Full wwPDB X-ray Structure Validation Report (i)

Dec 11, 2023 – 08:18 PM JST

PDB ID	:	8HTG
Title	:	Crystal structure of Golf in complex with GTP-gamma S and Mg
Authors	:	Kang, H.; Choi, H.-J.
Deposited on	:	2022-12-21
Resolution	:	2.91 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 (i) 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 (i)) were used in the production of this report:

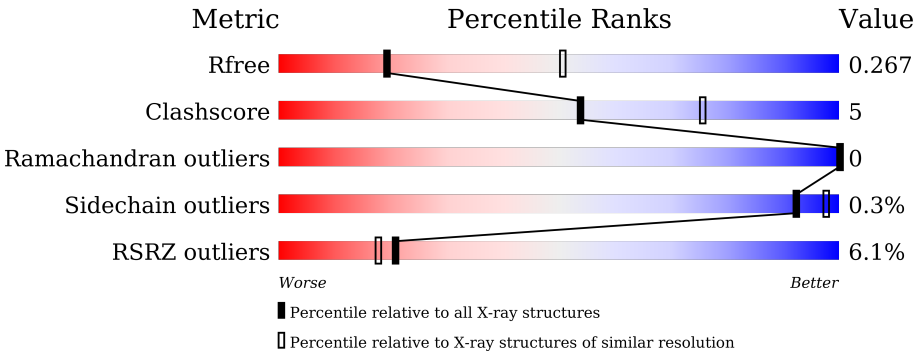
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.91 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	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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	A	395	70% 14% 16%
1	B	395	74% 11% 15%
1	C	395	74% 10% 16%
1	D	395	17% 72% 11% 17%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11035 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 Guanine nucleotide-binding protein G(olf) subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	0	0
			2714	1723	470	507	14			
1	B	334	Total	C	N	O	S	0	0	0
			2733	1734	474	511	14			
1	C	332	Total	C	N	O	S	0	0	0
			2715	1723	470	509	13			
1	D	326	Total	C	N	O	S	0	0	0
			2666	1692	463	498	13			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP Q8CGK7
A	-12	HIS	-	expression tag	UNP Q8CGK7
A	-11	HIS	-	expression tag	UNP Q8CGK7
A	-10	HIS	-	expression tag	UNP Q8CGK7
A	-9	HIS	-	expression tag	UNP Q8CGK7
A	-8	HIS	-	expression tag	UNP Q8CGK7
A	-7	HIS	-	expression tag	UNP Q8CGK7
A	-6	LEU	-	expression tag	UNP Q8CGK7
A	-5	GLU	-	expression tag	UNP Q8CGK7
A	-4	VAL	-	expression tag	UNP Q8CGK7
A	-3	LEU	-	expression tag	UNP Q8CGK7
A	-2	PHE	-	expression tag	UNP Q8CGK7
A	-1	GLN	-	expression tag	UNP Q8CGK7
A	0	GLY	-	expression tag	UNP Q8CGK7
A	1	PRO	-	expression tag	UNP Q8CGK7
A	3	SER	CYS	engineered mutation	UNP Q8CGK7
B	-13	MET	-	initiating methionine	UNP Q8CGK7
B	-12	HIS	-	expression tag	UNP Q8CGK7
B	-11	HIS	-	expression tag	UNP Q8CGK7
B	-10	HIS	-	expression tag	UNP Q8CGK7
B	-9	HIS	-	expression tag	UNP Q8CGK7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	HIS	-	expression tag	UNP Q8CGK7
B	-7	HIS	-	expression tag	UNP Q8CGK7
B	-6	LEU	-	expression tag	UNP Q8CGK7
B	-5	GLU	-	expression tag	UNP Q8CGK7
B	-4	VAL	-	expression tag	UNP Q8CGK7
B	-3	LEU	-	expression tag	UNP Q8CGK7
B	-2	PHE	-	expression tag	UNP Q8CGK7
B	-1	GLN	-	expression tag	UNP Q8CGK7
B	0	GLY	-	expression tag	UNP Q8CGK7
B	1	PRO	-	expression tag	UNP Q8CGK7
B	3	SER	CYS	engineered mutation	UNP Q8CGK7
C	-13	MET	-	initiating methionine	UNP Q8CGK7
C	-12	HIS	-	expression tag	UNP Q8CGK7
C	-11	HIS	-	expression tag	UNP Q8CGK7
C	-10	HIS	-	expression tag	UNP Q8CGK7
C	-9	HIS	-	expression tag	UNP Q8CGK7
C	-8	HIS	-	expression tag	UNP Q8CGK7
C	-7	HIS	-	expression tag	UNP Q8CGK7
C	-6	LEU	-	expression tag	UNP Q8CGK7
C	-5	GLU	-	expression tag	UNP Q8CGK7
C	-4	VAL	-	expression tag	UNP Q8CGK7
C	-3	LEU	-	expression tag	UNP Q8CGK7
C	-2	PHE	-	expression tag	UNP Q8CGK7
C	-1	GLN	-	expression tag	UNP Q8CGK7
C	0	GLY	-	expression tag	UNP Q8CGK7
C	1	PRO	-	expression tag	UNP Q8CGK7
C	3	SER	CYS	engineered mutation	UNP Q8CGK7
D	-13	MET	-	initiating methionine	UNP Q8CGK7
D	-12	HIS	-	expression tag	UNP Q8CGK7
D	-11	HIS	-	expression tag	UNP Q8CGK7
D	-10	HIS	-	expression tag	UNP Q8CGK7
D	-9	HIS	-	expression tag	UNP Q8CGK7
D	-8	HIS	-	expression tag	UNP Q8CGK7
D	-7	HIS	-	expression tag	UNP Q8CGK7
D	-6	LEU	-	expression tag	UNP Q8CGK7
D	-5	GLU	-	expression tag	UNP Q8CGK7
D	-4	VAL	-	expression tag	UNP Q8CGK7
D	-3	LEU	-	expression tag	UNP Q8CGK7
D	-2	PHE	-	expression tag	UNP Q8CGK7
D	-1	GLN	-	expression tag	UNP Q8CGK7
D	0	GLY	-	expression tag	UNP Q8CGK7
D	1	PRO	-	expression tag	UNP Q8CGK7

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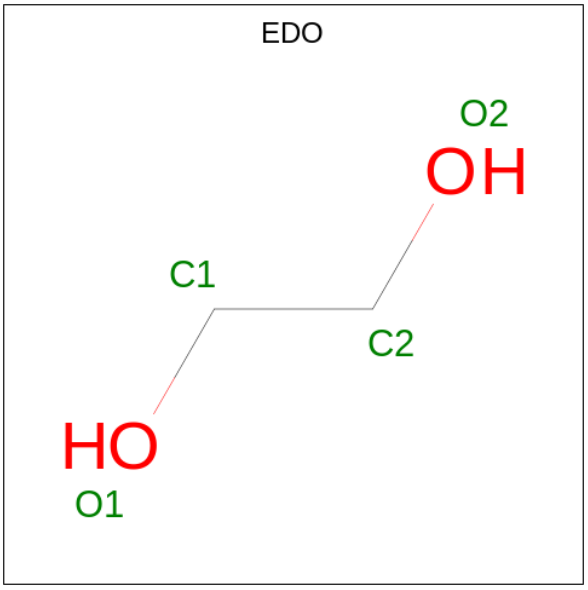
Chain	Residue	Modelled	Actual	Comment	Reference
D	3	SER	CYS	engineered mutation	UNP Q8CGK7

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

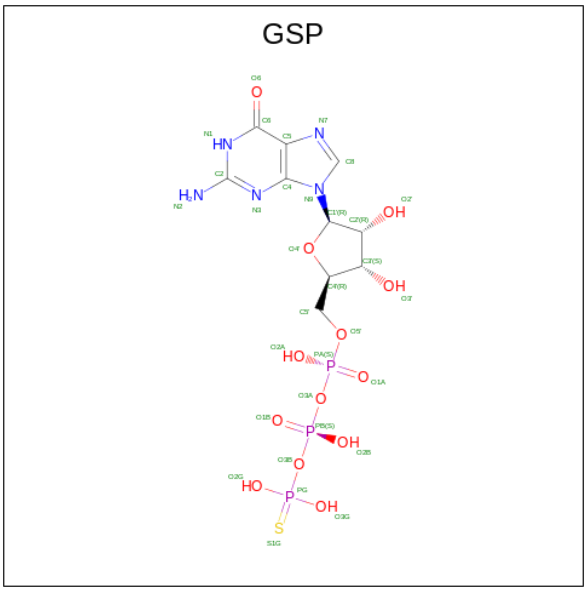


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

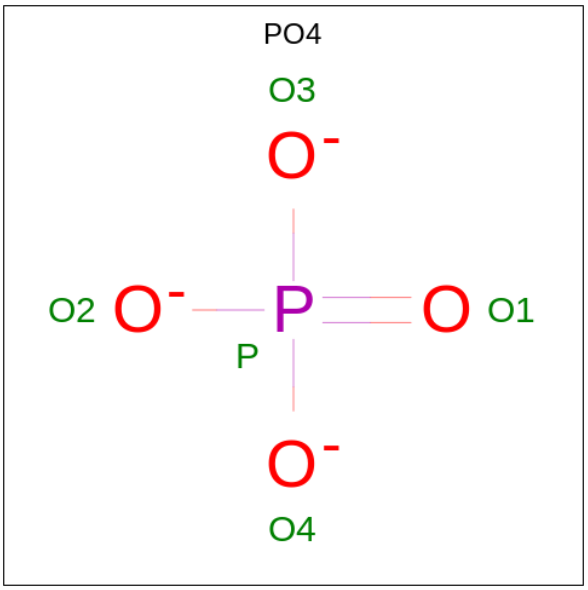
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0

- Molecule 4 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (three-letter code: GSP) (formula: $C_{10}H_{16}N_5O_{13}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
4	B	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
4	C	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
4	D	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 6 is water.

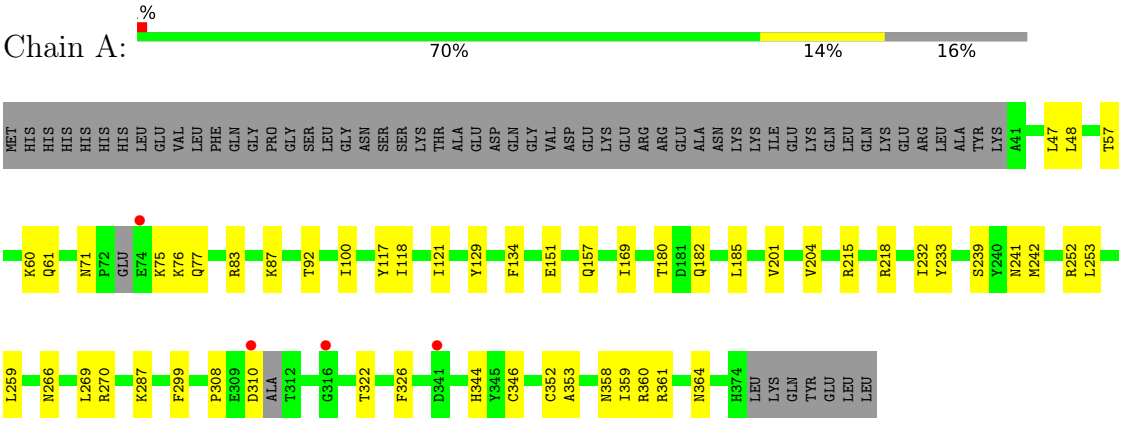
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	21	Total O 21 21	0	0
6	B	15	Total O 15 15	0	0
6	C	16	Total O 16 16	0	0

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.

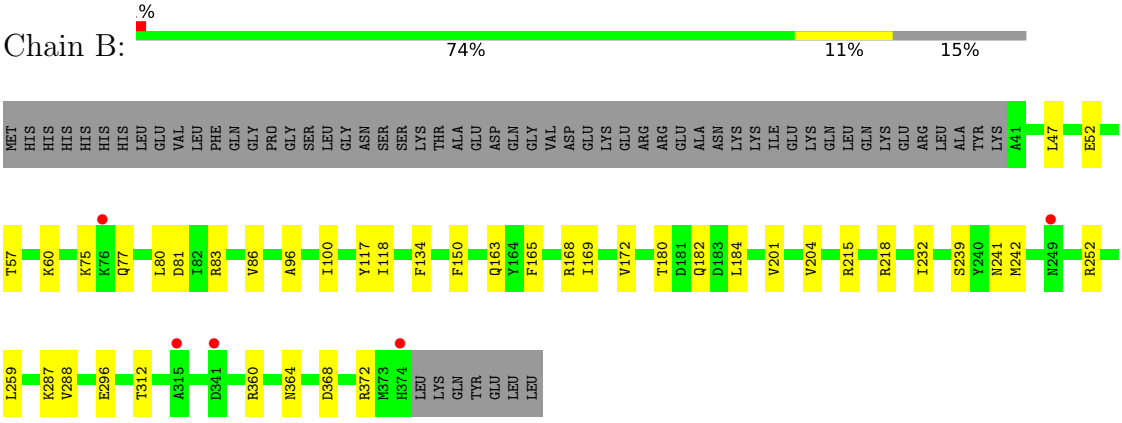
• Molecule 1: Guanine nucleotide-binding protein G(olf) subunit alpha

Chain A:



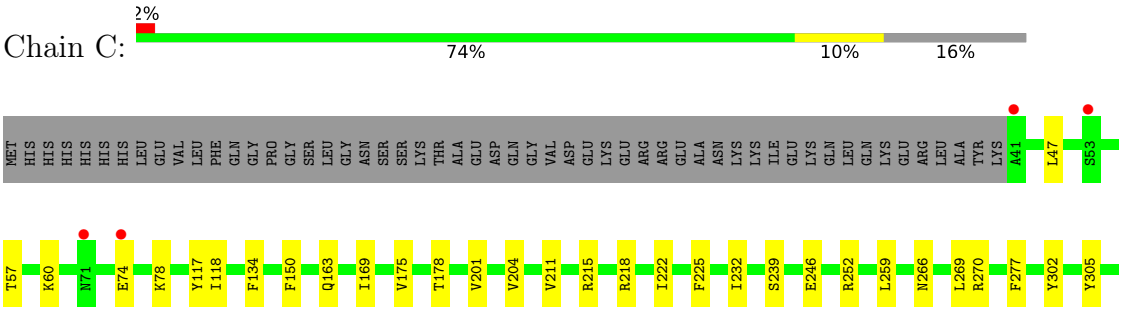
• Molecule 1: Guanine nucleotide-binding protein G(olf) subunit alpha

Chain B:



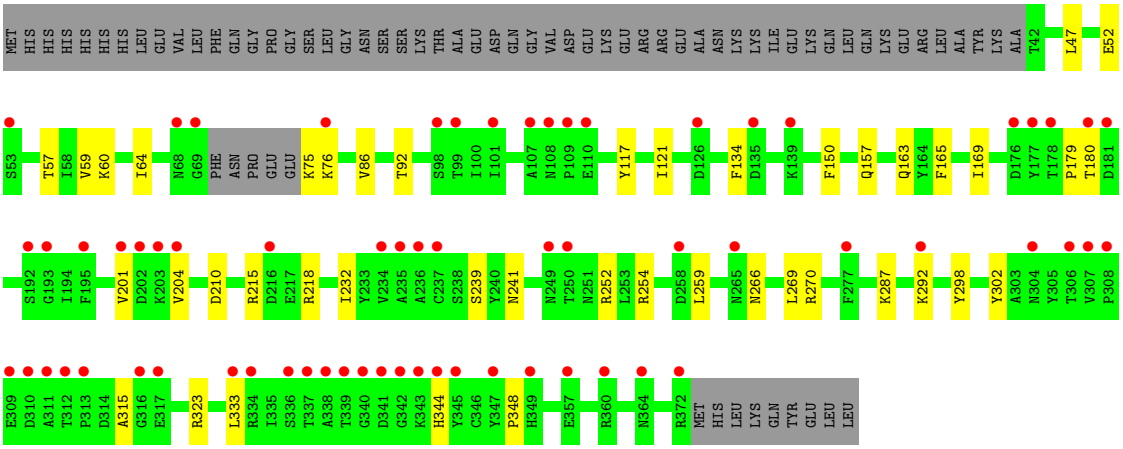
• Molecule 1: Guanine nucleotide-binding protein G(olf) subunit alpha

Chain C:



• Molecule 1: Guanine nucleotide-binding protein G(olf) subunit alpha

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	121.73Å 52.36Å 125.51Å 90.00° 118.53° 90.00°	Depositor
Resolution (Å)	27.57 – 2.91 27.57 – 2.91	Depositor EDS
% Data completeness (in resolution range)	99.6 (27.57-2.91) 99.7 (27.57-2.91)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.19.2-4158	Depositor
R, R_{free}	0.230 , 0.267 0.230 , 0.267	Depositor DCC
R_{free} test set	1547 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	43.2	Xtriage
Anisotropy	0.630	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 43.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.016 for -h-l,k,h 0.016 for l,k,-h-l 0.011 for h,-k,-h-l 0.013 for -h-l,-k,l 0.023 for l,-k,h	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	11035	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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: MG, PO4, EDO, GSP

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	0.25	0/2769	0.48	0/3742
1	B	0.25	0/2791	0.48	0/3775
1	C	0.25	0/2772	0.48	0/3750
1	D	0.25	0/2720	0.48	0/3677
All	All	0.25	0/11052	0.48	0/14944

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	A	2714	0	2672	35	0
1	B	2733	0	2690	29	0
1	C	2715	0	2674	25	0
1	D	2666	0	2634	27	0
2	A	4	0	6	1	0
2	B	4	0	6	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	0	0
4	A	32	0	12	0	0
4	B	32	0	12	0	0
4	C	32	0	12	0	0
4	D	32	0	12	0	0
5	A	10	0	0	0	0
5	C	5	0	0	0	0
6	A	21	0	0	1	0
6	B	15	0	0	2	0
6	C	16	0	0	0	0
All	All	11035	0	10730	114	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 (114) 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:B:172:VAL:O	6:B:501:HOH:O	2.01	0.79
1:D:218:ARG:HH21	1:D:259:LEU:HD22	1.48	0.79
1:B:218:ARG:HH21	1:B:259:LEU:HD22	1.48	0.78
1:C:218:ARG:HH21	1:C:259:LEU:HD22	1.49	0.75
1:B:57:THR:HA	1:B:60:LYS:HD2	1.69	0.74
1:A:218:ARG:HH21	1:A:259:LEU:HD22	1.52	0.74
1:A:215:ARG:HA	1:A:218:ARG:HH11	1.53	0.74
1:C:215:ARG:HA	1:C:218:ARG:HH11	1.53	0.72
1:D:215:ARG:HA	1:D:218:ARG:HH11	1.54	0.71
1:B:215:ARG:HA	1:B:218:ARG:HH11	1.56	0.70
1:D:57:THR:HA	1:D:60:LYS:HD2	1.75	0.68
1:A:180:THR:HG22	1:A:182:GLN:H	1.62	0.65
1:B:47:LEU:HD23	1:B:232:ILE:HB	1.81	0.63
1:C:57:THR:HA	1:C:60:LYS:HD2	1.80	0.61
1:B:241:ASN:OD1	1:B:287:LYS:NZ	2.34	0.60
1:C:47:LEU:HD23	1:C:232:ILE:HB	1.82	0.60
1:A:57:THR:HA	1:A:60:LYS:HD2	1.84	0.59
1:A:47:LEU:HD23	1:A:232:ILE:HB	1.84	0.58
1:D:47:LEU:HD23	1:D:232:ILE:HB	1.84	0.58
1:D:150:PHE:CZ	1:D:163:GLN:HB2	2.39	0.58
1:D:241:ASN:OD1	1:D:287:LYS:NZ	2.37	0.57
1:A:117:TYR:HD2	1:A:118:ILE:HD12	1.70	0.56
1:A:185:LEU:O	6:A:501:HOH:O	2.17	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ARG:NH2	1:A:259:LEU:HD22	2.20	0.56
1:C:270:ARG:O	1:C:344:HIS:ND1	2.39	0.56
1:B:218:ARG:HE	1:B:259:LEU:HD13	1.71	0.56
1:B:180:THR:HG22	1:B:182:GLN:H	1.70	0.55
1:A:218:ARG:HE	1:A:259:LEU:HD13	1.71	0.55
1:B:368:ASP:O	1:B:372:ARG:HG3	2.07	0.55
1:A:360:ARG:O	1:A:364:ASN:HB2	2.06	0.55
1:C:150:PHE:CZ	1:C:163:GLN:HB2	2.42	0.54
1:D:52:GLU:OE1	1:D:252:ARG:NH2	2.35	0.54
1:B:360:ARG:O	1:B:364:ASN:HB2	2.07	0.54
1:A:134:PHE:HD1	1:A:169:ILE:HD11	1.73	0.54
1:C:218:ARG:HE	1:C:259:LEU:HD13	1.72	0.54
1:A:239:SER:HB3	1:A:252:ARG:HD3	1.90	0.54
1:C:117:TYR:HD2	1:C:118:ILE:HD12	1.73	0.53
1:A:353:ALA:HA	1:A:359:ILE:HD11	1.91	0.52
1:B:288:VAL:HA	2:B:401:EDO:H11	1.92	0.52
1:C:134:PHE:HD1	1:C:169:ILE:HD11	1.75	0.52
1:B:134:PHE:HD1	1:B:169:ILE:HD11	1.76	0.51
1:A:241:ASN:OD1	1:A:287:LYS:NZ	2.41	0.51
1:B:77:GLN:NE2	1:B:81:ASP:OD1	2.44	0.51
1:C:366:CYS:O	1:C:370:ILE:HG12	2.11	0.51
1:A:358:ASN:HD22	1:A:361:ARG:NH2	2.09	0.51
1:D:270:ARG:O	1:D:344:HIS:ND1	2.44	0.51
1:D:333:LEU:HD21	1:D:348:PRO:HG3	1.93	0.51
1:B:239:SER:HA	1:B:242:MET:HE2	1.92	0.50
1:C:305:TYR:O	1:C:323:ARG:NH2	2.42	0.50
1:C:74:GLU:O	1:C:78:LYS:HG2	2.11	0.50
1:A:61:GLN:HG3	1:A:359:ILE:HG13	1.94	0.50
1:B:150:PHE:CZ	1:B:163:GLN:HB2	2.47	0.50
1:B:201:VAL:O	1:B:204:VAL:HG12	2.12	0.50
1:B:117:TYR:HD2	1:B:118:ILE:HD12	1.77	0.49
1:D:266:ASN:HB3	1:D:269:LEU:HB2	1.95	0.48
1:A:75:LYS:C	1:A:77:GLN:H	2.16	0.48
1:C:360:ARG:O	1:C:364:ASN:HB2	2.14	0.47
1:D:239:SER:HB3	1:D:252:ARG:HD3	1.95	0.47
1:A:87:LYS:NZ	1:A:121:ILE:O	2.42	0.47
1:B:218:ARG:NH2	1:B:259:LEU:HD22	2.23	0.47
1:C:218:ARG:NH2	1:C:259:LEU:HD22	2.25	0.47
1:C:150:PHE:HZ	1:C:163:GLN:HB2	1.79	0.47
1:B:52:GLU:OE1	1:B:252:ARG:NH2	2.48	0.47
1:A:346:CYS:HB3	2:A:401:EDO:H21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:VAL:O	1:D:204:VAL:HG12	2.15	0.46
1:A:201:VAL:O	1:A:204:VAL:HG12	2.16	0.46
1:A:239:SER:HA	1:A:242:MET:HE2	1.99	0.45
1:D:302:TYR:O	1:D:323:ARG:NH2	2.49	0.45
1:B:77:GLN:HE21	1:B:80:LEU:HD23	1.82	0.44
1:C:277:PHE:CG	1:C:351:THR:HG21	2.52	0.44
1:D:218:ARG:HE	1:D:259:LEU:HD13	1.83	0.44
1:D:218:ARG:NH2	1:D:259:LEU:HD22	2.25	0.44
1:A:83:ARG:HB3	1:A:129:TYR:CE1	2.53	0.43
1:A:270:ARG:O	1:A:344:HIS:ND1	2.51	0.43
1:B:75:LYS:HE3	1:B:184:LEU:HD11	2.01	0.43
1:C:201:VAL:O	1:C:204:VAL:HG12	2.18	0.43
1:D:117:TYR:CE2	1:D:121:ILE:HD13	2.53	0.43
1:B:239:SER:HB3	1:B:252:ARG:HD3	2.01	0.43
1:A:308:PRO:HB2	1:A:310:ASP:OD1	2.18	0.43
1:B:150:PHE:HZ	1:B:163:GLN:HB2	1.84	0.43
1:D:59:VAL:HG21	1:D:210:ASP:HB2	2.00	0.43
1:D:75:LYS:NZ	1:D:179:PRO:HD2	2.34	0.43
1:D:134:PHE:HD1	1:D:169:ILE:HD11	1.83	0.43
1:D:75:LYS:HD3	1:D:76:LYS:H	1.85	0.42
1:A:48:LEU:O	1:A:233:TYR:HA	2.19	0.42
1:D:75:LYS:O	1:D:76:LYS:HB2	2.19	0.42
1:A:151:GLU:CD	1:C:175:VAL:HG22	2.40	0.42
1:B:100:ILE:HD13	1:B:100:ILE:HA	1.88	0.42
1:A:215:ARG:HG2	1:A:218:ARG:NH1	2.35	0.42
1:A:352:CYS:N	1:A:358:ASN:OD1	2.45	0.42
1:A:253:LEU:HD23	1:A:299:PHE:CE1	2.54	0.42
1:A:92:THR:HG21	1:A:157:GLN:O	2.19	0.42
1:C:266:ASN:HB3	1:C:269:LEU:HB2	2.02	0.42
1:A:266:ASN:HB3	1:A:269:LEU:HB2	2.02	0.42
1:D:92:THR:HG21	1:D:157:GLN:O	2.20	0.42
1:C:347:TYR:CE2	1:D:315:ALA:HB1	2.55	0.42
1:B:168:ARG:O	1:B:172:VAL:HG23	2.20	0.41
1:C:222:ILE:HD12	1:C:225:PHE:CD2	2.56	0.41
1:C:351:THR:HG22	1:C:362:VAL:HG11	2.02	0.41
1:B:83:ARG:NE	6:B:501:HOH:O	2.47	0.41
1:D:292:LYS:HA	1:D:292:LYS:HD2	1.89	0.41
1:A:71:ASN:O	1:A:75:LYS:HB3	2.21	0.41
1:C:302:TYR:HD1	1:C:327:PHE:CG	2.38	0.41
1:B:296:GLU:H	1:B:296:GLU:HG3	1.62	0.41
1:C:239:SER:HB3	1:C:252:ARG:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:ARG:NH2	1:D:298:TYR:O	2.52	0.41
1:A:322:THR:O	1:A:326:PHE:HD2	2.04	0.41
1:A:75:LYS:O	1:A:76:LYS:HB2	2.21	0.40
1:B:86:VAL:HG22	1:B:165:PHE:HB3	2.03	0.40
1:D:60:LYS:O	1:D:64:ILE:HG12	2.21	0.40
1:D:86:VAL:HG22	1:D:165:PHE:HB3	2.04	0.40
1:B:96:ALA:HB1	1:B:100:ILE:HG12	2.03	0.40
1:C:215:ARG:HG3	1:C:246:GLU:HG2	2.03	0.40
1:A:100:ILE:HD13	1:A:100:ILE:HA	1.88	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	326/395 (82%)	320 (98%)	6 (2%)	0	100	100
1	B	332/395 (84%)	326 (98%)	6 (2%)	0	100	100
1	C	330/395 (84%)	324 (98%)	6 (2%)	0	100	100
1	D	322/395 (82%)	314 (98%)	8 (2%)	0	100	100
All	All	1310/1580 (83%)	1284 (98%)	26 (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	301/357 (84%)	301 (100%)	0	100 100
1	B	303/357 (85%)	302 (100%)	1 (0%)	92 98
1	C	301/357 (84%)	299 (99%)	2 (1%)	84 95
1	D	296/357 (83%)	295 (100%)	1 (0%)	92 98
All	All	1201/1428 (84%)	1197 (100%)	4 (0%)	92 98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	312	THR
1	C	178	THR
1	C	211	VAL
1	D	180	THR

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)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 for Mogul analysis.

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	$\#\|Z\|>2$
5	PO4	C	403	-	4,4,4	0.94	0	6,6,6	0.40	0
5	PO4	A	404	-	4,4,4	0.96	0	6,6,6	0.43	0
4	GSP	D	402	3	26,34,34	2.15	3 (11%)	27,54,54	1.52	6 (22%)
5	PO4	A	405	-	4,4,4	0.92	0	6,6,6	0.45	0
4	GSP	B	403	3	26,34,34	2.07	3 (11%)	27,54,54	1.49	4 (14%)
4	GSP	C	402	3	26,34,34	2.08	3 (11%)	27,54,54	1.44	5 (18%)
2	EDO	A	401	-	3,3,3	0.46	0	2,2,2	0.32	0
2	EDO	B	401	-	3,3,3	0.47	0	2,2,2	0.32	0
4	GSP	A	403	3	26,34,34	2.09	3 (11%)	27,54,54	1.50	4 (14%)

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	GSP	D	402	3	-	2/17/38/38	0/3/3/3
4	GSP	B	403	3	-	1/17/38/38	0/3/3/3
4	GSP	C	402	3	-	0/17/38/38	0/3/3/3
2	EDO	A	401	-	-	0/1/1/1	-
2	EDO	B	401	-	-	1/1/1/1	-
4	GSP	A	403	3	-	0/17/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	402	GSP	PG-S1G	-9.28	1.70	1.90
4	A	403	GSP	PG-S1G	-9.05	1.71	1.90
4	C	402	GSP	PG-S1G	-8.91	1.71	1.90
4	B	403	GSP	PG-S1G	-8.88	1.71	1.90
4	D	402	GSP	C5-C6	-3.88	1.39	1.47
4	C	402	GSP	C5-C6	-3.83	1.39	1.47
4	B	403	GSP	C5-C6	-3.72	1.39	1.47
4	A	403	GSP	C5-C6	-3.63	1.40	1.47
4	D	402	GSP	C2-N3	2.22	1.38	1.33
4	B	403	GSP	C2-N3	2.15	1.38	1.33
4	A	403	GSP	C2-N3	2.10	1.38	1.33
4	C	402	GSP	C2-N3	2.07	1.38	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	403	GSP	PA-O3A-PB	-3.57	120.59	132.83
4	B	403	GSP	PA-O3A-PB	-3.56	120.63	132.83
4	B	403	GSP	C5-C6-N1	3.27	119.73	113.95
4	C	402	GSP	C5-C6-N1	3.25	119.69	113.95
4	A	403	GSP	C5-C6-N1	3.23	119.66	113.95
4	D	402	GSP	C5-C6-N1	3.21	119.61	113.95
4	D	402	GSP	PA-O3A-PB	-3.14	122.05	132.83
4	C	402	GSP	PA-O3A-PB	-3.07	122.29	132.83
4	D	402	GSP	C8-N7-C5	3.07	108.84	102.99
4	A	403	GSP	C8-N7-C5	2.94	108.59	102.99
4	B	403	GSP	C8-N7-C5	2.92	108.56	102.99
4	C	402	GSP	C8-N7-C5	2.88	108.47	102.99
4	D	402	GSP	C2-N1-C6	-2.83	119.89	125.10
4	C	402	GSP	C2-N1-C6	-2.73	120.06	125.10
4	B	403	GSP	C2-N1-C6	-2.72	120.10	125.10
4	A	403	GSP	C2-N1-C6	-2.72	120.10	125.10
4	D	402	GSP	C3'-C2'-C1'	2.40	104.59	100.98
4	D	402	GSP	O6-C6-C5	-2.10	120.28	124.37
4	C	402	GSP	O6-C6-C5	-2.02	120.43	124.37

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	402	GSP	PA-O3A-PB-O1B
2	B	401	EDO	O1-C1-C2-O2
4	B	403	GSP	PA-O3A-PB-O1B
4	D	402	GSP	PA-O3A-PB-O2B

There are no ring outliers.

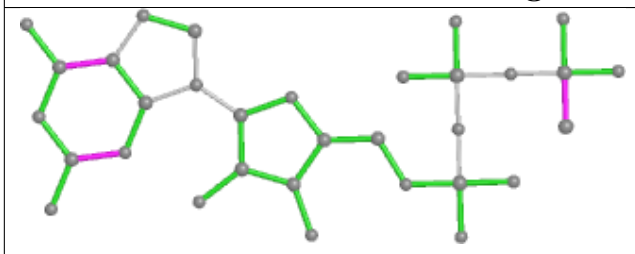
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	EDO	1	0
2	B	401	EDO	1	0

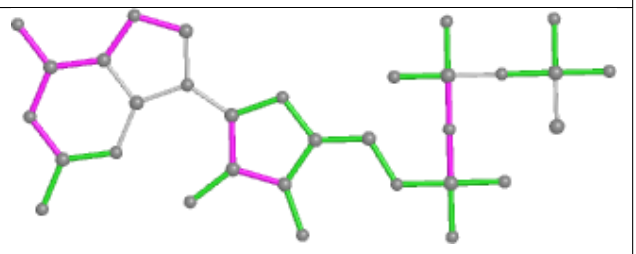
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

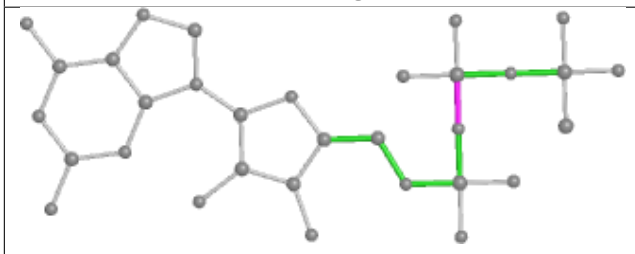
Ligand GSP D 402



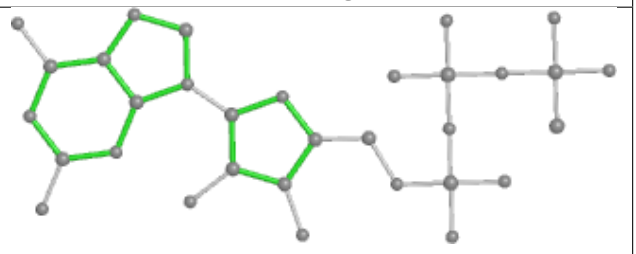
Bond lengths



Bond angles

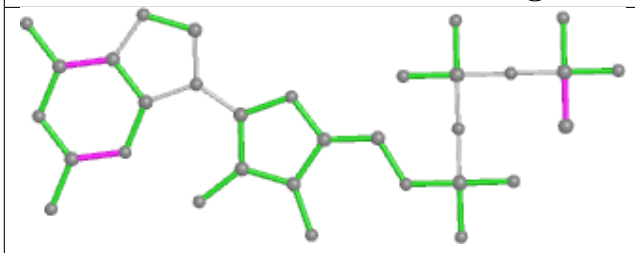


Torsions

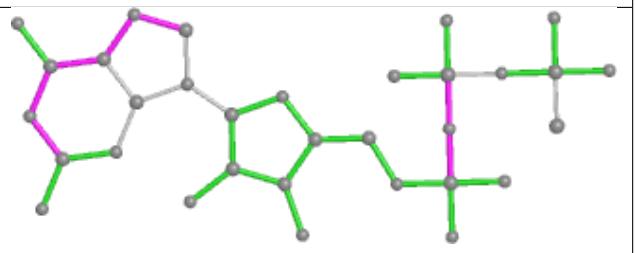


Rings

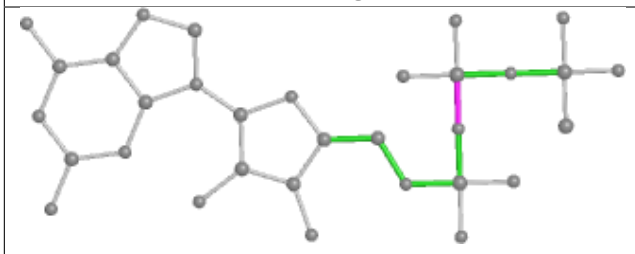
Ligand GSP B 403



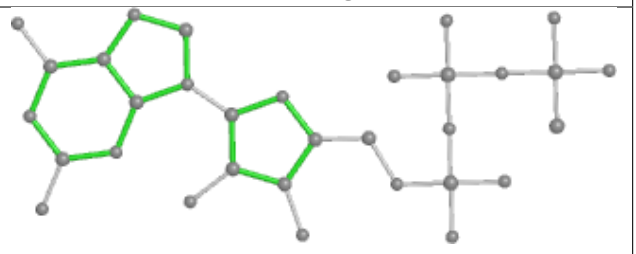
Bond lengths



Bond angles

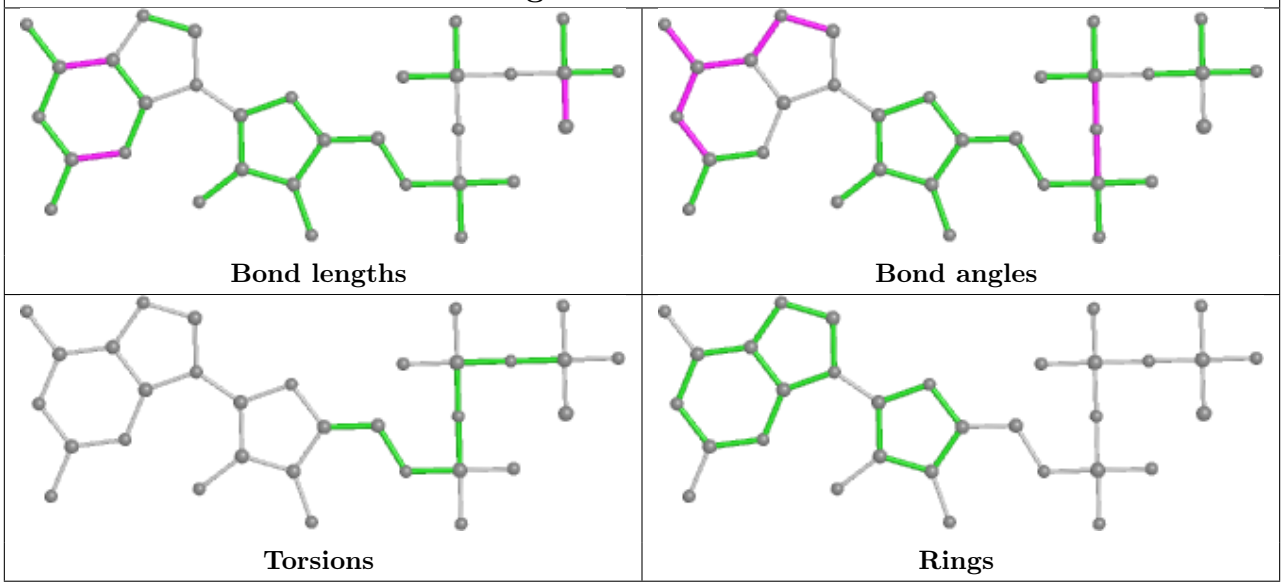


Torsions

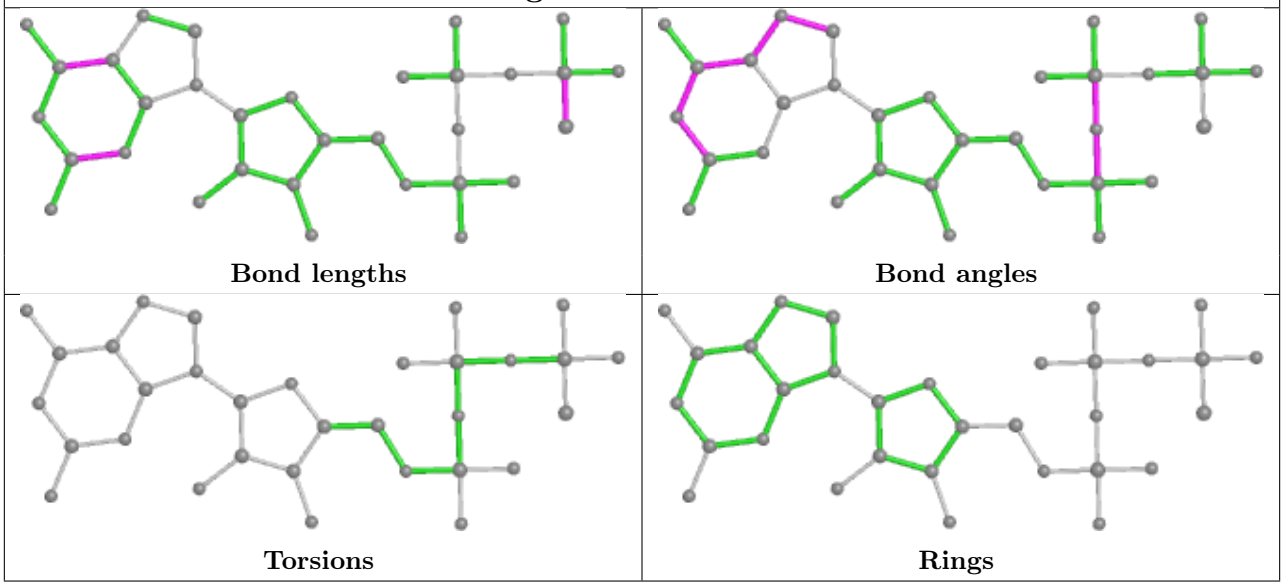


Rings

Ligand GSP C 402



Ligand GSP A 403



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	332/395 (84%)	-0.05	4 (1%) 79 79	23, 37, 64, 102	0
1	B	334/395 (84%)	-0.13	5 (1%) 73 73	24, 37, 67, 97	0
1	C	332/395 (84%)	-0.01	6 (1%) 68 67	25, 41, 73, 97	0
1	D	326/395 (82%)	1.21	66 (20%) 1 0	61, 85, 108, 147	0
All	All	1324/1580 (83%)	0.25	81 (6%) 21 18	23, 44, 96, 147	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	338	ALA	7.0
1	D	312	THR	6.1
1	D	76	LYS	5.5
1	D	339	THR	5.3
1	D	234	VAL	4.7
1	D	203	LYS	4.7
1	D	201	VAL	4.4
1	D	68	ASN	4.4
1	D	202	ASP	4.3
1	D	101	ILE	4.3
1	D	309	GLU	4.2
1	D	341	ASP	4.1
1	D	304	ASN	4.1
1	C	74	GLU	4.1
1	D	235	ALA	3.9
1	D	347	TYR	3.8
1	D	249	ASN	3.7
1	D	107	ALA	3.7
1	D	180	THR	3.7
1	D	307	VAL	3.7
1	D	345	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	135	ASP	3.6
1	D	311	ALA	3.6
1	D	337	THR	3.6
1	D	109	PRO	3.6
1	D	310	ASP	3.5
1	D	258	ASP	3.5
1	D	53	SER	3.4
1	B	76	LYS	3.4
1	B	315	ALA	3.3
1	D	313	PRO	3.2
1	D	292	LYS	3.1
1	D	277	PHE	3.1
1	B	249	ASN	3.0
1	D	317	GLU	3.0
1	D	236	ALA	3.0
1	D	334	ARG	3.0
1	D	340	GLY	2.9
1	D	192	SER	2.9
1	D	372	ARG	2.9
1	D	336	SER	2.8
1	D	316	GLY	2.8
1	A	74	GLU	2.7
1	D	204	VAL	2.6
1	D	343	LYS	2.6
1	C	41	ALA	2.6
1	D	349	HIS	2.6
1	D	98	SER	2.6
1	D	342	GLY	2.6
1	D	108	ASN	2.6
1	D	216	ASP	2.5
1	B	374	HIS	2.5
1	D	195	PHE	2.5
1	D	360	ARG	2.5
1	A	310	ASP	2.5
1	D	110	GLU	2.5
1	C	341	ASP	2.4
1	C	315	ALA	2.4
1	D	250	THR	2.4
1	A	341	ASP	2.4
1	D	181	ASP	2.3
1	D	176	ASP	2.2
1	D	333	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	308	PRO	2.2
1	D	237	CYS	2.2
1	B	341	ASP	2.2
1	D	193	GLY	2.2
1	C	53	SER	2.1
1	D	69	GLY	2.1
1	D	126	ASP	2.1
1	D	177	TYR	2.1
1	A	316	GLY	2.1
1	D	364	ASN	2.1
1	D	178	THR	2.1
1	D	344	HIS	2.0
1	D	265	ASN	2.0
1	D	306	THR	2.0
1	D	357	GLU	2.0
1	C	71	ASN	2.0
1	D	139	LYS	2.0
1	D	99	THR	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 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
5	PO4	C	403	5/5	0.84	0.26	80,85,89,92	0
5	PO4	A	405	5/5	0.89	0.22	88,90,92,99	0
2	EDO	B	401	4/4	0.90	0.28	30,34,38,44	0
3	MG	C	401	1/1	0.90	0.12	29,29,29,29	0
4	GSP	D	402	32/32	0.91	0.22	72,85,98,106	0

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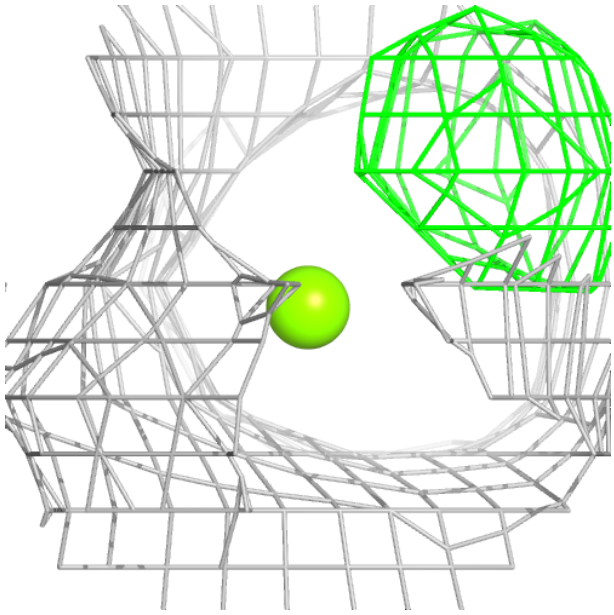
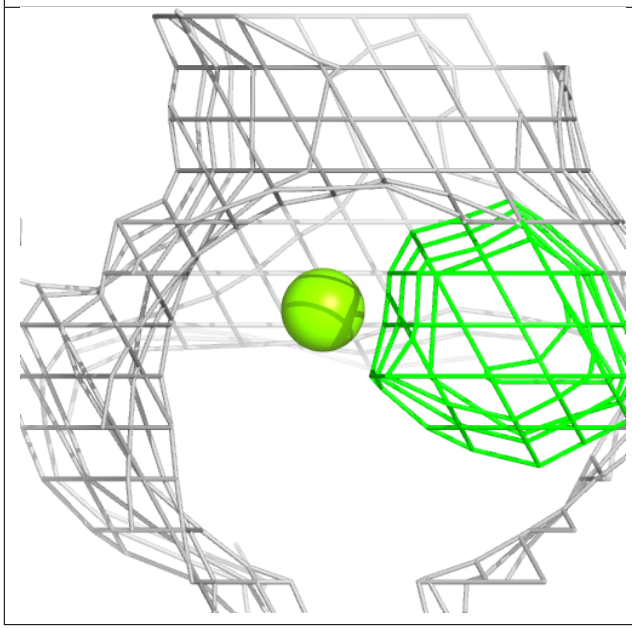
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PO4	A	404	5/5	0.93	0.29	89,97,100,101	0
2	EDO	A	401	4/4	0.94	0.18	37,42,45,48	0
3	MG	D	401	1/1	0.95	0.28	87,87,87,87	0
3	MG	B	402	1/1	0.96	0.21	29,29,29,29	0
4	GSP	B	403	32/32	0.97	0.17	18,25,37,46	0
4	GSP	C	402	32/32	0.97	0.19	22,29,43,44	0
4	GSP	A	403	32/32	0.98	0.18	20,31,36,37	0
3	MG	A	402	1/1	0.99	0.22	20,20,20,20	0

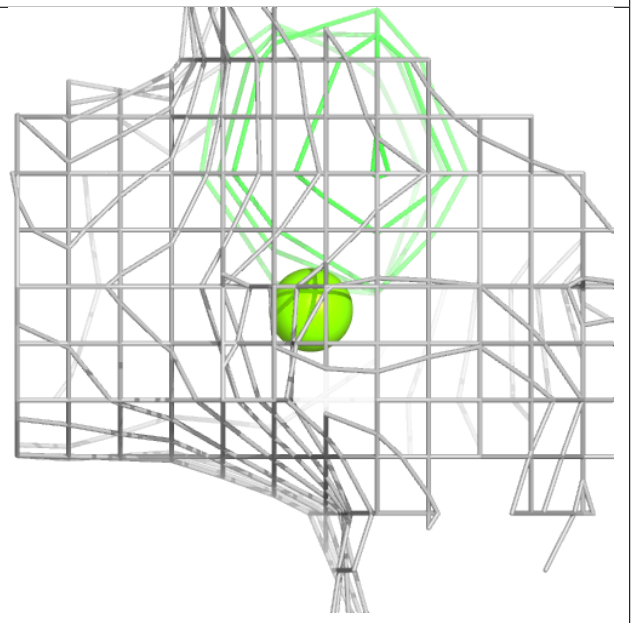
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MG C 401:

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

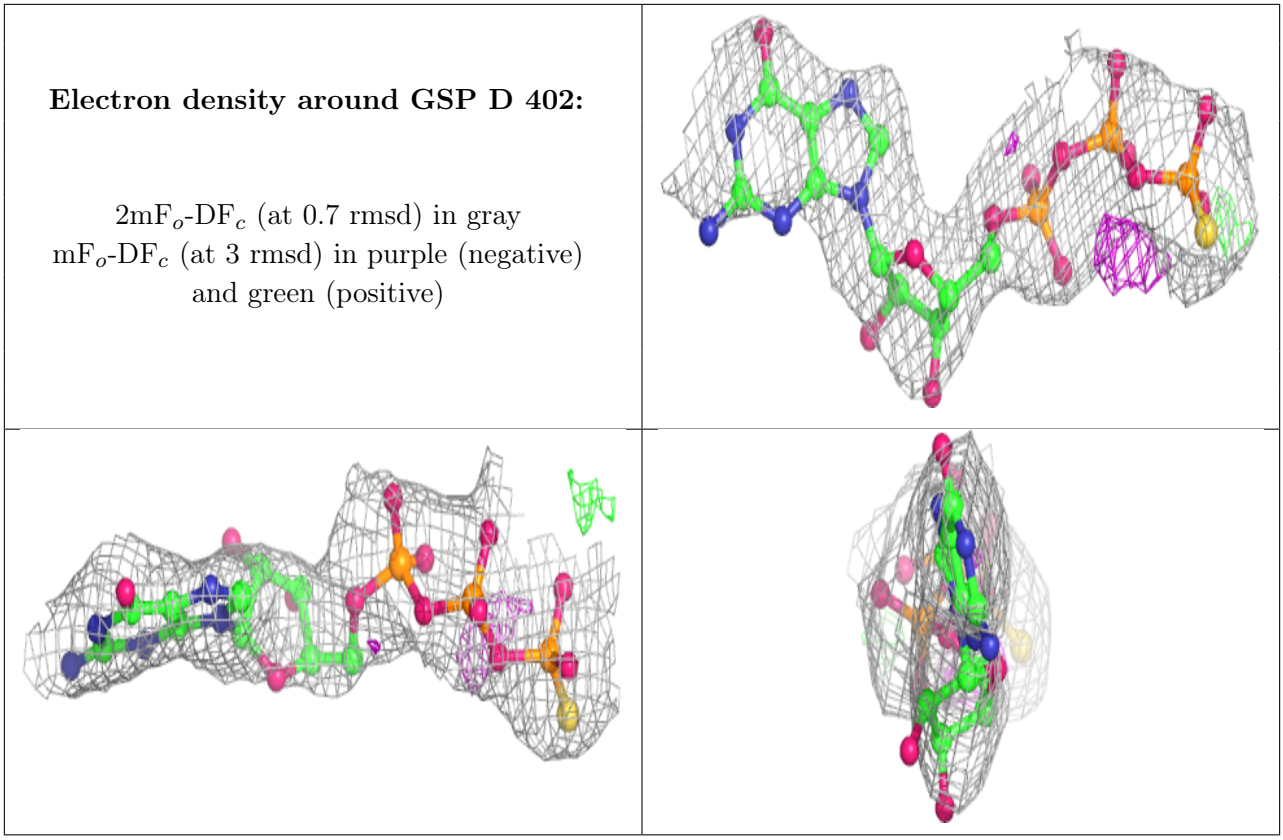






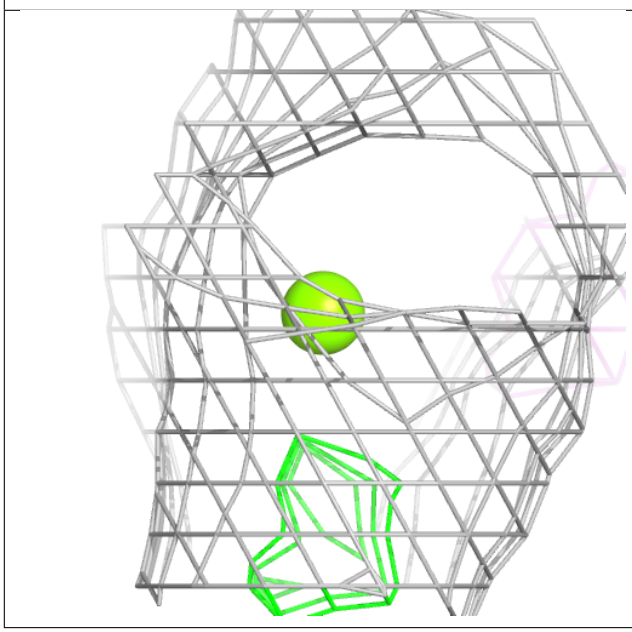
Electron density around GSP D 402:

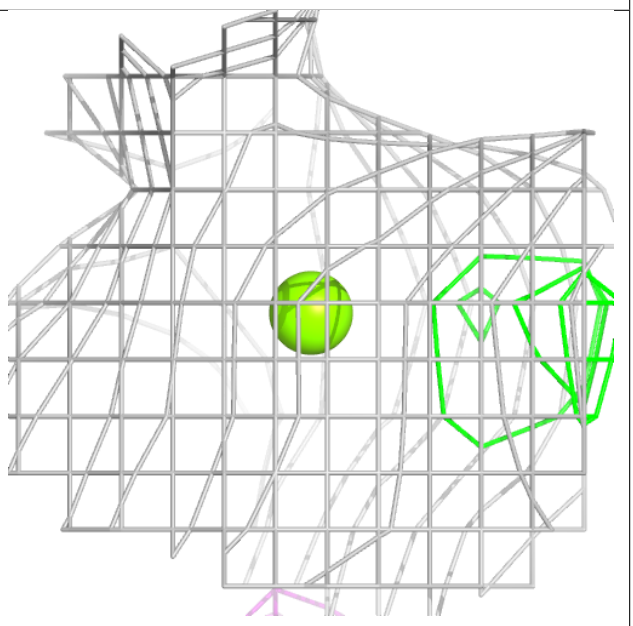
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around MG D 401:

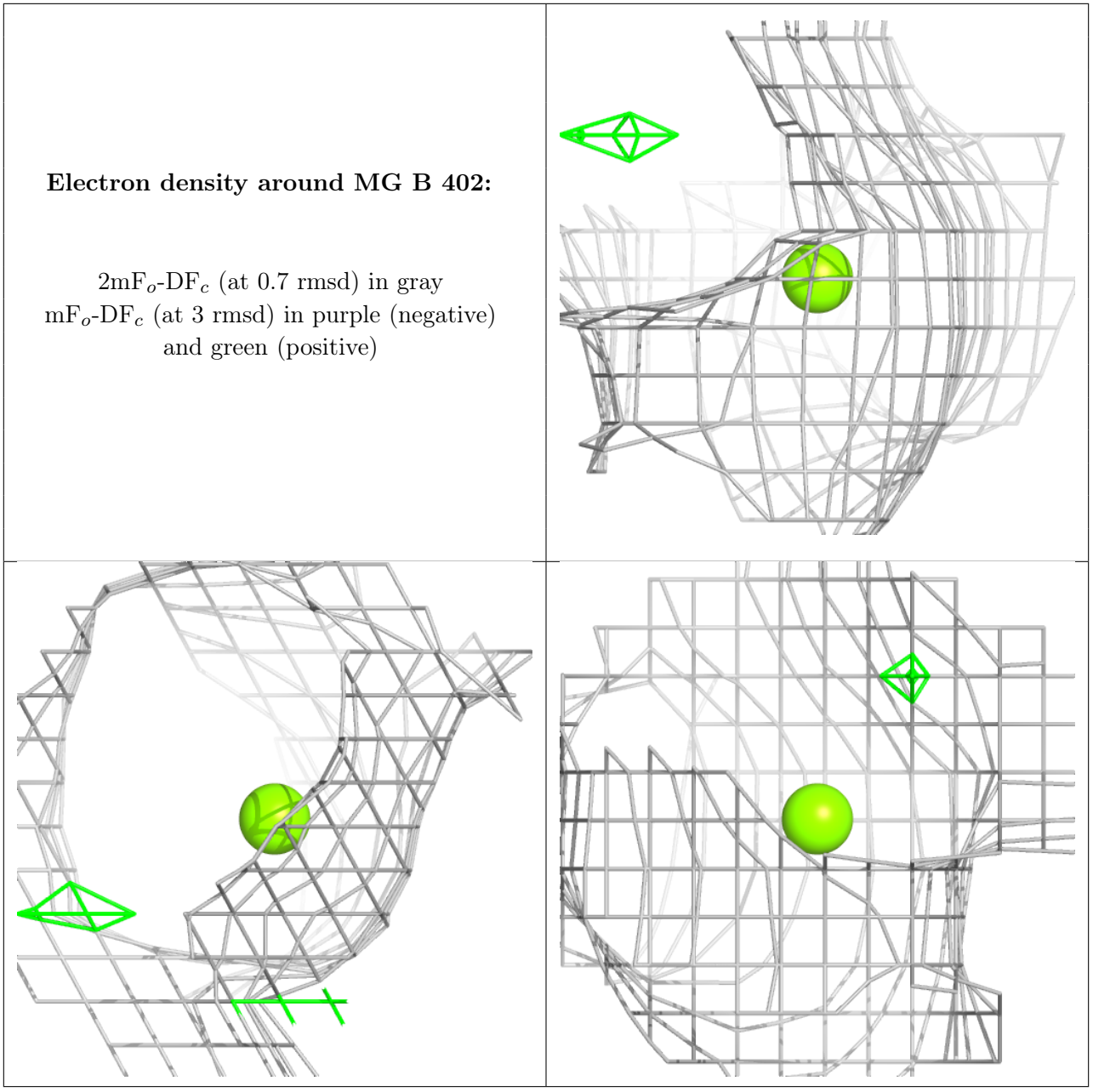
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





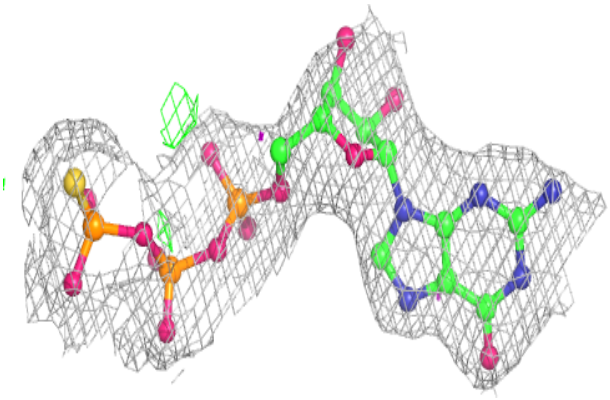
Electron density around MG B 402:

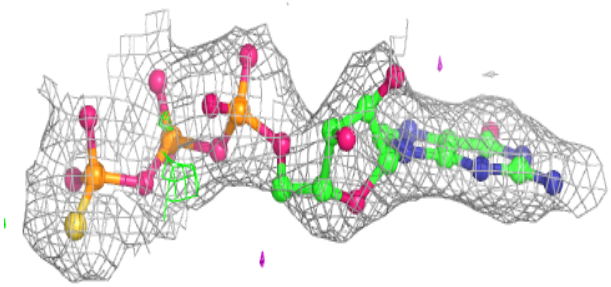
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

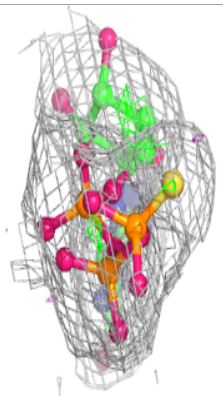


Electron density around GSP B 403:

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

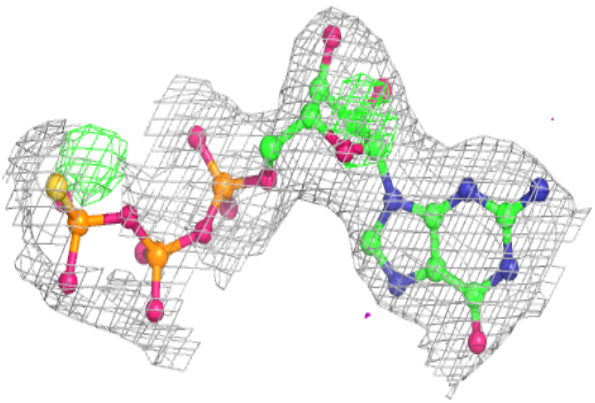


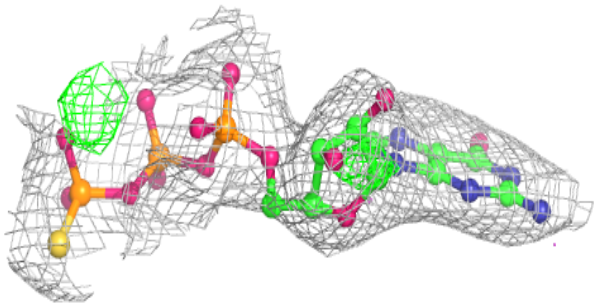


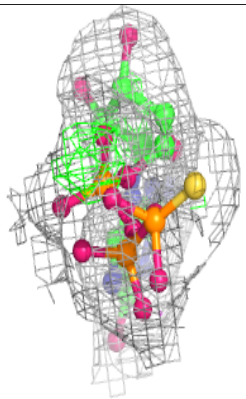


Electron density around GSP C 402:

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

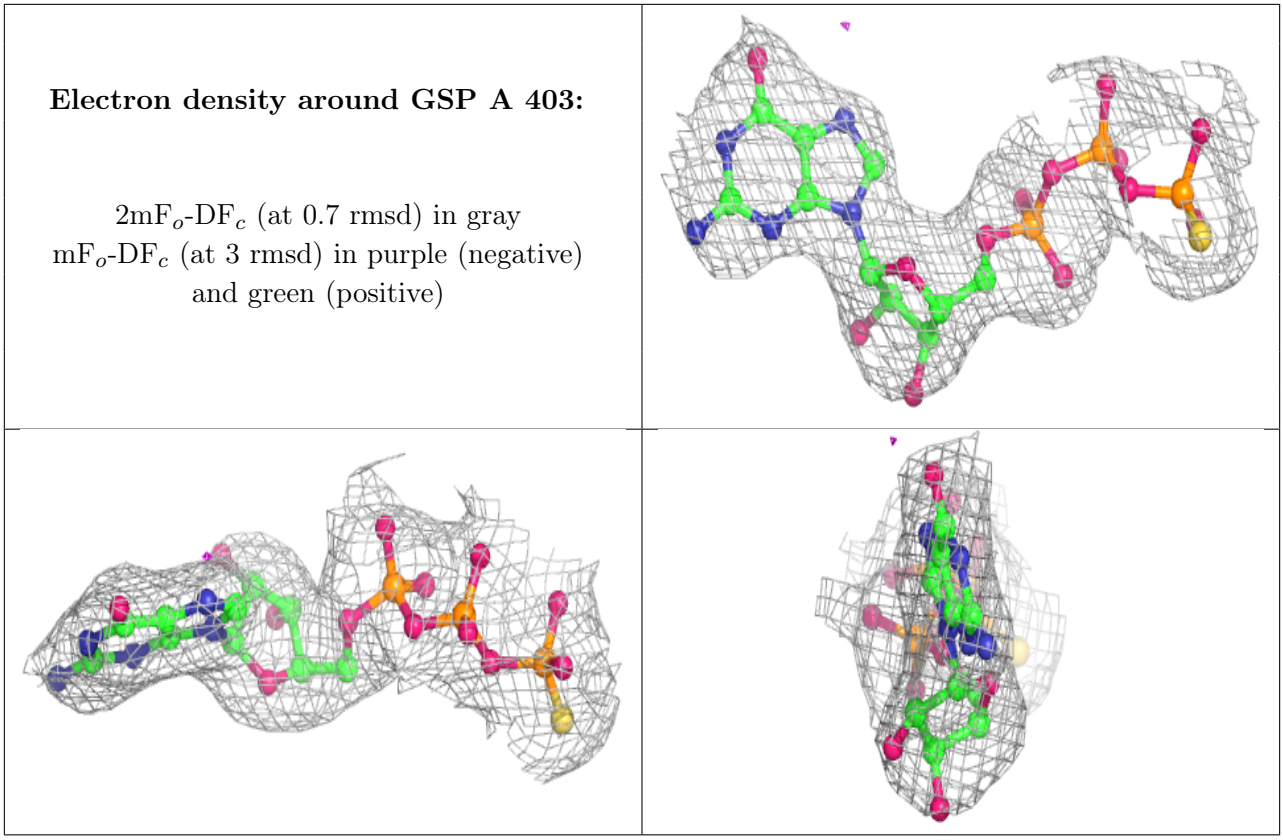






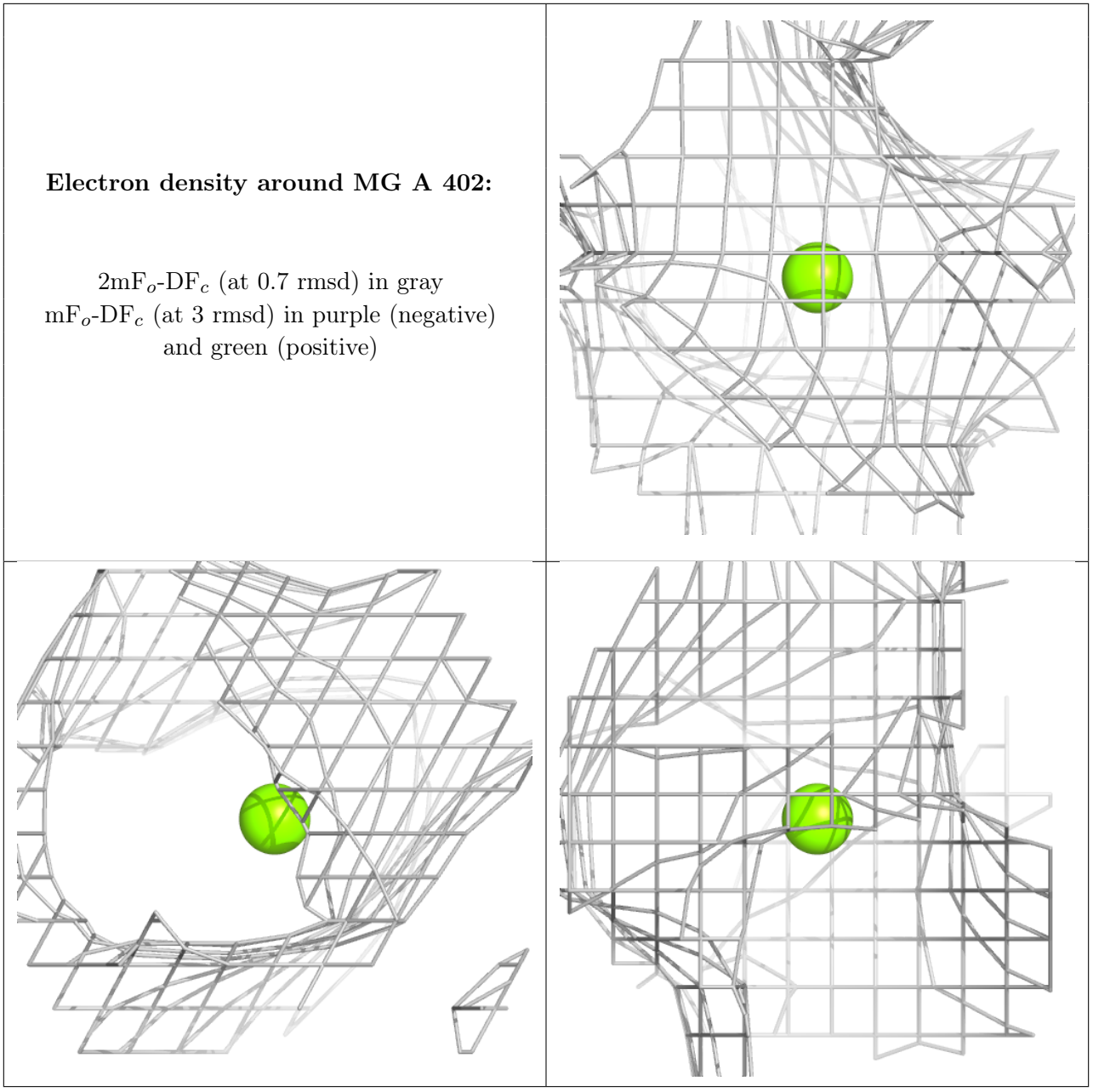
Electron density around GSP A 403:

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



Electron density around MG A 402:

$2mF_o$-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.