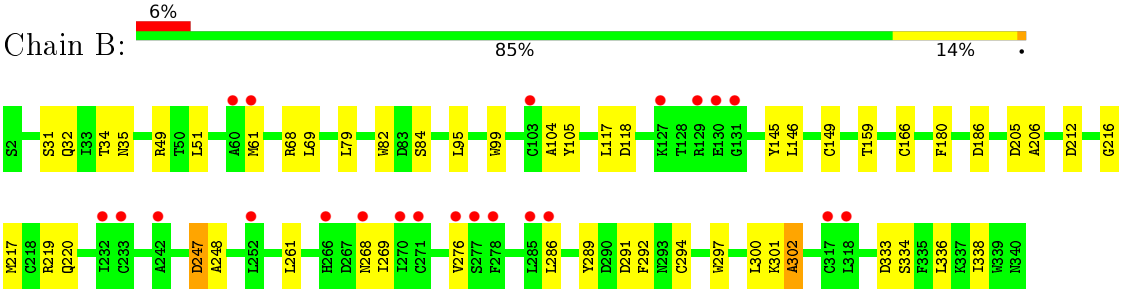
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

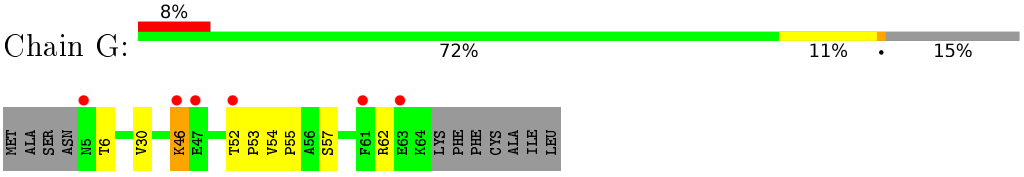
- Molecule 1: Beta-adrenergic receptor kinase 1



- 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 (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	60.55Å 239.93Å 208.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.56 29.83 – 2.56	Depositor EDS
% Data completeness (in resolution range)	94.5 (30.00-2.56) 94.6 (29.83-2.56)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 2.57Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.202 , 0.264 0.205 , 0.262	Depositor DCC
R_{free} test set	2316 reflections (5.19%)	DCC
Wilson B-factor (Å^2)	58.3	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 31.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8248	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 453

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	0.66	0/5210	0.81	1/7001 (0.0%)
2	B	0.74	1/2666 (0.0%)	0.92	5/3613 (0.1%)
3	G	0.64	0/468	0.77	0/631
All	All	0.69	1/8344 (0.0%)	0.84	6/11245 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	297	TRP	CB-CG	-5.22	1.40	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	212	ASP	CB-CG-OD1	8.21	125.69	118.30
2	B	118	ASP	CB-CG-OD2	-6.06	112.84	118.30
1	A	392	ARG	NE-CZ-NH1	5.76	123.18	120.30
2	B	118	ASP	CB-CG-OD1	5.63	123.36	118.30
2	B	212	ASP	CB-CG-OD2	-5.61	113.25	118.30
2	B	247	ASP	CB-CG-OD1	5.40	123.16	118.30

There are no chirality outliers.

There are no planarity outliers.

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	5094	0	5102	56	0
2	B	2619	0	2518	22	0
3	G	462	0	473	5	0
4	A	37	0	22	1	0
5	A	17	0	0	1	0
5	B	19	0	0	0	0
All	All	8248	0	8115	83	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 5.

All (83) 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:212:ASP:HB3	1:A:213:THR:HG23	1.60	0.81
3:G:54:VAL:HG22	3:G:55:PRO:HD2	1.66	0.74
1:A:565:MET:HE1	1:A:632:LEU:HD13	1.76	0.66
2:B:32:GLN:O	2:B:35:ASN:HB2	1.95	0.66
1:A:361:VAL:HA	1:A:368:TYR:CE2	2.34	0.62
1:A:237:LEU:O	1:A:241:ILE:HD12	2.02	0.59
2:B:180:PHE:CE1	2:B:216:GLY:HA2	2.36	0.59
2:B:51:LEU:HB2	2:B:336:LEU:HB2	1.84	0.58
1:A:470:LEU:HD23	1:A:470:LEU:C	2.26	0.56
1:A:430:GLN:HG3	1:A:435:ARG:O	2.06	0.55
2:B:247:ASP:O	2:B:248:ALA:HB3	2.07	0.54
1:A:644:LYS:NZ	5:A:801:HOH:O	2.40	0.53
1:A:256:CYS:N	1:A:272:ASP:OD2	2.37	0.53
3:G:54:VAL:CG2	3:G:55:PRO:HD2	2.37	0.53
1:A:240:ARG:CZ	1:A:511:LEU:HD21	2.38	0.53
1:A:245:LEU:O	1:A:311:ARG:HD3	2.09	0.52
2:B:205:ASP:O	2:B:206:ALA:HB3	2.10	0.52
1:A:252:PRO:HG2	1:A:253:PHE:CE2	2.46	0.51
1:A:570:ASN:HB2	1:A:573:LEU:HB3	1.93	0.51
2:B:79:LEU:HG	2:B:95:LEU:HD21	1.93	0.51
2:B:261:LEU:HD22	3:G:30:VAL:HG13	1.94	0.50
4:A:701:453:H18	4:A:701:453:OAL	2.12	0.49
1:A:603:MET:HB3	1:A:651:TYR:HA	1.94	0.49
1:A:262:HIS:HB2	1:A:266:LYS:O	2.14	0.48
1:A:570:ASN:CB	1:A:573:LEU:HB3	2.44	0.47
3:G:52:THR:O	3:G:53:PRO:C	2.51	0.47
1:A:125:SER:O	1:A:129:ILE:HD12	2.14	0.47
1:A:385:LEU:HD13	1:A:421:LEU:HD21	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:68:ARG:O	2:B:84:SER:OG	2.32	0.47
1:A:625:ARG:HD2	1:A:625:ARG:HA	1.77	0.47
1:A:242:MET:HA	1:A:242:MET:HE2	1.97	0.47
1:A:315:TYR:O	1:A:316:ARG:HB2	2.12	0.47
1:A:325:LEU:N	1:A:325:LEU:HD12	2.30	0.47
1:A:457:ASP:OD1	1:A:457:ASP:C	2.53	0.47
2:B:276:VAL:HA	2:B:286:LEU:O	2.15	0.46
1:A:294:MET:C	1:A:294:MET:SD	2.94	0.46
1:A:470:LEU:HD23	1:A:471:ILE:N	2.30	0.46
1:A:315:TYR:OH	1:A:322:ASN:HB3	2.16	0.45
1:A:349:ALA:O	1:A:368:TYR:OH	2.29	0.45
1:A:509:PHE:HB3	1:A:510:PRO:HD3	1.99	0.45
1:A:436:ARG:O	1:A:440:LEU:HD13	2.17	0.45
1:A:566:SER:HA	1:A:577:GLN:O	2.16	0.45
1:A:319:LYS:O	1:A:320:PRO:C	2.55	0.45
1:A:472:PRO:HA	1:A:473:PRO:HD3	1.89	0.44
1:A:525:VAL:O	1:A:529:ILE:HG12	2.17	0.44
2:B:145:TYR:OH	2:B:186:ASP:OD2	2.23	0.44
2:B:104:ALA:HB2	2:B:149:CYS:O	2.17	0.44
1:A:188:MET:HE1	1:A:221:CYS:SG	2.58	0.44
1:A:525:VAL:O	1:A:529:ILE:CG1	2.66	0.43
1:A:69:ARG:HB2	1:A:83:VAL:HG11	2.00	0.43
1:A:147:GLN:N	1:A:148:PRO:HD2	2.34	0.43
1:A:196:ILE:HD12	1:A:196:ILE:H	1.83	0.43
2:B:301:LYS:O	2:B:302:ALA:HB3	2.18	0.43
2:B:49:ARG:HB2	2:B:338:ILE:HG12	1.99	0.43
2:B:34:THR:HG21	2:B:300:LEU:HB3	2.01	0.43
1:A:223:ASP:OD2	1:A:226:ARG:HG3	2.18	0.42
1:A:430:GLN:HA	1:A:430:GLN:OE1	2.19	0.42
2:B:146:LEU:HD11	2:B:159:THR:HB	2.00	0.42
1:A:259:TYR:OH	1:A:517:TRP:HD1	2.02	0.42
1:A:278:ASP:OD2	1:A:321:ALA:HA	2.19	0.42
1:A:80:LYS:N	1:A:81:PRO:CD	2.82	0.42
2:B:291:ASP:C	2:B:291:ASP:OD1	2.58	0.42
1:A:314:VAL:HG12	1:A:370:SER:HA	2.02	0.42
1:A:468:PRO:HA	1:A:469:PRO:HD3	1.85	0.42
1:A:66:LEU:HD23	1:A:66:LEU:HA	1.87	0.42
1:A:80:LYS:HB3	1:A:81:PRO:HD3	2.02	0.42
2:B:269:ILE:HG21	2:B:289:TYR:CE2	2.55	0.41
1:A:279:LEU:HB2	1:A:320:PRO:O	2.20	0.41
2:B:333:ASP:O	2:B:334:SER:CB	2.68	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:ILE:HD13	1:A:380:MET:HE1	2.03	0.41
2:B:99:TRP:CB	2:B:117:LEU:HB2	2.51	0.41
2:B:219:ARG:C	2:B:220:GLN:HG3	2.40	0.41
2:B:166:CYS:HB2	2:B:180:PHE:HB2	2.02	0.41
1:A:377:LEU:O	1:A:381:LEU:HG	2.20	0.41
1:A:65:TYR:O	1:A:66:LEU:C	2.58	0.41
2:B:69:LEU:HA	2:B:82:TRP:O	2.20	0.41
1:A:246:VAL:O	1:A:307:HIS:HE1	2.04	0.40
1:A:199:ARG:HG3	1:A:204:GLU:HG3	2.02	0.40
1:A:305:LEU:HD23	1:A:305:LEU:HA	1.94	0.40
1:A:357:MET:CE	1:A:362:LEU:HD21	2.51	0.40
1:A:509:PHE:N	1:A:510:PRO:CD	2.84	0.40
1:A:648:ARG:HA	1:A:651:TYR:CD2	2.56	0.40
3:G:46:LYS:HD2	3:G:46:LYS:N	2.36	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	617/641 (96%)	564 (91%)	46 (8%)	7 (1%)	17 33
2	B	339/339 (100%)	319 (94%)	19 (6%)	1 (0%)	46 68
3	G	58/71 (82%)	53 (91%)	5 (9%)	0	100 100
All	All	1014/1051 (96%)	936 (92%)	70 (7%)	8 (1%)	24 43

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	LYS
1	A	212	ASP
2	B	302	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	370	SER
1	A	625	ARG
1	A	76	LEU
1	A	361	VAL
1	A	495	GLY

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	559/574 (97%)	542 (97%)	17 (3%)	48	73
2	B	284/282 (101%)	277 (98%)	7 (2%)	55	79
3	G	49/58 (84%)	45 (92%)	4 (8%)	14	25
All	All	892/914 (98%)	864 (97%)	28 (3%)	47	73

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LYS
1	A	38	SER
1	A	69	ARG
1	A	237	LEU
1	A	240	ARG
1	A	244	SER
1	A	262	HIS
1	A	401	GLU
1	A	412	GLU
1	A	415	ASP
1	A	419	PRO
1	A	440	LEU
1	A	474	ARG
1	A	511	LEU
1	A	595	GLU
1	A	625	ARG
1	A	651	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	31	SER
2	B	61	MET
2	B	105	TYR
2	B	217	MET
2	B	268	ASN
2	B	292	PHE
2	B	294	CYS
3	G	6	THR
3	G	46	LYS
3	G	57	SER
3	G	62	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	A	275	ASN
1	A	307	HIS
3	G	11	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

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	453	A	701	-	39,41,41	1.43	5 (12%)	51,58,58	2.07	16 (31%)

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	453	A	701	-	-	0/21/37/37	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	453	CAN-CAM	-4.92	1.47	1.51
4	A	701	453	CAR-NAQ	-3.35	1.32	1.38
4	A	701	453	CAP-NAQ	-3.03	1.32	1.37
4	A	701	453	CAG-NAJ	-2.00	1.37	1.41
4	A	701	453	CAR-CAM	2.84	1.46	1.36

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	701	453	CAW-CAX-CAY	-3.90	118.85	123.16
4	A	701	453	CBF-CBE-NBD	-3.38	105.50	112.72
4	A	701	453	OAL-CAK-CAM	-3.34	115.42	121.17
4	A	701	453	CAR-NAQ-CAP	-2.64	121.64	123.81
4	A	701	453	CAX-CAY-CBB	-2.57	119.03	125.05
4	A	701	453	OAT-CAP-NAQ	-2.56	116.56	121.82
4	A	701	453	CAS-CAR-CAM	-2.29	124.13	127.67
4	A	701	453	CAH-CAI-CAE	-2.20	118.43	120.86
4	A	701	453	CAG-NAJ-CAK	-2.10	123.86	127.60
4	A	701	453	CAY-CBB-NBD	2.31	122.26	117.52
4	A	701	453	CAV-CAW-CAX	2.56	121.86	118.96
4	A	701	453	CBH-NBG-CBF	2.66	120.91	117.35
4	A	701	453	CAZ-CAY-CAX	2.67	119.21	116.83
4	A	701	453	CAI-CAE-NAA	3.26	135.65	130.23
4	A	701	453	CAM-CAN-NAO	3.69	111.91	109.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	701	453	NAQ-CAP-NAO	7.06	124.34	116.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	701	453	1	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, 95^{th} 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	621/641 (96%)	0.44	64 (10%) 9 7	41, 71, 116, 155	0
2	B	339/339 (100%)	0.29	22 (6%) 22 20	41, 58, 87, 152	0
3	G	60/71 (84%)	0.51	6 (10%) 9 8	47, 65, 116, 138	0
All	All	1020/1051 (97%)	0.39	92 (9%) 12 10	41, 65, 112, 155	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	129	ARG	6.6
1	A	475	GLY	6.5
1	A	474	ARG	5.5
1	A	395	LYS	5.5
3	G	46	LYS	5.2
1	A	547	LEU	4.8
1	A	99	GLU	4.8
1	A	394	HIS	4.7
1	A	318	LEU	4.1
1	A	301	ILE	4.0
1	A	408	THR	3.8
3	G	52	THR	3.8
2	B	233[A]	CYS	3.7
1	A	550	GLU	3.6
1	A	499	LEU	3.6
1	A	549	HIS	3.5
1	A	409	MET	3.5
1	A	377	LEU	3.5
3	G	61	PHE	3.4
2	B	317	CYS	3.4
1	A	312	PHE	3.4
1	A	97	THR	3.4
1	A	359	PRO	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	333	ILE	3.3
1	A	543	LYS	3.3
2	B	60	ALA	3.3
2	B	61	MET	3.3
1	A	363	GLN	3.3
2	B	286	LEU	3.3
1	A	334	SER	3.2
1	A	668	PRO	3.2
2	B	318	LEU	3.1
1	A	572	PHE	3.1
3	G	5	ASN	3.0
1	A	393	GLN	3.0
1	A	548	GLY	3.0
1	A	376	SER	2.9
1	A	545	LYS	2.9
2	B	277	SER	2.8
1	A	473	PRO	2.8
2	B	127	LYS	2.8
2	B	103	CYS	2.8
1	A	315	TYR	2.7
1	A	342	PHE	2.7
2	B	268	ASN	2.7
1	A	380	MET	2.7
1	A	365	GLY	2.7
1	A	298	ALA	2.6
1	A	102	LEU	2.6
1	A	126	LYS	2.6
1	A	118	LEU	2.5
2	B	276	VAL	2.5
2	B	285	LEU	2.5
1	A	405	MET	2.5
1	A	501	SER	2.5
2	B	130	GLU	2.5
2	B	131	GLY	2.5
2	B	271[A]	CYS	2.4
1	A	494	LYS	2.4
3	G	47	GLU	2.4
1	A	540	LYS	2.4
1	A	297	TYR	2.4
1	A	375	PHE	2.4
1	A	618	LYS	2.4
1	A	505	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	507	ARG	2.4
2	B	242	ALA	2.3
1	A	569	GLY	2.3
1	A	402	ILE	2.3
1	A	95	LEU	2.3
1	A	498	LEU	2.3
1	A	362	LEU	2.3
1	A	404	ARG	2.2
1	A	415	ASP	2.2
1	A	551	GLU	2.2
2	B	232	ILE	2.2
1	A	435	ARG	2.2
1	A	546	GLN	2.2
1	A	397	LYS	2.2
1	A	336	LEU	2.1
1	A	613	GLN	2.1
2	B	266	HIS	2.1
1	A	378	GLY	2.1
1	A	229	MET	2.1
1	A	323	ILE	2.1
2	B	252	LEU	2.1
3	G	63	GLU	2.1
2	B	270	ILE	2.1
1	A	364	LYS	2.0
2	B	278	PHE	2.0
1	A	77	GLU	2.0
1	A	379	CYS	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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, 95^{th} 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	453	A	701	37/37	0.95	0.17	-0.45	45,70,81,82	0

6.5 Other polymers (i)

There are no such residues in this entry.