



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 29, 2022 – 03:20 pm GMT

PDB ID : 7Q9U
Title : Crystal structure of the high affinity KRas mutant PDE6D complex
Authors : Yelland, T.; Ismail, I.
Deposited on : 2021-11-14
Resolution : 2.24 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

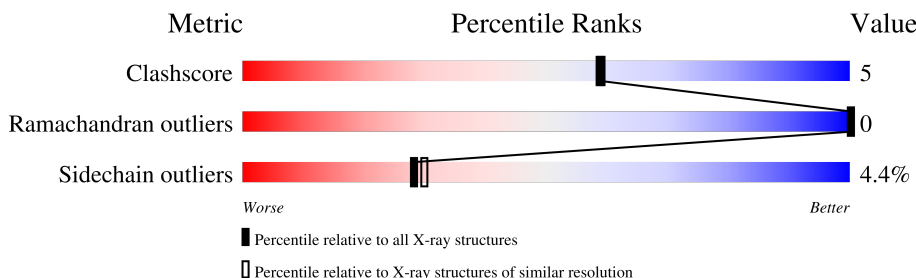
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 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))
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)

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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	AAA	185	81% 10% • 8%
1	BBB	185	84% 9% • 6%
2	CCC	150	86% 13% •
2	DDD	150	84% 13% ••

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	EDO	CCC	204	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5483 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 GTPase KRas.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	170	Total	C	N	O	S	0	3	0
			1372	854	240	269	9			
1	BBB	174	Total	C	N	O	S	0	2	0
			1400	872	246	274	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	182	SER	LYS	conflict	UNP P01116
AAA	184	ILE	LYS	conflict	UNP P01116
BBB	182	SER	LYS	conflict	UNP P01116
BBB	184	ILE	LYS	conflict	UNP P01116

- Molecule 2 is a protein called Retinal rod rhodopsin-sensitive cGMP 3',5'-cyclic phosphodiesterase subunit delta.

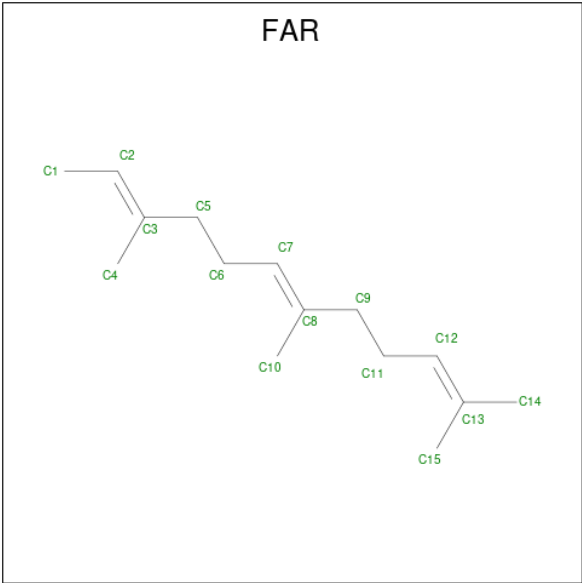
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	DDD	147	Total	C	N	O	S	0	0	0
			1202	771	202	223	6			
2	CCC	150	Total	C	N	O	S	0	1	0
			1236	791	210	228	7			

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



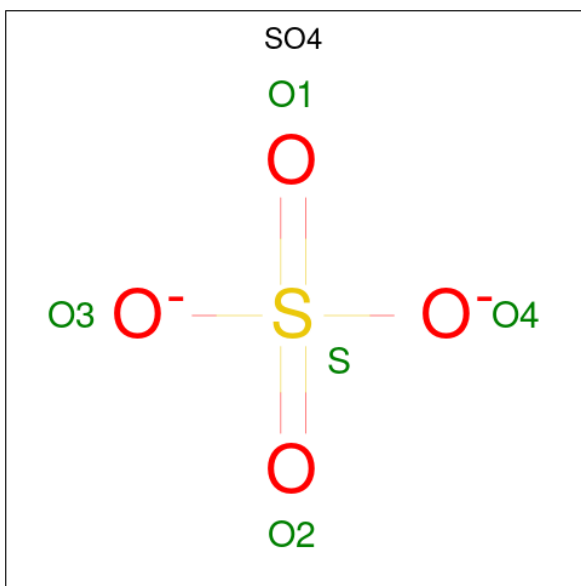
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	AAA	1	Total 28	C 10	N 5	O 11	P 2	0	0
3	BBB	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 4 is FARNESYL (three-letter code: FAR) (formula: C₁₅H₂₆).



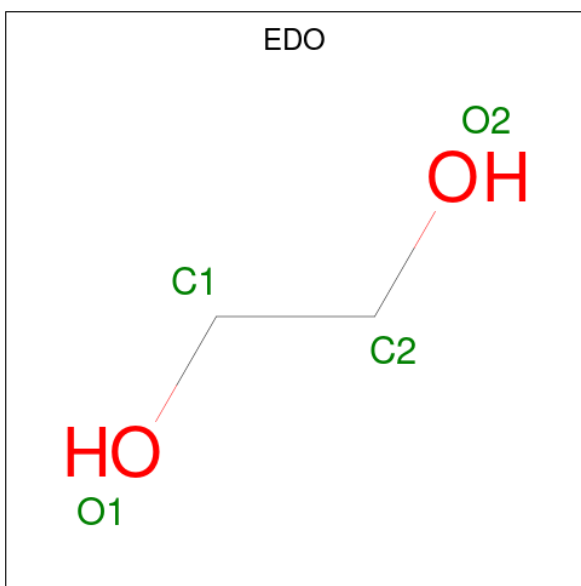
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	1	Total	C	0	0
			15	15		
4	BBB	1	Total	C	0	0
			15	15		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	BBB	1	Total	O	S	0	0
			5	4	1		
5	DDD	1	Total	O	S	0	0
			5	4	1		
5	CCC	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	DDD	1	Total C O 4 2 2	0	0
6	DDD	1	Total C O 4 2 2	0	0
6	CCC	1	Total C O 4 2 2	0	0
6	CCC	1	Total C O 4 2 2	0	0
6	CCC	1	Total C O 4 2 2	0	0

- Molecule 7 is water.


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	32	Total O 32 32	0	0
7	BBB	45	Total O 45 45	0	0
7	DDD	29	Total O 29 29	0	0
7	CCC	46	Total O 46 46	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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.


Note EDS failed to run properly.

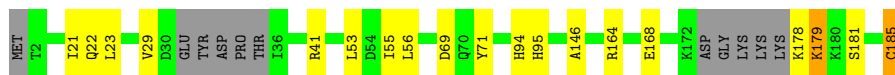
- Molecule 1: GTPase KRas

Chain AAA: 




- Molecule 1: GTPase KRas

Chain BBB: 



- Molecule 2: Retinal rod rhodopsin-sensitive cGMP 3',5'-cyclic phosphodiesterase subunit delta

Chain DDD: 



- Molecule 2: Retinal rod rhodopsin-sensitive cGMP 3',5'-cyclic phosphodiesterase subunit delta

Chain CCC: 



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.09Å 57.92Å 78.91Å 82.77° 81.71° 68.45°	Depositor
Resolution (Å)	53.71 – 2.24	Depositor
% Data completeness (in resolution range)	93.5 (53.71-2.24)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.25Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.199 , 0.255	Depositor
Wilson B-factor (Å ²)	41.7	Xtriage
Anisotropy	0.063	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5483	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.30% 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: GDP, EDO, FAR, CMT, SO4

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	AAA	0.66	0/1382	0.87	0/1855
1	BBB	0.65	0/1409	0.85	0/1889
2	CCC	0.63	0/1262	0.92	0/1699
2	DDD	0.63	0/1228	0.88	0/1656
All	All	0.64	0/5281	0.88	0/7099

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	AAA	1372	0	1352	13	0
1	BBB	1400	0	1393	11	0
2	CCC	1236	0	1234	19	0
2	DDD	1202	0	1189	12	0
3	AAA	28	0	12	0	0
3	BBB	28	0	12	0	0
4	AAA	15	0	24	1	0
4	BBB	15	0	24	3	0
5	BBB	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	CCC	5	0	0	0	0
5	DDD	5	0	0	0	0
6	CCC	12	0	18	8	0
6	DDD	8	0	12	0	0
7	AAA	32	0	0	4	0
7	BBB	45	0	0	2	0
7	CCC	46	0	0	2	0
7	DDD	29	0	0	2	0
All	All	5483	0	5270	50	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.

The worst 5 of 50 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:91:PHE:HB3	6:CCC:204:EDO:H12	1.35	1.06
2:CCC:93:GLU:HG2	6:CCC:204:EDO:H21	1.59	0.83
1:AAA:184:ILE:HG21	2:DDD:80:VAL:HG11	1.67	0.74
2:CCC:91:PHE:HB3	6:CCC:204:EDO:C1	2.16	0.71
2:CCC:93:GLU:HG3	6:CCC:204:EDO:O1	1.93	0.68

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	AAA	167/185 (90%)	163 (98%)	4 (2%)	0	100	100
1	BBB	170/185 (92%)	163 (96%)	7 (4%)	0	100	100
2	CCC	149/150 (99%)	147 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	DDD	145/150 (97%)	143 (99%)	2 (1%)	0	100	100
All	All	631/670 (94%)	616 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	151/163 (93%)	145 (96%)	6 (4%)	31	34
1	BBB	154/163 (94%)	151 (98%)	3 (2%)	57	64
2	CCC	136/135 (101%)	127 (93%)	9 (7%)	16	14
2	DDD	132/135 (98%)	124 (94%)	8 (6%)	18	16
All	All	573/596 (96%)	547 (96%)	26 (4%)	28	29

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	DDD	87	LEU
2	CCC	1	MET
2	CCC	122	VAL
2	DDD	147	LEU
2	CCC	9	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are 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
1	CMT	AAA	185	4,1	7,7,7	2.00	1 (14%)	6,8,8	3.68	4 (66%)
1	CMT	BBB	185	4,1	7,7,7	1.96	1 (14%)	6,8,8	1.85	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
1	CMT	AAA	185	4,1	-	3/8/8/8	-
1	CMT	BBB	185	4,1	-	4/8/8/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	185	CMT	OXT-C	5.16	1.45	1.33
1	BBB	185	CMT	OXT-C	5.00	1.45	1.33

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	185	CMT	OXT-C-O	-5.75	112.59	123.84
1	AAA	185	CMT	OXT-C-CA	5.41	125.38	111.52
1	AAA	185	CMT	CA-CB-SG	3.18	121.28	114.44
1	BBB	185	CMT	OXT-C-O	-2.89	118.20	123.84
1	AAA	185	CMT	C-CA-N	2.42	118.41	110.79

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AAA	185	CMT	N-CA-CB-SG
1	BBB	185	CMT	CA-C-OXT-C1
1	BBB	185	CMT	O-C-OXT-C1
1	BBB	185	CMT	N-CA-CB-SG
1	AAA	185	CMT	O-C-CA-N

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AAA	185	CMT	2	0
1	BBB	185	CMT	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are 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	$\# Z > 2$
6	EDO	CCC	204	-	3,3,3	0.06	0	2,2,2	0.94	0
3	GDP	AAA	201	-	24,30,30	0.99	2 (8%)	30,47,47	1.33	2 (6%)
4	FAR	AAA	202	1	14,14,14	0.24	0	16,16,16	0.98	1 (6%)
3	GDP	BBB	202	-	24,30,30	0.98	2 (8%)	30,47,47	1.26	4 (13%)
6	EDO	CCC	203	-	3,3,3	0.05	0	2,2,2	0.14	0
6	EDO	CCC	202	-	3,3,3	0.08	0	2,2,2	0.41	0
5	SO4	BBB	201	-	4,4,4	0.39	0	6,6,6	0.12	0
6	EDO	DDD	202	-	3,3,3	0.06	0	2,2,2	0.68	0
5	SO4	DDD	201	-	4,4,4	0.39	0	6,6,6	0.05	0
5	SO4	CCC	201	-	4,4,4	0.38	0	6,6,6	0.14	0
6	EDO	DDD	203	-	3,3,3	0.05	0	2,2,2	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FAR	BBB	203	1	14,14,14	0.29	0	16,16,16	0.67	0

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
6	EDO	CCC	204	-	-	1/1/1/1	-
3	GDP	AAA	201	-	-	1/12/32/32	0/3/3/3
4	FAR	AAA	202	1	-	6/14/14/14	-
3	GDP	BBB	202	-	-	1/12/32/32	0/3/3/3
6	EDO	CCC	203	-	-	1/1/1/1	-
6	EDO	CCC	202	-	-	1/1/1/1	-
6	EDO	DDD	202	-	-	0/1/1/1	-
6	EDO	DDD	203	-	-	1/1/1/1	-
4	FAR	BBB	203	1	-	5/14/14/14	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AAA	201	GDP	C6-N1	-2.44	1.34	1.37
3	BBB	202	GDP	C5-C4	2.41	1.49	1.43
3	BBB	202	GDP	C6-N1	-2.35	1.34	1.37
3	AAA	201	GDP	C5-C4	2.35	1.49	1.43

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AAA	201	GDP	PA-O3A-PB	-3.09	122.23	132.83
3	BBB	202	GDP	O6-C6-N1	2.89	124.06	120.65
3	BBB	202	GDP	O3'-C3'-C2'	-2.36	104.17	111.82
3	BBB	202	GDP	O5'-PA-O1A	-2.26	100.24	109.07
3	BBB	202	GDP	O2A-PA-O1A	2.25	123.38	112.24

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AAA	202	FAR	C1-C2-C3-C5
4	AAA	202	FAR	C1-C2-C3-C4

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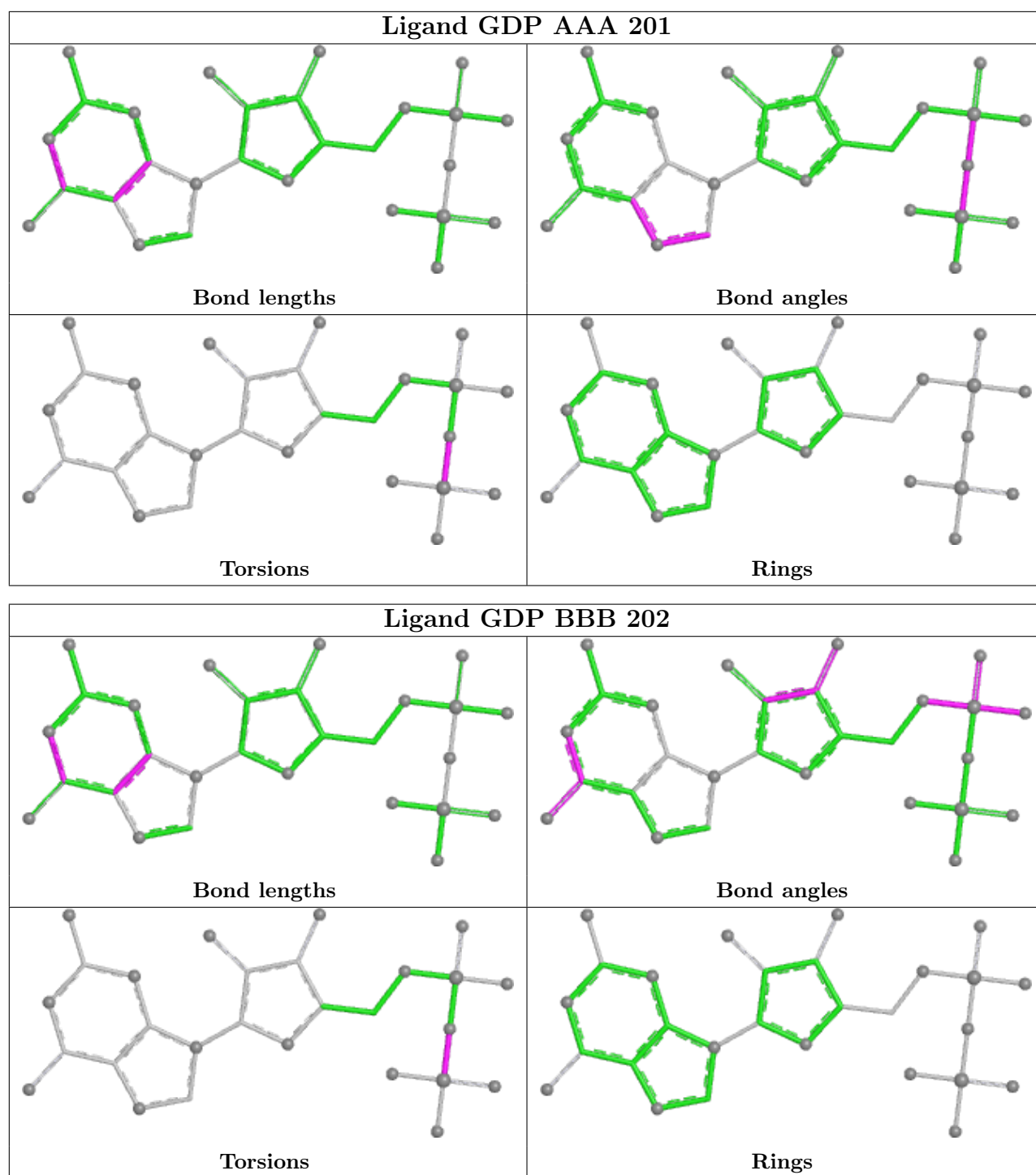
Mol	Chain	Res	Type	Atoms
4	BBB	203	FAR	C6-C7-C8-C9
4	BBB	203	FAR	C6-C7-C8-C10
4	BBB	203	FAR	C4-C3-C5-C6

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	CCC	204	EDO	8	0
4	AAA	202	FAR	1	0
5	BBB	201	SO4	1	0
4	BBB	203	FAR	3	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 [i](#)

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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.