Full wwPDB X-ray Structure Validation Report ⓘ

Jan 20, 2024 – 05:23 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 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:

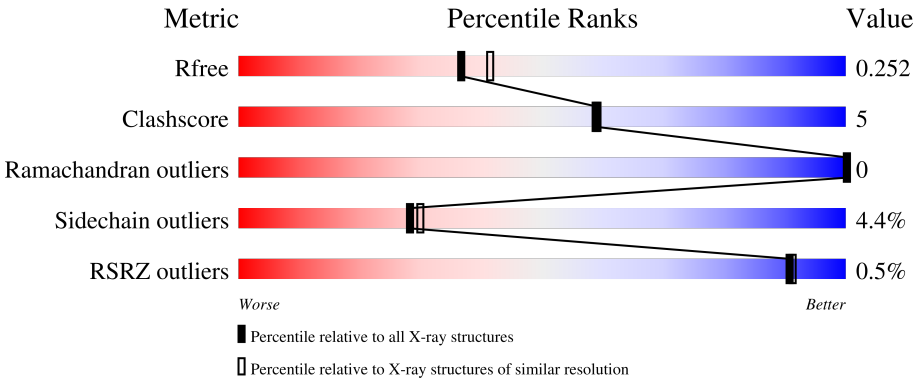
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.24 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))
R_{free}	130704	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (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 <=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	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 (i)

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			

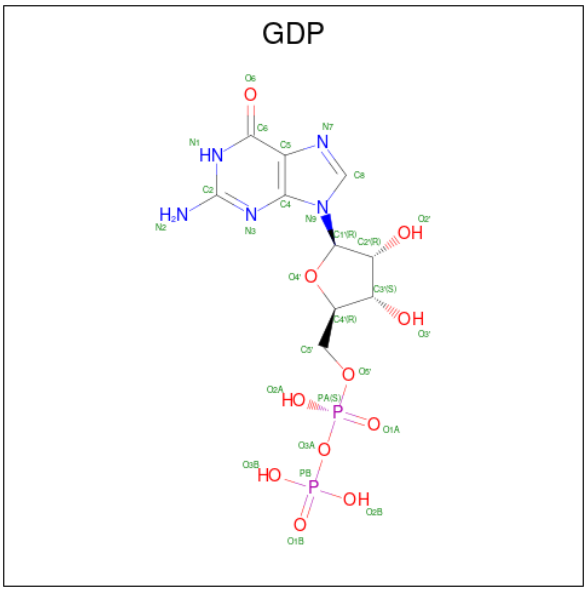
There are 4 discrepancies between the modelled and reference sequences:

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.

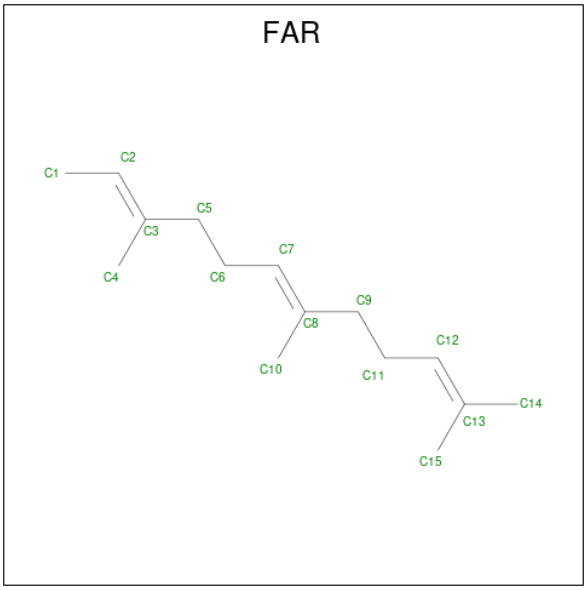
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	DDD	147	Total	C	N	O	S	0	0	0
			1202	771	202	223	6			
2	CCC	150	Total	C	N	O	S	0	1	0
			1236	791	210	228	7			

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



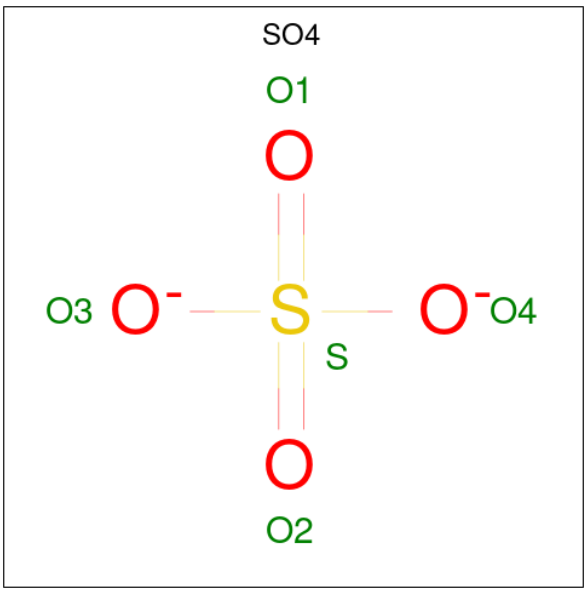
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	AAA	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	BBB	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 4 is FARNESYL (three-letter code: FAR) (formula: $C_{15}H_{26}$).



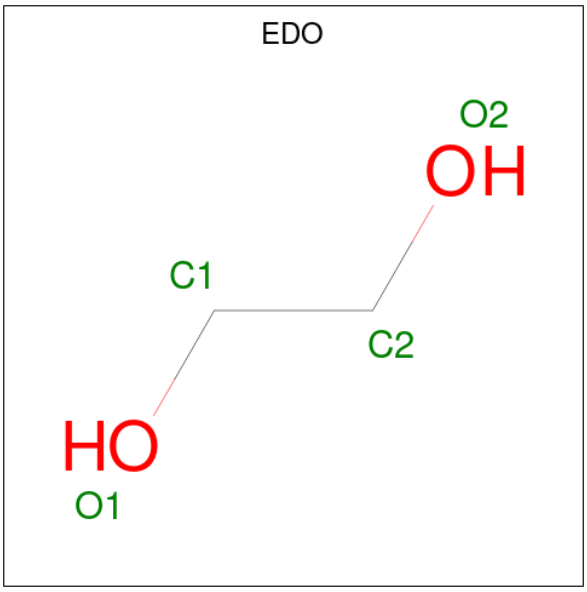
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	1	Total	C	0	0
			15	15		
4	BBB	1	Total	C	0	0
			15	15		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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.

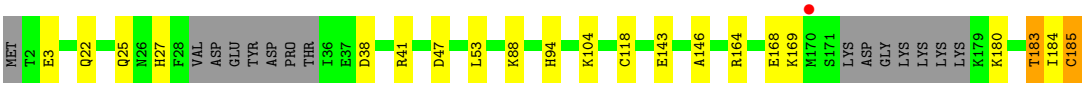
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	32	Total O 32 32	0	0
7	BBB	45	Total O 45 45	0	0
7	DDD	29	Total O 29 29	0	0
7	CCC	46	Total O 46 46	0	0

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 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.

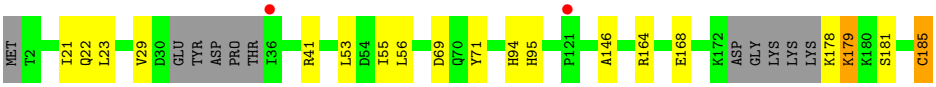
• Molecule 1: GTPase KRas

Chain AAA:



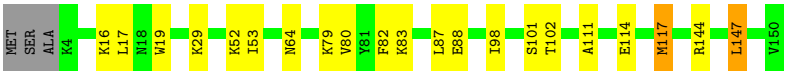
• Molecule 1: GTPase KRas

Chain BBB:



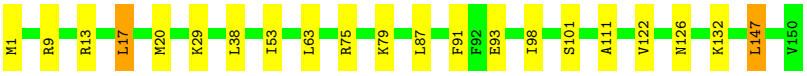
• Molecule 2: Retinal rod rhodopsin-sensitive cGMP 3',5'-cyclic phosphodiesterase subunit delta

Chain DDD:



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

Chain CCC:



4 Data and refinement statistics (i)

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 53.71 – 2.24	Depositor EDS
% Data completeness (in resolution range)	93.5 (53.71-2.24) 93.5 (53.71-2.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 2.25Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.199 , 0.255 0.202 , 0.252	Depositor DCC
R_{free} test set	1774 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å^2)	41.7	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 34.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: SO4, CMT, EDO, GDP, FAR

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

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.

All (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
2:CCC:75:ARG:HD2	6:CCC:204:EDO:H22	1.76	0.67
2:CCC:20:MET:HE2	2:CCC:63:LEU:CD2	2.28	0.63
4:BBB:203:FAR:H12A	2:CCC:53:ILE:CD1	2.29	0.63
1:AAA:118[B]:CYS:SG	1:AAA:143:GLU:HB3	2.39	0.63
1:BBB:95:HIS:ND1	7:BBB:303:HOH:O	2.31	0.61
4:BBB:203:FAR:H12A	2:CCC:53:ILE:HD13	1.83	0.61
1:BBB:179:LYS:HD3	1:BBB:181:SER:HB3	1.86	0.57
1:BBB:94:HIS:ND1	5:BBB:201:SO4:O1	2.37	0.56
2:CCC:75:ARG:HD2	6:CCC:204:EDO:C2	2.37	0.54
2:CCC:132:LYS:HE2	7:CCC:313:HOH:O	2.08	0.54
1:AAA:183:THR:HB	2:DDD:88:GLU:OE1	2.08	0.53
1:AAA:185:CMT:H11	2:DDD:53:ILE:O	2.09	0.53
1:AAA:94:HIS:ND1	7:AAA:302:HOH:O	2.35	0.51
2:DDD:114:GLU:HA	2:DDD:117:MET:HG3	1.92	0.50
2:CCC:17:LEU:HD11	2:CCC:63:LEU:HD22	1.94	0.49
2:CCC:93:GLU:CG	6:CCC:204:EDO:O1	2.60	0.49
1:AAA:47:ASP:OD2	1:AAA:164:ARG:NH1	2.43	0.48
2:DDD:144:ARG:HD3	7:DDD:302:HOH:O	2.13	0.48
1:BBB:21:ILE:HD13	1:BBB:29:VAL:HG11	1.95	0.48
2:CCC:20:MET:HE2	2:CCC:63:LEU:HD21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:126:ASN:ND2	7:CCC:305:HOH:O	2.47	0.47
1:AAA:180:LYS:NZ	7:AAA:304:HOH:O	2.46	0.47
1:AAA:88:LYS:HE3	7:AAA:322:HOH:O	2.14	0.47
1:BBB:23:LEU:HD23	1:BBB:55:ILE:CD1	2.45	0.46
1:AAA:22:GLN:HG3	1:AAA:146:ALA:O	2.16	0.46
1:BBB:178:LYS:HG2	1:BBB:178:LYS:O	2.16	0.46
1:AAA:185:CMT:H13	2:DDD:111:ALA:HB2	1.96	0.46
2:DDD:102:THR:HG22	7:DDD:322:HOH:O	2.17	0.44
1:BBB:22:GLN:HG3	1:BBB:146:ALA:O	2.18	0.44
1:AAA:25:GLN:NE2	1:AAA:27:HIS:NE2	2.65	0.44
4:AAA:202:FAR:H52	2:DDD:147:LEU:HD21	1.99	0.44
4:BBB:203:FAR:H61	2:CCC:147:LEU:HD21	1.99	0.44
2:CCC:20:MET:HE3	2:CCC:38:LEU:HD12	1.99	0.44
2:DDD:82:PHE:CE1	2:DDD:83:LYS:HD2	2.53	0.43
2:DDD:98:ILE:O	2:DDD:101:SER:OG	2.29	0.43
1:BBB:185:CMT:H13	2:CCC:111:ALA:HB2	2.00	0.43
2:DDD:19:TRP:CE2	2:DDD:64:ASN:CB	3.03	0.42
2:CCC:93:GLU:CG	6:CCC:204:EDO:H21	2.40	0.42
1:AAA:104:LYS:NZ	7:AAA:305:HOH:O	2.47	0.42
1:BBB:41[B]:ARG:HA	1:BBB:53:LEU:O	2.19	0.41
1:BBB:56:LEU:HD23	1:BBB:71:TYR:HB2	2.01	0.41
2:CCC:98:ILE:O	2:CCC:101:SER:OG	2.26	0.41
1:AAA:41:ARG:HA	1:AAA:53:LEU:O	2.21	0.41
2:DDD:19:TRP:CZ2	2:DDD:64:ASN:HB2	2.56	0.41
1:BBB:164:ARG:HD3	7:BBB:339:HOH:O	2.21	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	AAA	167/185 (90%)	163 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BBB	170/185 (92%)	163 (96%)	7 (4%)	0	100	100
2	CCC	149/150 (99%)	147 (99%)	2 (1%)	0	100	100
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 (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	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

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

Mol	Chain	Res	Type
1	AAA	3	GLU
1	AAA	38[A]	ASP
1	AAA	38[B]	ASP
1	AAA	168	GLU
1	AAA	169	LYS
1	AAA	183	THR
1	BBB	69	ASP
1	BBB	168	GLU
1	BBB	179	LYS
2	DDD	16	LYS
2	DDD	17	LEU
2	DDD	29	LYS
2	DDD	52	LYS

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Mol	Chain	Res	Type
2	DDD	79	LYS
2	DDD	87	LEU
2	DDD	117	MET
2	DDD	147	LEU
2	CCC	1	MET
2	CCC	9	ARG
2	CCC	13	ARG
2	CCC	17	LEU
2	CCC	29	LYS
2	CCC	79	LYS
2	CCC	87	LEU
2	CCC	122	VAL
2	CCC	147	LEU

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
1	BBB	185	CMT	OXT-C-CA	2.08	116.84	111.52
1	BBB	185	CMT	CA-CB-SG	-2.00	110.13	114.44

There are no chirality outliers.

All (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
1	BBB	185	CMT	O-C-CA-N
1	AAA	185	CMT	C-CA-CB-SG

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	DDD	203	-	3,3,3	0.05	0	2,2,2	0.26	0
5	SO4	CCC	201	-	4,4,4	0.38	0	6,6,6	0.14	0
6	EDO	CCC	202	-	3,3,3	0.08	0	2,2,2	0.41	0
6	EDO	DDD	202	-	3,3,3	0.06	0	2,2,2	0.68	0
3	GDP	BBB	202	-	24,30,30	0.98	2 (8%)	30,47,47	1.26	4 (13%)
5	SO4	BBB	201	-	4,4,4	0.39	0	6,6,6	0.12	0
6	EDO	CCC	203	-	3,3,3	0.05	0	2,2,2	0.14	0
6	EDO	CCC	204	-	3,3,3	0.06	0	2,2,2	0.94	0
5	SO4	DDD	201	-	4,4,4	0.39	0	6,6,6	0.05	0
3	GDP	AAA	201	-	24,30,30	0.99	2 (8%)	30,47,47	1.33	2 (6%)
4	FAR	BBB	203	1	14,14,14	0.29	0	16,16,16	0.67	0
4	FAR	AAA	202	1	14,14,14	0.24	0	16,16,16	0.98	1 (6%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FAR	BBB	203	1	-	5/14/14/14	-
4	FAR	AAA	202	1	-	6/14/14/14	-

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

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
3	AAA	201	GDP	C8-N7-C5	2.21	107.20	102.99
4	AAA	202	FAR	C5-C3-C2	2.10	125.08	120.27

There are no chirality outliers.

All (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
4	BBB	203	FAR	C6-C7-C8-C9
4	BBB	203	FAR	C6-C7-C8-C10
4	BBB	203	FAR	C4-C3-C5-C6
4	BBB	203	FAR	C2-C3-C5-C6
4	AAA	202	FAR	C10-C8-C9-C11
4	AAA	202	FAR	C7-C8-C9-C11
4	AAA	202	FAR	C2-C3-C5-C6
4	AAA	202	FAR	C4-C3-C5-C6
6	CCC	203	EDO	O1-C1-C2-O2
6	CCC	204	EDO	O1-C1-C2-O2
3	AAA	201	GDP	PA-O3A-PB-O2B
3	BBB	202	GDP	PA-O3A-PB-O3B
6	DDD	203	EDO	O1-C1-C2-O2

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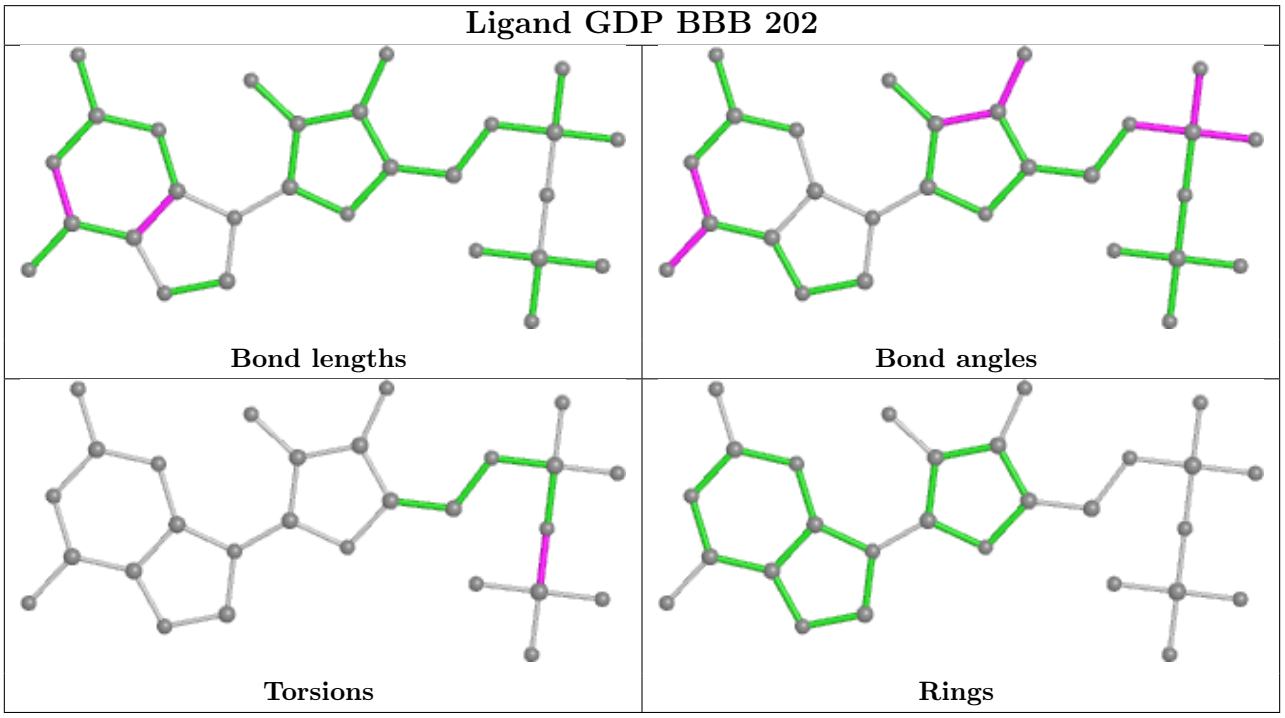
Mol	Chain	Res	Type	Atoms
6	CCC	202	EDO	O1-C1-C2-O2
4	BBB	203	FAR	C10-C8-C9-C11

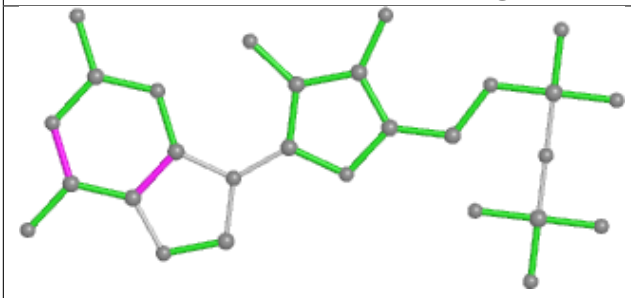
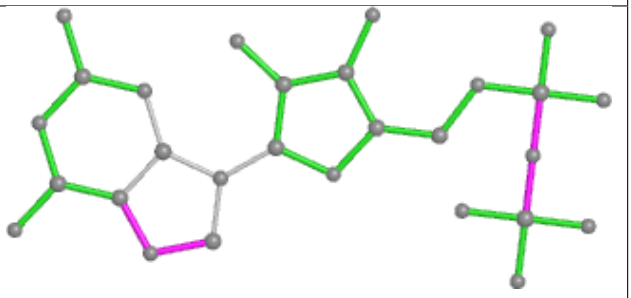
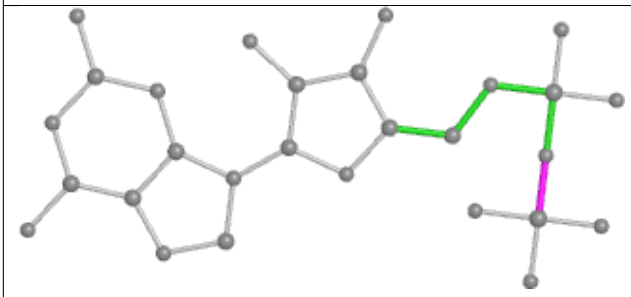
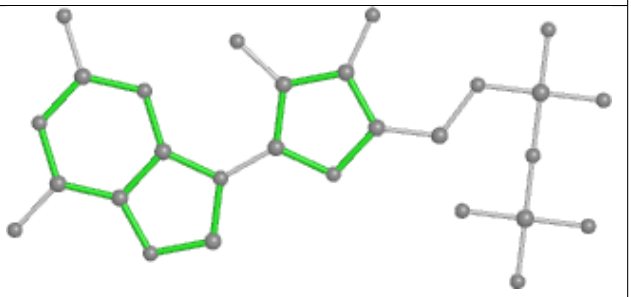
There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	BBB	201	SO4	1	0
6	CCC	204	EDO	8	0
4	BBB	203	FAR	3	0
4	AAA	202	FAR	1	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 then 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.



Ligand GDP AAA 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	AAA	169/185 (91%)	-0.08	1 (0%) 89 89	36, 49, 71, 109	0
1	BBB	173/185 (93%)	0.01	2 (1%) 79 80	31, 47, 88, 103	0
2	CCC	150/150 (100%)	-0.08	0 100 100	31, 41, 58, 73	0
2	DDD	147/150 (98%)	-0.05	0 100 100	30, 48, 82, 108	0
All	All	639/670 (95%)	-0.05	3 (0%) 91 91	30, 46, 78, 109	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	36	ILE	3.8
1	AAA	170	MET	2.5
1	BBB	121	PRO	2.3

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

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^{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	B-factors(Å^2)	Q<0.9
1	CMT	AAA	185	8/8	0.94	0.16	45,49,55,55	0
1	CMT	BBB	185	8/8	0.98	0.12	35,40,47,53	0

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

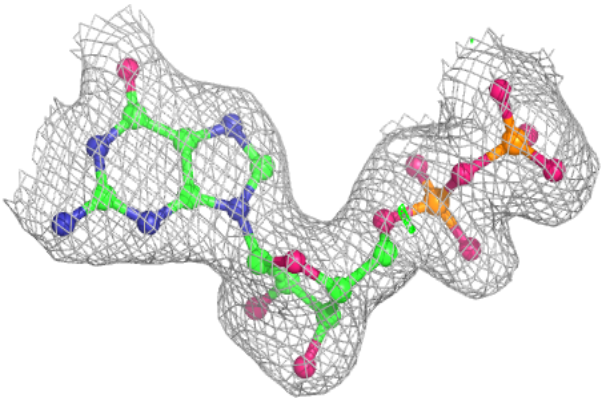
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

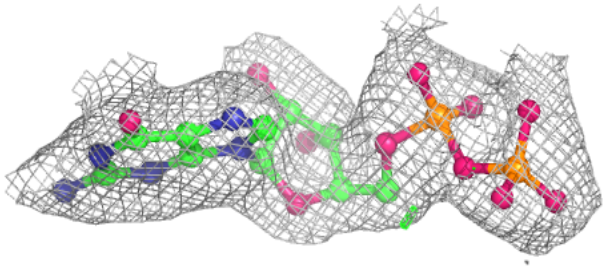
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	DDD	203	4/4	0.87	0.17	62,68,68,73	0
6	EDO	CCC	204	4/4	0.88	0.34	48,59,61,62	0
6	EDO	CCC	203	4/4	0.91	0.16	52,58,59,60	0
4	FAR	AAA	202	15/15	0.92	0.23	44,54,62,68	0
4	FAR	BBB	203	15/15	0.95	0.17	37,42,46,46	0
5	SO4	CCC	201	5/5	0.96	0.22	72,76,92,93	0
3	GDP	BBB	202	28/28	0.97	0.11	41,48,55,57	0
5	SO4	BBB	201	5/5	0.97	0.12	62,62,69,70	0
5	SO4	DDD	201	5/5	0.98	0.29	80,85,92,94	0
6	EDO	CCC	202	4/4	0.98	0.14	41,45,48,49	0
3	GDP	AAA	201	28/28	0.98	0.11	43,50,55,57	0
6	EDO	DDD	202	4/4	0.98	0.15	39,44,45,47	0

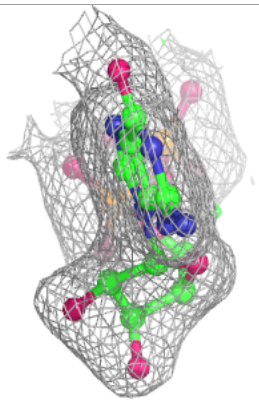
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP BBB 202:

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

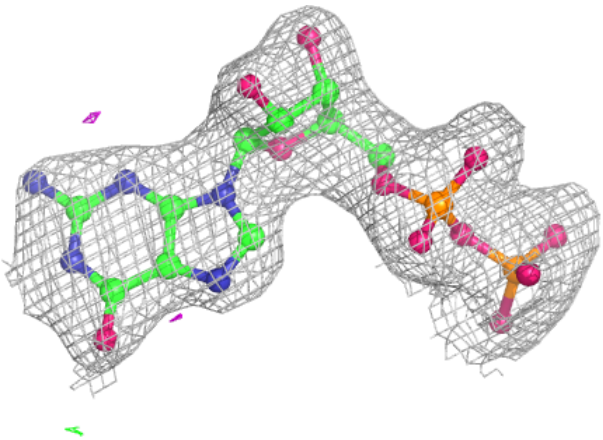


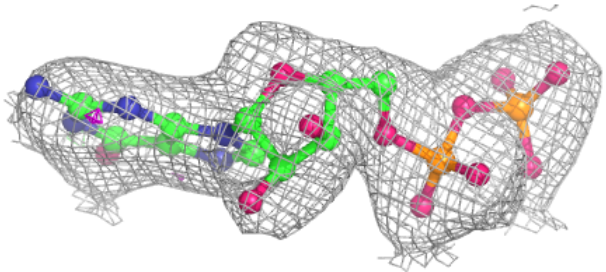


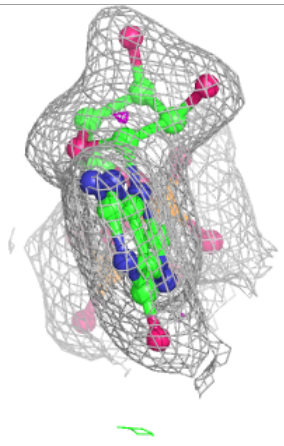


Electron density around GDP AAA 201:

$2mF_o$-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.