



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 12:34 am BST

PDB ID : 4LYH
Title : Crystal Structure of small molecule vinylsulfonamide 9 covalently bound to K-Ras G12C
Authors : Ostrem, J.M.; Peters, U.; Sos, M.L.; Wells, J.A.; Shokat, K.M.
Deposited on : 2013-07-31
Resolution : 1.37 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

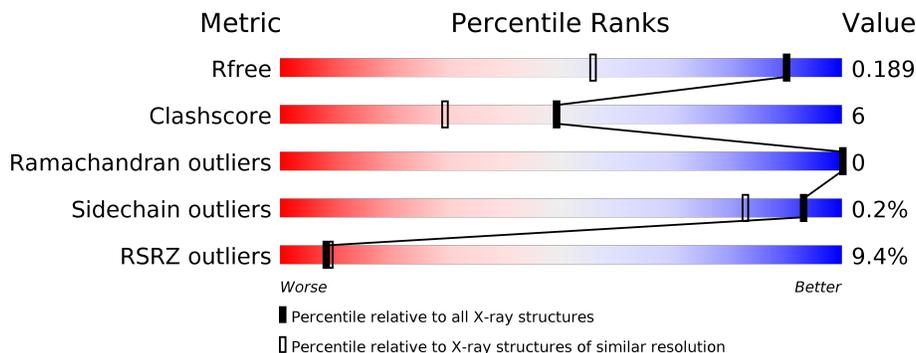
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.37 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	2907 (1.40-1.36)
Clashscore	141614	3037 (1.40-1.36)
Ramachandran outliers	138981	2970 (1.40-1.36)
Sidechain outliers	138945	2969 (1.40-1.36)
RSRZ outliers	127900	2846 (1.40-1.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	170	
1	B	170	
1	C	170	

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
2	SO4	C	201	-	-	X	-
4	21F	C	202	-	-	X	-

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 8321 atoms, of which 3931 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	
			Total	C	H	N	O				S
1	A	163	2639	830	1317	228	258	6	0	6	0
1	B	159	2604	815	1310	229	245	5	0	5	0
1	C	156	2471	781	1232	219	235	4	0	3	0

There are 33 discrepancies between the modelled and reference sequences:

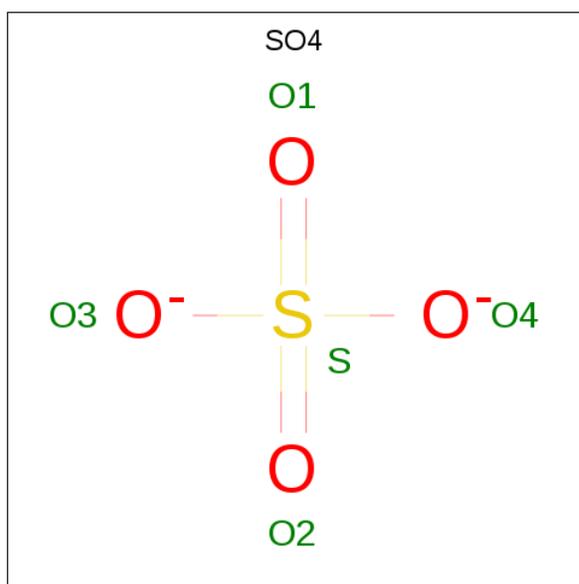
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	EXPRESSION TAG	UNP P01116
A	12	CYS	GLY	VARIANT	UNP P01116
A	51	SER	CYS	ENGINEERED MUTATION	UNP P01116
A	80	LEU	CYS	ENGINEERED MUTATION	UNP P01116
A	118	SER	CYS	ENGINEERED MUTATION	UNP P01116
A	151	GLY	ARG	SEE REMARK 999	UNP P01116
A	153	ASP	GLU	SEE REMARK 999	UNP P01116
A	165	LYS	GLN	SEE REMARK 999	UNP P01116
A	166	HIS	TYR	SEE REMARK 999	UNP P01116
A	167	LYS	ARG	SEE REMARK 999	UNP P01116
A	168	GLU	LEU	SEE REMARK 999	UNP P01116
B	0	GLY	-	EXPRESSION TAG	UNP P01116
B	12	CYS	GLY	VARIANT	UNP P01116
B	51	SER	CYS	ENGINEERED MUTATION	UNP P01116
B	80	LEU	CYS	ENGINEERED MUTATION	UNP P01116
B	118	SER	CYS	ENGINEERED MUTATION	UNP P01116
B	151	GLY	ARG	SEE REMARK 999	UNP P01116
B	153	ASP	GLU	SEE REMARK 999	UNP P01116
B	165	LYS	GLN	SEE REMARK 999	UNP P01116
B	166	HIS	TYR	SEE REMARK 999	UNP P01116
B	167	LYS	ARG	SEE REMARK 999	UNP P01116
B	168	GLU	LEU	SEE REMARK 999	UNP P01116
C	0	GLY	-	EXPRESSION TAG	UNP P01116

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Chain	Residue	Modelled	Actual	Comment	Reference
C	12	CYS	GLY	VARIANT	UNP P01116
C	51	SER	CYS	ENGINEERED MUTATION	UNP P01116
C	80	LEU	CYS	ENGINEERED MUTATION	UNP P01116
C	118	SER	CYS	ENGINEERED MUTATION	UNP P01116
C	151	GLY	ARG	SEE REMARK 999	UNP P01116
C	153	ASP	GLU	SEE REMARK 999	UNP P01116
C	165	LYS	GLN	SEE REMARK 999	UNP P01116
C	166	HIS	TYR	SEE REMARK 999	UNP P01116
C	167	LYS	ARG	SEE REMARK 999	UNP P01116
C	168	GLU	LEU	SEE REMARK 999	UNP P01116

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf		
2	A	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

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

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	
			Total	C	Cl	H	I	N	O			S
4	B	1	48	16	1	22	1	3	4	1	0	0
4	C	1	46	16	1	20	1	3	4	1	0	0

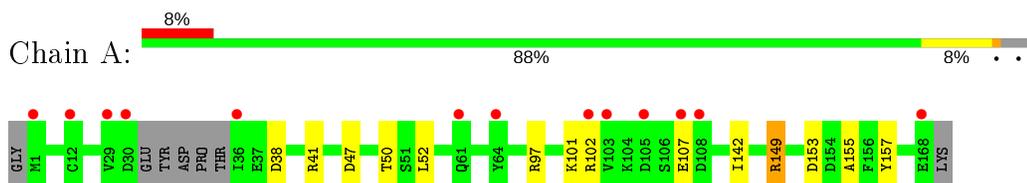
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	154	Total 154	O 154	0	0
5	B	142	Total 142	O 142	0	0
5	C	93	Total 93	O 93	0	0

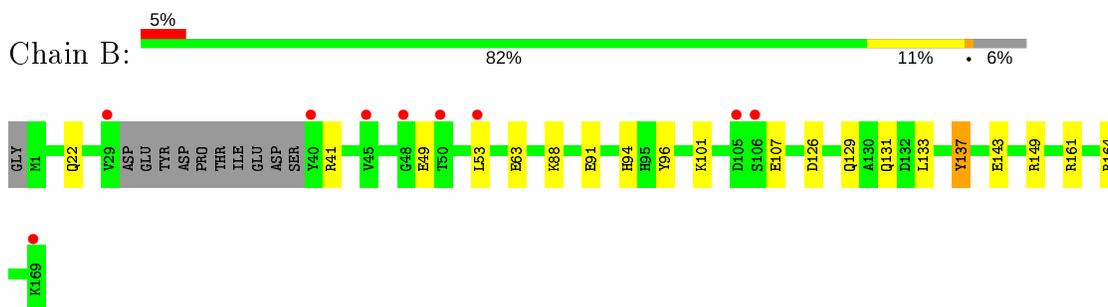
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

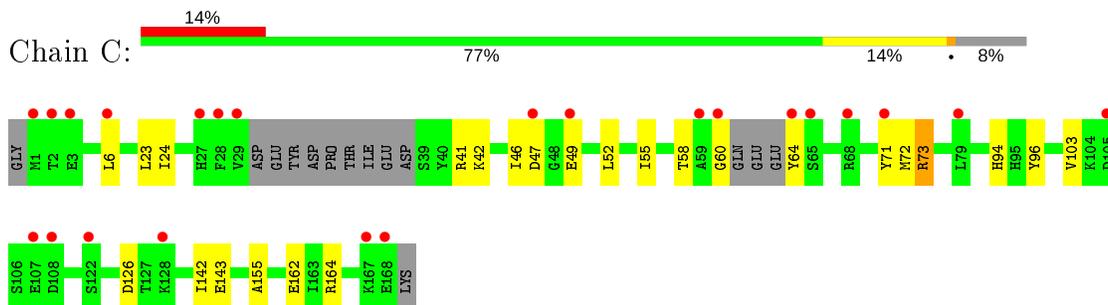
- Molecule 1: GTPase KRas



- Molecule 1: GTPase KRas



- Molecule 1: GTPase KRas



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	68.03Å 83.53Å 86.97Å 90.00° 111.13° 90.00°	Depositor
Resolution (Å)	19.12 – 1.37 19.12 – 1.37	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.12-1.37) 96.8 (19.12-1.37)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.24 (at 1.37Å)	Xtrriage
Refinement program	PHENIX dev_1402	Depositor
R, R_{free}	0.165 , 0.188 0.166 , 0.189	Depositor DCC
R_{free} test set	2007 reflections (2.12%)	wwPDB-VP
Wilson B-factor (Å ²)	15.3	Xtrriage
Anisotropy	0.083	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.46 , 56.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8321	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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: GDP, 21F, 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	A	0.96	1/1358 (0.1%)	1.08	7/1828 (0.4%)
1	B	0.91	1/1327 (0.1%)	0.91	2/1782 (0.1%)
1	C	0.87	0/1265	0.95	3/1703 (0.2%)
All	All	0.92	2/3950 (0.1%)	0.99	12/5313 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	96	TYR	CE2-CZ	-8.57	1.27	1.38
1	A	157	TYR	CE1-CZ	-5.99	1.30	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	73	ARG	NE-CZ-NH1	9.36	124.98	120.30
1	C	73	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	A	97[A]	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	A	97[B]	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	A	38	ASP	CB-CG-OD1	6.92	124.53	118.30
1	A	153	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	B	91	GLU	OE1-CD-OE2	-5.78	116.36	123.30
1	A	149	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	97[A]	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	97[B]	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	B	137	TYR	CB-CG-CD1	5.51	124.30	121.00
1	C	162	GLU	OE1-CD-OE2	-5.17	117.10	123.30

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	A	1322	1317	1325	6	1
1	B	1294	1310	1315	11	0
1	C	1239	1232	1241	26	0
2	A	5	0	0	0	0
2	C	5	0	0	5	0
3	A	28	10	12	0	0
3	B	28	10	12	0	0
3	C	28	10	12	0	0
4	B	26	22	22	0	0
4	C	26	20	22	10	0
5	A	154	0	0	2	1
5	B	142	0	0	4	0
5	C	93	0	0	8	0
All	All	4390	3931	3961	47	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (47) 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:C:201:SO4:O3	2:C:201:SO4:S	0.77	1.16
1:C:94[B]:HIS:ND1	5:C:362:HOH:O	1.88	1.03
2:C:201:SO4:O1	2:C:201:SO4:O3	1.77	1.01
2:C:201:SO4:O4	2:C:201:SO4:O3	1.80	0.96
2:C:201:SO4:O3	2:C:201:SO4:O2	1.86	0.93
1:C:94[B]:HIS:CG	5:C:362:HOH:O	2.24	0.90
1:C:64:TYR:N	5:C:368:HOH:O	2.06	0.87
1:C:143:GLU:OE1	5:C:376:HOH:O	1.96	0.83
1:C:49:GLU:OE1	5:C:391:HOH:O	1.96	0.81
1:C:60:GLY:O	5:C:380:HOH:O	2.07	0.72
1:B:94:HIS:ND1	5:B:427:HOH:O	2.21	0.71
1:C:126:ASP:OD2	5:C:372:HOH:O	2.09	0.69
1:B:63:GLU:OE2	5:B:404:HOH:O	2.15	0.64
1:B:143:GLU:OE1	5:B:324:HOH:O	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ARG:HG3	1:A:52:LEU:HD21	1.89	0.55
1:C:72:MET:HE2	4:C:202:21F:C26	2.37	0.55
1:C:47:ASP:CG	1:C:164:ARG:HH12	2.10	0.55
1:A:149:ARG:NE	5:A:450:HOH:O	2.27	0.55
1:C:58:THR:HG22	4:C:202:21F:I04	2.79	0.53
1:C:72:MET:CE	4:C:202:21F:H253	2.39	0.53
1:C:96:TYR:HD1	4:C:202:21F:H251	1.73	0.53
1:C:73:ARG:HD2	1:C:103:VAL:O	2.08	0.52
1:A:142:ILE:HD12	1:A:155:ALA:HA	1.91	0.52
1:A:101:LYS:NZ	1:A:107:GLU:OE1	2.42	0.52
1:C:6:LEU:N	2:C:201:SO4:O1	2.43	0.52
1:C:71:TYR:HD2	4:C:202:21F:I04	2.63	0.51
1:B:49:GLU:OE2	1:B:164:ARG:NH2	2.44	0.51
1:B:126:ASP:OD1	1:B:129:GLN:HG3	2.11	0.50
1:A:102:ARG:HG3	5:A:358:HOH:O	2.12	0.49
1:C:72:MET:HE1	4:C:202:21F:H253	1.95	0.49
1:B:22:GLN:OE1	1:B:149:ARG:NE	2.34	0.48
1:C:46:ILE:O	1:C:164:ARG:NH2	2.46	0.48
1:A:47:ASP:O	1:B:131[B]:GLN:HG3	2.14	0.48
1:B:161:ARG:NH1	5:B:423:HOH:O	2.45	0.47
1:C:71:TYR:HB2	4:C:202:21F:CL1	2.51	0.47
1:C:71:TYR:CD2	4:C:202:21F:I04	3.39	0.46
1:C:142:ILE:HD12	1:C:155:ALA:HA	1.97	0.45
1:C:49:GLU:CD	5:C:391:HOH:O	2.48	0.44
1:B:101:LYS:HE3	1:B:107:GLU:HA	2.00	0.43
1:C:23:LEU:HD23	1:C:55:ILE:CD1	2.49	0.43
1:B:133:LEU:HD11	1:B:137:TYR:CZ	2.54	0.43
1:C:41[A]:ARG:HG2	1:C:52:LEU:HD11	2.00	0.42
1:C:24:ILE:HD13	1:C:42:LYS:HB2	2.00	0.42
1:C:24:ILE:CD1	1:C:42:LYS:HB2	2.49	0.42
4:C:202:21F:H131	4:C:202:21F:H161	1.82	0.41
1:C:72:MET:HE2	4:C:202:21F:H261	2.02	0.40
1:B:41:ARG:HA	1:B:53:LEU:O	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:THR:HG1	1:A:50:THR:HG1[2_1059]	1.27	0.33
5:A:427:HOH:O	5:A:429:HOH:O[2_1059]	1.95	0.25

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	165/170 (97%)	164 (99%)	1 (1%)	0	100	100
1	B	160/170 (94%)	156 (98%)	4 (2%)	0	100	100
1	C	153/170 (90%)	150 (98%)	3 (2%)	0	100	100
All	All	478/510 (94%)	470 (98%)	8 (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	A	148/150 (99%)	148 (100%)	0	100	100
1	B	143/150 (95%)	142 (99%)	1 (1%)	84	65
1	C	135/150 (90%)	135 (100%)	0	100	100
All	All	426/450 (95%)	425 (100%)	1 (0%)	93	83

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	88	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	C	99	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

7 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
4	21F	C	202	1	27,27,27	1.81	4 (14%)	33,38,38	3.79	13 (39%)
4	21F	B	201	1	27,27,27	1.33	3 (11%)	33,38,38	1.51	7 (21%)
3	GDP	A	202	-	24,30,30	1.41	2 (8%)	31,47,47	1.95	7 (22%)
3	GDP	B	202	-	24,30,30	1.68	5 (20%)	31,47,47	1.72	6 (19%)
2	SO4	C	201	-	4,4,4	4.30	1 (25%)	6,6,6	0.74	0
2	SO4	A	201	-	4,4,4	0.53	0	6,6,6	0.26	0
3	GDP	C	203	-	24,30,30	1.17	2 (8%)	31,47,47	1.58	7 (22%)

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	21F	B	201	1	-	0/19/29/29	0/2/2/2
3	GDP	A	202	-	-	2/12/32/32	0/3/3/3
4	21F	C	202	1	-	5/19/29/29	0/2/2/2
3	GDP	B	202	-	-	1/12/32/32	0/3/3/3
3	GDP	C	203	-	-	2/12/32/32	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	201	SO4	O3-S	-8.55	0.77	1.47
4	C	202	21F	C09-N10	5.86	1.47	1.35
3	B	202	GDP	C6-N1	3.95	1.39	1.33
4	B	201	21F	C03-I04	-3.46	2.02	2.10
4	C	202	21F	S15-N14	3.35	1.67	1.61
3	B	202	GDP	O4'-C1'	2.97	1.45	1.41
3	A	202	GDP	C8-N7	-2.79	1.29	1.34
3	A	202	GDP	PA-O2A	-2.77	1.42	1.55
4	B	201	21F	C02-C03	2.67	1.42	1.39
4	C	202	21F	C08-N07	-2.51	1.41	1.45
4	B	201	21F	S15-N14	2.51	1.65	1.61
3	B	202	GDP	C8-N7	-2.45	1.30	1.34
4	C	202	21F	C06-N07	2.41	1.44	1.37
3	B	202	GDP	PA-O1A	-2.39	1.42	1.50
3	C	203	GDP	O4'-C1'	2.11	1.44	1.41
3	C	203	GDP	C8-N7	-2.08	1.31	1.34
3	B	202	GDP	O2'-C2'	2.02	1.47	1.43

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	202	21F	O19-S15-O18	-14.23	98.73	119.35
4	C	202	21F	C13-N14-S15	-10.35	105.24	122.37
3	B	202	GDP	C5-C6-N1	-6.21	114.94	123.43
4	C	202	21F	C08-N07-C06	-6.11	115.23	123.98
3	A	202	GDP	C5-C6-N1	-4.94	116.68	123.43
4	C	202	21F	C12-C13-C20	4.47	118.56	110.82
3	A	202	GDP	C6-N1-C2	4.19	122.59	115.93
3	B	202	GDP	C6-N1-C2	4.16	122.54	115.93
3	A	202	GDP	N2-C2-N3	4.01	124.32	117.79
3	A	202	GDP	C6-C5-C4	-3.88	117.09	120.80
4	C	202	21F	O19-S15-N14	3.84	112.64	107.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	203	GDP	C5-C6-N1	-3.81	118.22	123.43
4	C	202	21F	C03-C02-CL1	3.65	123.83	121.11
3	C	203	GDP	C6-C5-C4	-3.61	117.35	120.80
3	C	203	GDP	C6-N1-C2	3.56	121.59	115.93
4	B	201	21F	C13-N14-S15	-3.51	116.57	122.37
4	B	201	21F	C08-N07-C06	-3.43	119.06	123.98
4	C	202	21F	C17-C16-S15	3.31	117.60	112.93
3	A	202	GDP	N2-C2-N1	-3.30	112.12	117.25
4	C	202	21F	C11-N10-C21	3.25	118.88	112.62
4	C	202	21F	C20-C21-N10	3.25	115.76	110.82
4	B	201	21F	C11-C12-C13	3.25	116.20	110.50
4	C	202	21F	C21-C20-C13	2.86	115.52	110.50
3	A	202	GDP	N3-C2-N1	-2.86	123.41	127.22
3	C	203	GDP	C1'-N9-C4	-2.60	122.08	126.64
4	B	201	21F	C02-C03-I04	2.39	124.24	121.72
3	A	202	GDP	O4'-C1'-C2'	-2.32	103.53	106.93
4	C	202	21F	O24-C23-C06	2.32	117.64	114.80
3	C	203	GDP	O2'-C2'-C3'	2.26	119.15	111.82
4	B	201	21F	C05-C06-C23	2.23	121.60	118.91
4	B	201	21F	C12-C11-N10	-2.23	107.43	110.82
4	B	201	21F	C03-C02-CL1	-2.20	119.47	121.11
4	C	202	21F	C08-C09-N10	2.20	120.83	117.15
3	C	203	GDP	PA-O3A-PB	-2.19	125.32	132.83
3	B	202	GDP	O4'-C1'-C2'	-2.13	103.81	106.93
4	C	202	21F	O18-S15-N14	2.13	110.18	107.12
3	C	203	GDP	C4-C5-N7	-2.10	107.21	109.40
3	B	202	GDP	C4-C5-N7	-2.08	107.23	109.40
3	B	202	GDP	O3B-PB-O2B	2.08	115.59	107.64
3	B	202	GDP	C6-C5-C4	-2.06	118.83	120.80

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	202	21F	C13-N14-S15-O19
4	C	202	21F	C17-C16-S15-O19
3	B	202	GDP	PA-O3A-PB-O1B
3	C	203	GDP	PA-O3A-PB-O1B
3	A	202	GDP	PA-O3A-PB-O2B
3	C	203	GDP	PA-O3A-PB-O3B
4	C	202	21F	C17-C16-S15-N14
4	C	202	21F	C05-C06-N07-C08

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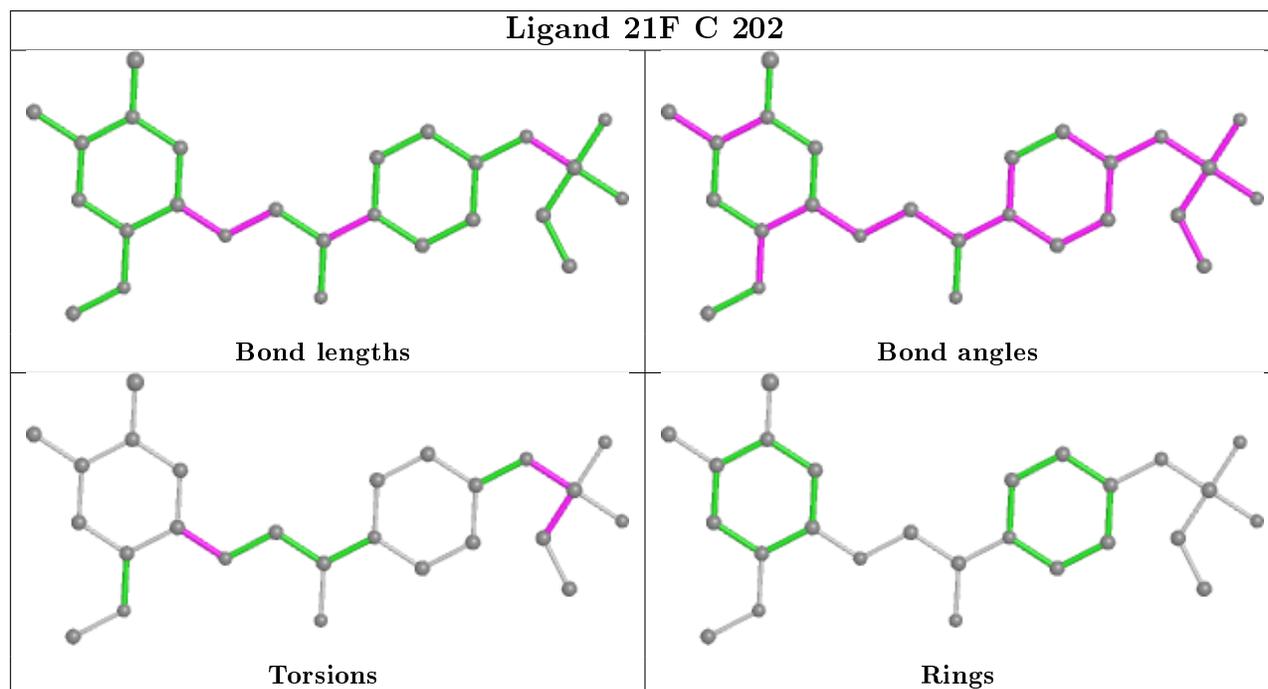
Mol	Chain	Res	Type	Atoms
3	A	202	GDP	PA-O3A-PB-O3B
4	C	202	21F	C23-C06-N07-C08

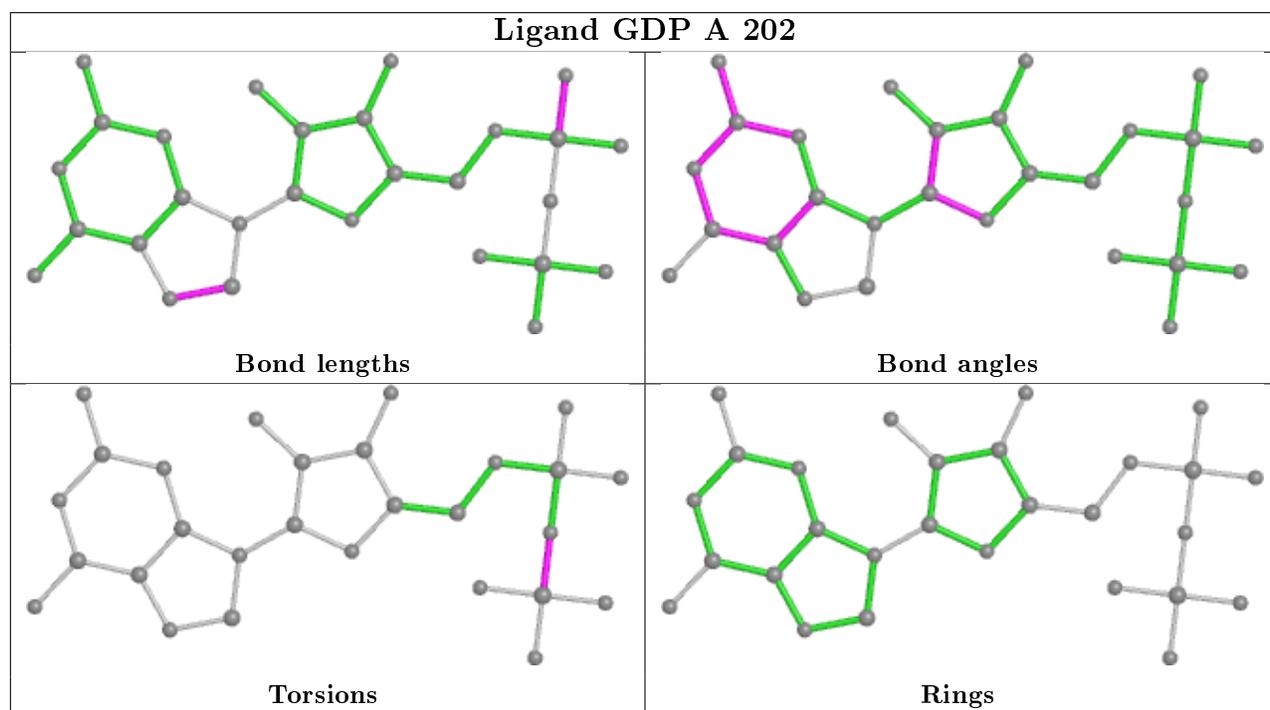
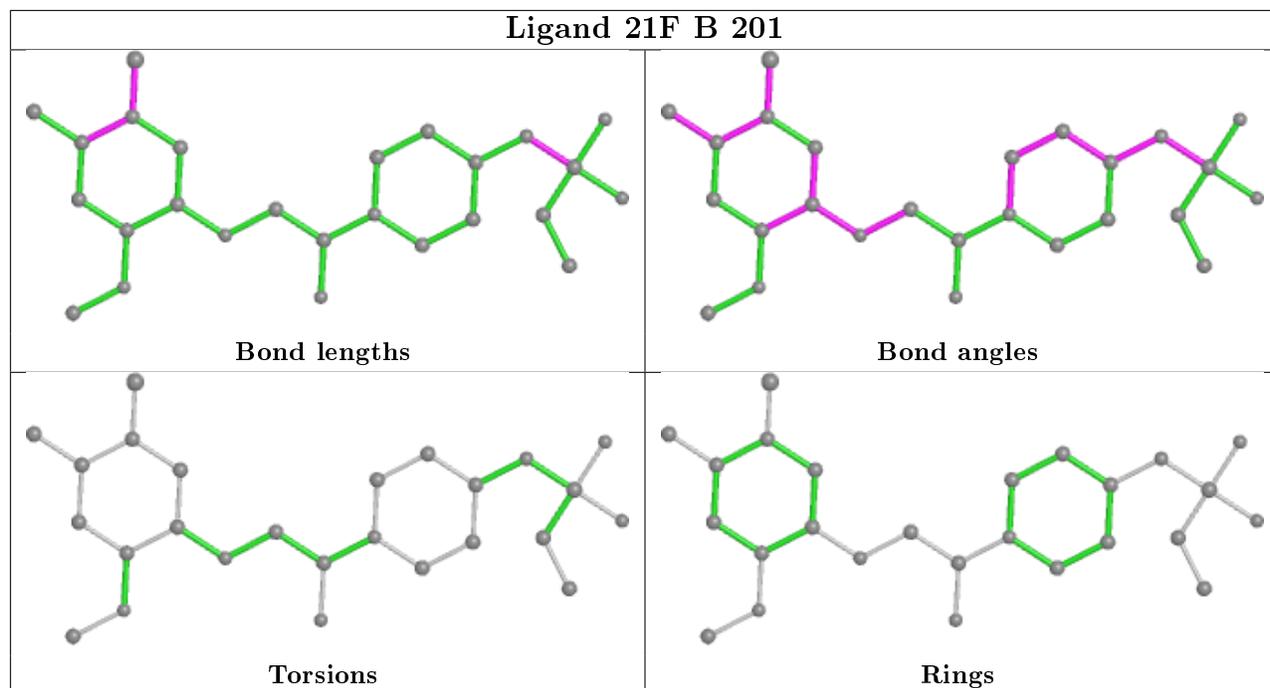
There are no ring outliers.

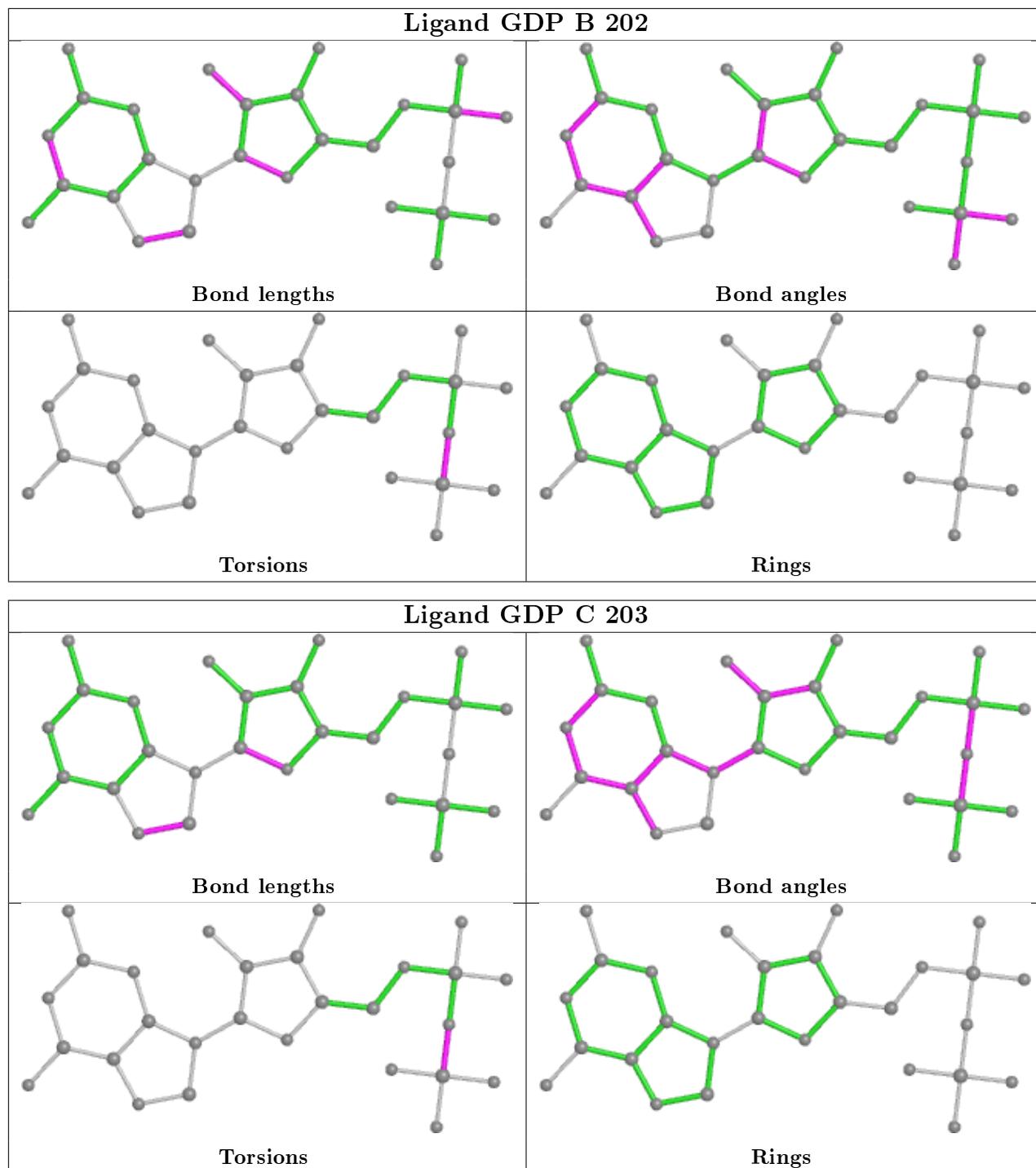
2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	202	21F	10	0
2	C	201	SO4	5	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](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	163/170 (95%)	0.48	13 (7%) 12 12	10, 20, 39, 57	0
1	B	159/170 (93%)	0.47	9 (5%) 23 23	11, 21, 41, 52	0
1	C	156/170 (91%)	0.89	23 (14%) 2 2	12, 25, 48, 56	0
All	All	478/510 (93%)	0.61	45 (9%) 8 9	10, 21, 43, 57	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	64	TYR	10.4
1	B	40	TYR	6.9
1	C	2	THR	6.2
1	A	29	VAL	5.7
1	B	29	VAL	5.7
1	C	71	TYR	5.2
1	A	30	ASP	4.5
1	C	59	ALA	4.4
1	C	65	SER	4.2
1	A	1	MET	4.2
1	C	105	ASP	4.0
1	C	29	VAL	3.9
1	B	48	GLY	3.8
1	A	36	ILE	3.7
1	C	60	GLY	3.6
1	A	61	GLN	3.5
1	C	168	GLU	3.4
1	C	108	ASP	3.4
1	C	28	PHE	3.4
1	B	45	VAL	3.4
1	A	107	GLU	3.3
1	C	27	HIS	3.2
1	C	1	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	107	GLU	3.2
1	C	122	SER	3.1
1	B	106	SER	3.1
1	A	102	ARG	3.0
1	C	68	ARG	3.0
1	B	169	LYS	3.0
1	C	3	GLU	2.9
1	A	105	ASP	2.8
1	C	6	LEU	2.8
1	A	168	GLU	2.7
1	C	167	LYS	2.7
1	A	108	ASP	2.6
1	A	64	TYR	2.6
1	A	103[A]	VAL	2.6
1	C	47	ASP	2.6
1	A	12[A]	CYS	2.4
1	B	105	ASP	2.3
1	B	50	THR	2.3
1	B	53	LEU	2.2
1	C	79	LEU	2.2
1	C	128	LYS	2.2
1	C	49	GLU	2.1

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

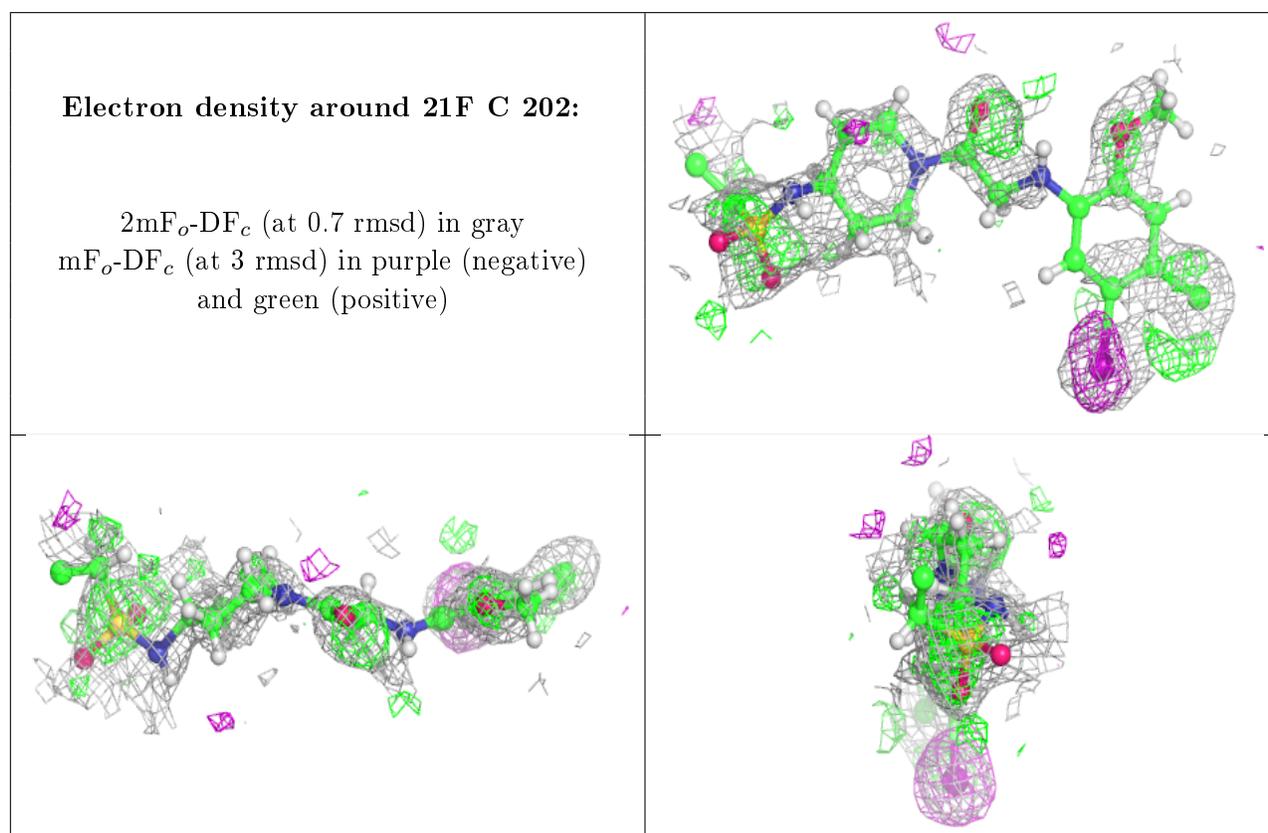
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	21F	C	202	26/26	0.79	0.31	17,29,87,103	46

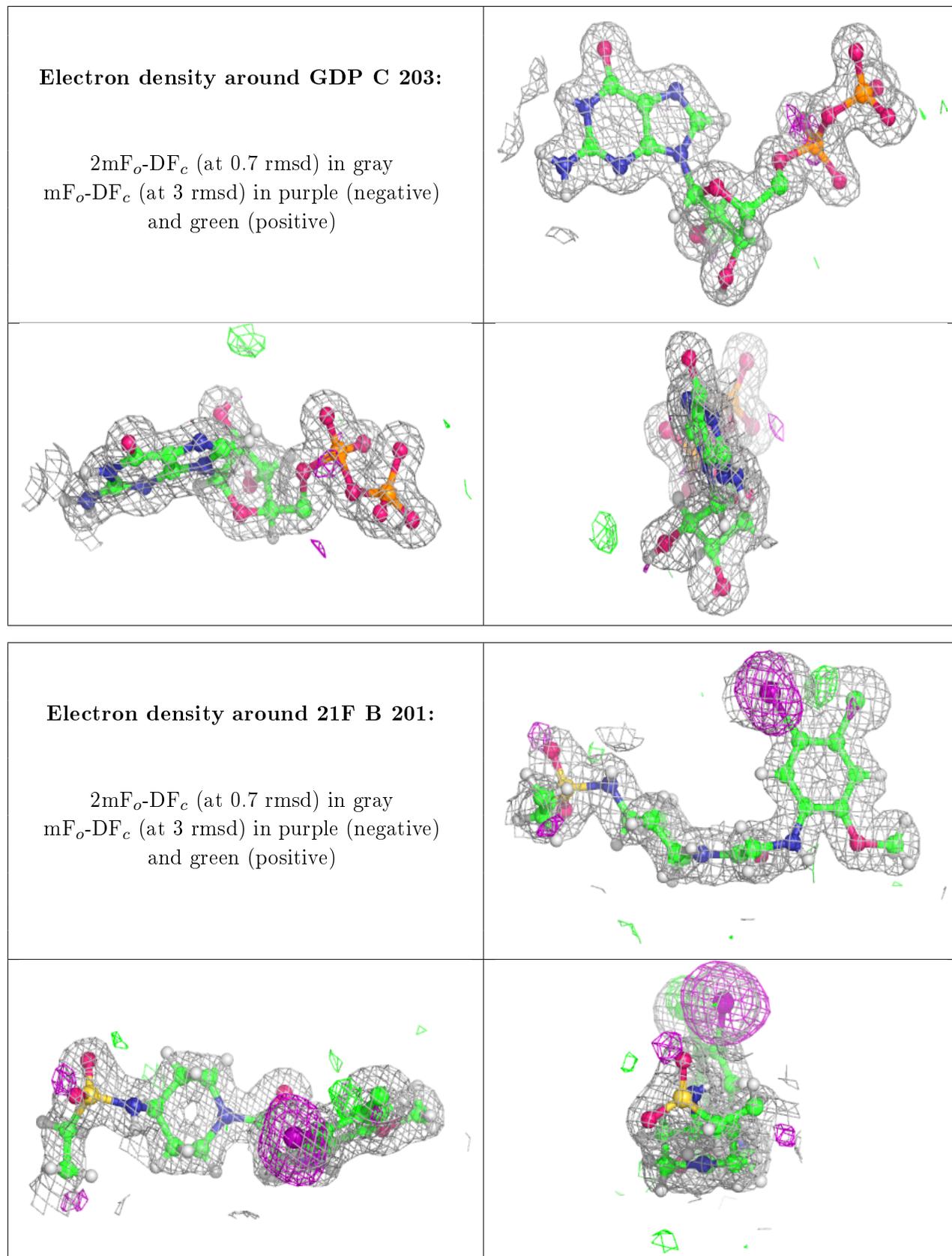
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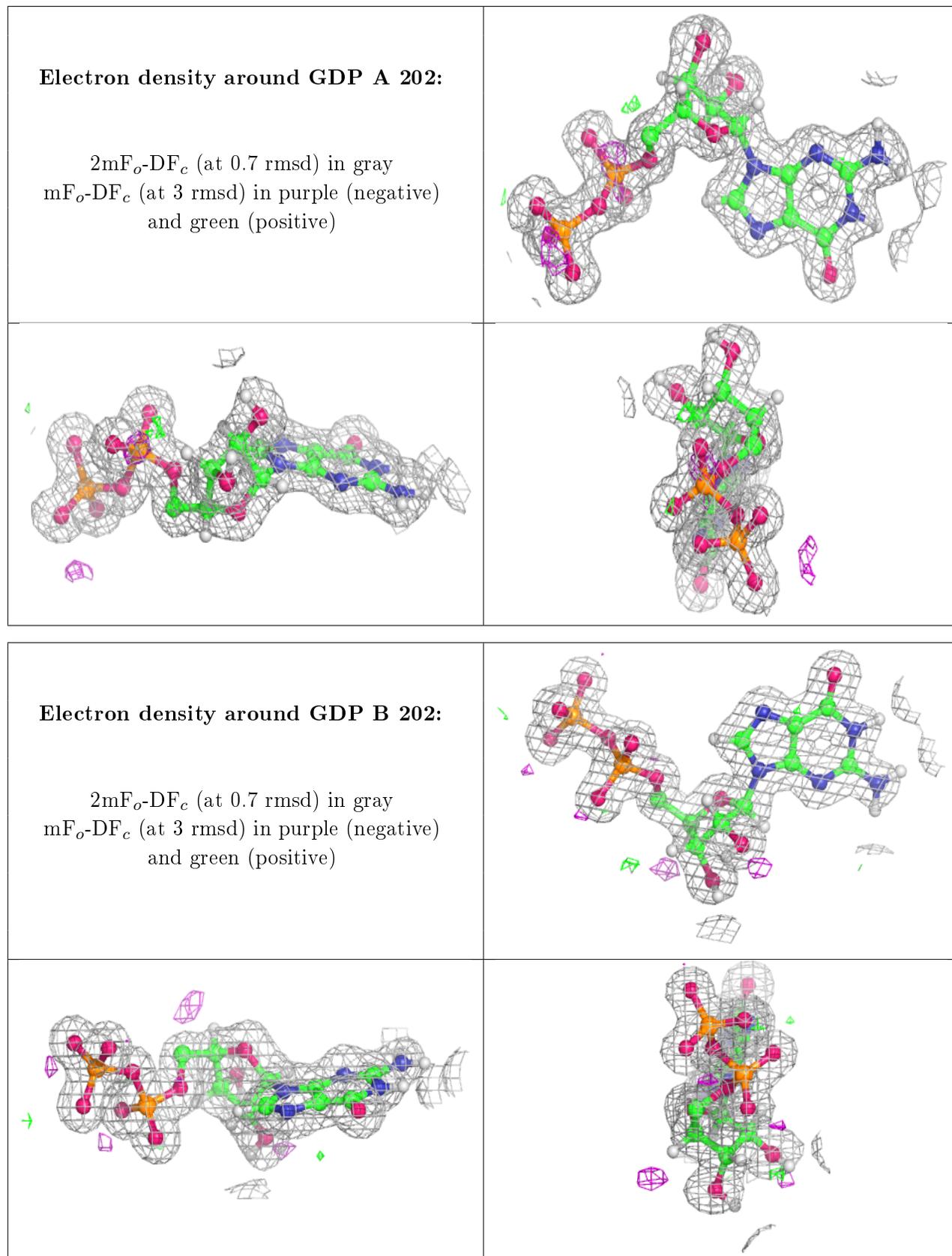
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	A	201	5/5	0.95	0.24	33,39,44,53	0
3	GDP	C	203	28/28	0.96	0.08	14,20,31,36	0
4	21F	B	201	26/26	0.97	0.07	15,19,24,31	0
3	GDP	A	202	28/28	0.97	0.07	12,17,26,29	0
3	GDP	B	202	28/28	0.98	0.06	13,16,22,26	0
2	SO4	C	201	5/5	0.99	0.19	12,13,49,51	0

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







6.5 Other polymers

There are no such residues in this entry.