



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2022 – 10:16 PM JST

PDB ID : 7E5E
Title : Crystal structure of GDP-bound GNAS in complex with the cyclic peptide inhibitor GD20
Authors : Hu, Q.; Dai, S.; Shokat, K.M.
Deposited on : 2021-02-18
Resolution : 1.95 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:

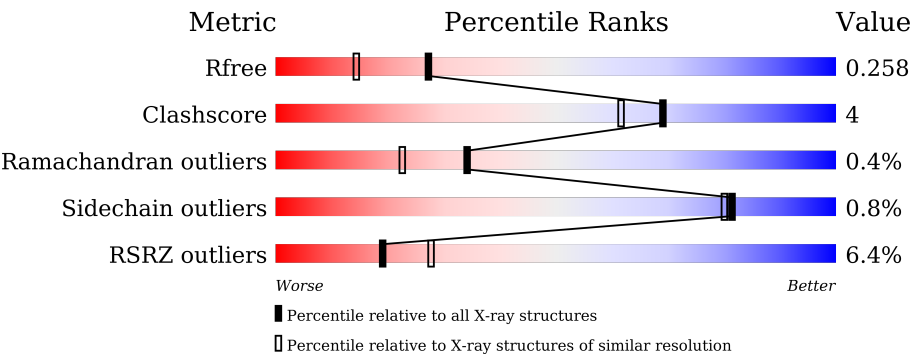
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.26
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.26

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 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	348	<div><div>2%</div><div>91%</div><div>6%</div><div>.</div></div>
1	B	348	<div><div>4%</div><div>85%</div><div>8%</div><div>7%</div></div>
1	C	348	<div><div>3%</div><div>85%</div><div>10%</div><div>5%</div></div>
1	D	348	<div><div>16%</div><div>77%</div><div>14%</div><div>9%</div></div>
2	E	17	<div><div>6%</div><div>100%</div></div>
2	F	17	<div><div>6%</div><div>94%</div><div>6%</div></div>

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Mol	Chain	Length	Quality of chain
2	G	17	<div><div></div><div>6%</div><div>76%</div><div>24%</div></div>
2	H	17	<div><div></div><div>6%</div><div>76%</div><div>18%</div><div>6%</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11740 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 Isoform Gnas-2 of Guanine nucleotide-binding protein G(s) subunit alpha isoforms short.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2778	1764	487	514	13			
1	B	324	Total	C	N	O	S	0	0	0
			2655	1688	460	494	13			
1	C	332	Total	C	N	O	S	0	0	0
			2731	1736	478	504	13			
1	D	317	Total	C	N	O	S	0	0	0
			2599	1654	447	486	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	GLY	-	expression tag	UNP P63092
A	34	PRO	-	expression tag	UNP P63092
B	33	GLY	-	expression tag	UNP P63092
B	34	PRO	-	expression tag	UNP P63092
C	33	GLY	-	expression tag	UNP P63092
C	34	PRO	-	expression tag	UNP P63092
D	33	GLY	-	expression tag	UNP P63092
D	34	PRO	-	expression tag	UNP P63092

- Molecule 2 is a protein called GD20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	17	Total	C	N	O	S	0	0	1
			133	90	22	20	1			
2	F	17	Total	C	N	O	S	0	0	1
			133	90	22	20	1			
2	G	17	Total	C	N	O	S	0	0	1
			133	90	22	20	1			
2	H	17	Total	C	N	O	S	0	0	1
			133	90	22	20	1			

-
- The image displays the chemical structure of GDP (Guanosine Diphosphate). It consists of a guanine base (a purine ring system with an amino group at C2 and a carbonyl group at C6) linked to a ribose sugar (a five-membered ring with hydroxyl groups at C2' and C3'). The ribose is further linked to two phosphate groups (P1 and P2) via phosphodiester bonds. The structure is labeled with atom names (N1, N2, N3, N7, N9, C2, C3, C4, C5, C6, C8, C1', C2', C3', C4', C5') and bond types (solid, dashed, wedged). The phosphate groups are labeled with their respective oxygen atoms (O1A, O1B, O2A, O2B, O3A, O3B).

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

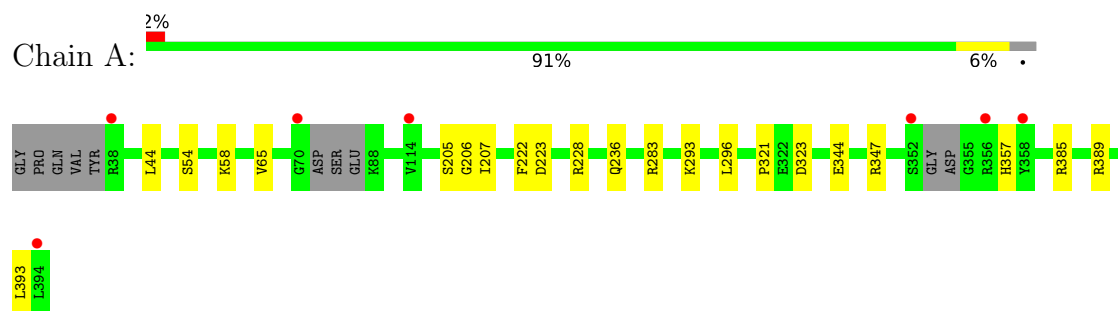
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	114	Total 114	O 114	0	0
5	B	88	Total 88	O 88	0	0
5	C	74	Total 74	O 74	0	0
5	D	21	Total 21	O 21	0	0
5	E	14	Total 14	O 14	0	0
5	F	5	Total 5	O 5	0	0
5	G	5	Total 5	O 5	0	0
5	H	8	Total 8	O 8	0	0

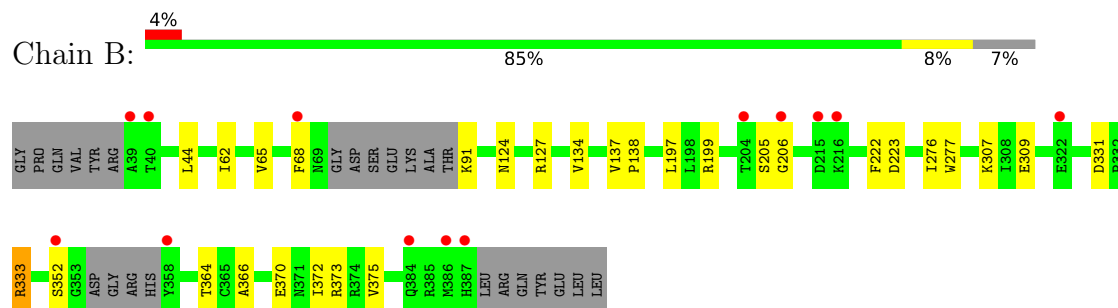
3 Residue-property plots [i](#)

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.

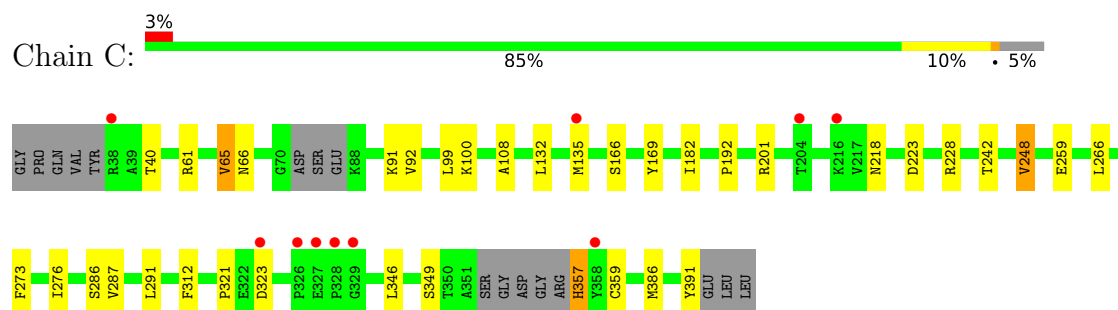
- Molecule 1: Isoform Gnas-2 of Guanine nucleotide-binding protein G(s) subunit alpha isoforms short



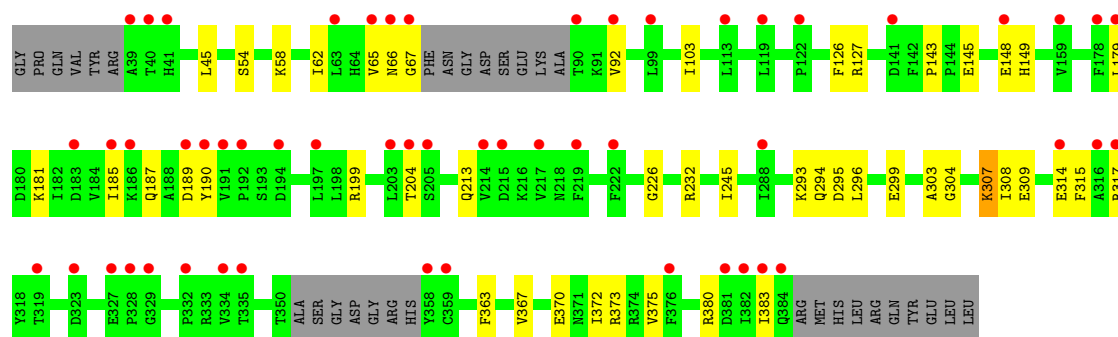
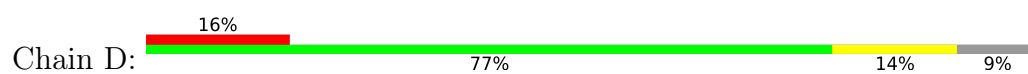
- Molecule 1: Isoform Gnas-2 of Guanine nucleotide-binding protein G(s) subunit alpha isoforms short



- Molecule 1: Isoform Gnas-2 of Guanine nucleotide-binding protein G(s) subunit alpha isoforms short



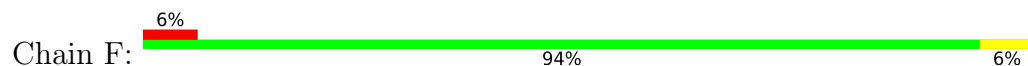
- Molecule 1: Isoform Gnas-2 of Guanine nucleotide-binding protein G(s) subunit alpha isoforms short



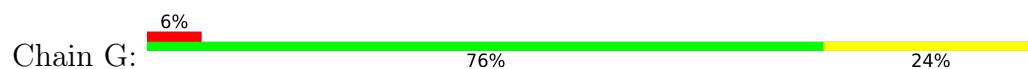
• Molecule 2: GD20



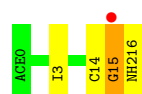
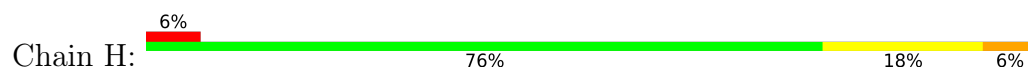
• Molecule 2: GD20



• Molecule 2: GD20



• Molecule 2: GD20



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	58.10Å 81.77Å 76.91Å 81.27° 83.84° 90.70°	Depositor
Resolution (Å)	48.54 – 1.95 48.54 – 1.95	Depositor EDS
% Data completeness (in resolution range)	80.7 (48.54-1.95) 80.7 (48.54-1.95)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.218 , 0.258 0.218 , 0.258	Depositor DCC
R_{free} test set	4043 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11740	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NH2, DTY, CL, GDP, ACE

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	0.28	0/2836	0.45	0/3833
1	B	0.27	0/2711	0.43	0/3668
1	C	0.26	0/2789	0.43	0/3772
1	D	0.25	0/2653	0.41	0/3592
2	E	0.26	0/121	0.48	0/164
2	F	0.34	0/121	0.44	0/164
2	G	0.27	0/121	0.38	0/164
2	H	0.26	0/121	0.42	0/164
All	All	0.27	0/11473	0.43	0/15521

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2778	0	2734	13	0
1	B	2655	0	2604	16	0
1	C	2731	0	2685	24	0
1	D	2599	0	2554	30	0
2	E	133	0	125	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	133	0	125	1	0
2	G	133	0	125	4	0
2	H	133	0	125	3	0
3	A	28	0	11	0	0
3	B	28	0	11	1	0
3	C	28	0	11	1	0
3	D	28	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	114	0	0	1	0
5	B	88	0	0	0	0
5	C	74	0	0	1	0
5	D	21	0	0	0	0
5	E	14	0	0	0	0
5	F	5	0	0	0	0
5	G	5	0	0	0	0
5	H	8	0	0	0	0
All	All	11740	0	11122	84	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 4.

All (84) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:GLY:HA2	1:B:205:SER:HB2	1.73	0.69
1:C:132:LEU:HD23	1:C:135:MET:HE3	1.75	0.67
1:D:370:GLU:OE2	1:D:373:ARG:NH2	2.35	0.60
1:B:276:ILE:HD11	2:F:5:PHE:HZ	1.68	0.59
1:D:380:ARG:HA	1:D:383:ILE:HD12	1.87	0.57
2:G:15:GLY:HA3	2:H:15:GLY:HA3	1.87	0.56
1:A:223:ASP:OD2	5:A:501:HOH:O	2.18	0.56
1:A:205:SER:HB2	1:B:206:GLY:HA2	1.87	0.55
1:B:331:ASP:OD1	1:B:333:ARG:NE	2.31	0.55
1:B:124:ASN:OD1	1:B:127:ARG:NH1	2.40	0.54
2:H:3:ILE:HG22	2:H:14:CYS:HB3	1.89	0.54
1:C:201:ARG:HD3	3:C:401:GDP:H5''	1.89	0.54
1:D:145:GLU:O	1:D:149:HIS:HD2	1.91	0.53
1:C:248:VAL:HG13	1:C:291:LEU:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:PRO:HB2	1:C:323:ASP:OD1	2.08	0.52
1:A:344:GLU:OE2	1:A:347:ARG:NH2	2.41	0.52
1:C:276:ILE:HD11	2:G:5:PHE:HZ	1.75	0.52
1:B:307:LYS:HE3	1:B:309:GLU:OE2	2.10	0.52
1:D:293:LYS:HD3	1:D:296:LEU:HD12	1.91	0.52
1:D:370:GLU:CD	1:D:373:ARG:HH21	2.13	0.52
1:B:91:LYS:HD3	1:B:197:LEU:HD22	1.91	0.52
1:D:187:GLN:HB3	1:D:189:ASP:OD1	2.10	0.51
1:D:62:ILE:HA	1:D:67:GLY:HA2	1.93	0.51
1:C:346:LEU:HA	1:C:349:SER:HB3	1.92	0.51
1:A:207:ILE:HD11	1:A:222:PHE:CD2	2.46	0.50
1:B:277:TRP:CD1	1:B:352:SER:HB3	2.47	0.50
1:C:40:THR:HG22	1:C:218:ASN:HB2	1.94	0.50
2:H:14:CYS:O	2:H:16:NH2:N	2.45	0.49
1:D:294:GLN:HG3	1:D:363:PHE:HB3	1.94	0.49
1:B:44:LEU:HD13	1:B:222:PHE:CE2	2.48	0.49
1:A:236:GLN:HE22	1:B:138:PRO:HA	1.78	0.49
1:A:385:ARG:O	1:A:389:ARG:NH1	2.45	0.49
1:A:321:PRO:HB2	1:A:323:ASP:OD1	2.12	0.49
1:C:100:LYS:NZ	1:C:135:MET:O	2.46	0.48
1:C:65:VAL:HG12	1:C:66:ASN:H	1.79	0.48
1:C:91:LYS:HE3	1:C:92:VAL:H	1.78	0.47
1:D:145:GLU:HA	1:D:148:GLU:HG2	1.95	0.47
1:B:199:ARG:HA	3:B:401:GDP:O2'	2.15	0.47
1:C:166:SER:HA	1:C:169:TYR:CE1	2.50	0.47
1:D:307:LYS:HA	1:D:307:LYS:HD2	1.58	0.47
1:C:242:THR:O	1:C:386:MET:HE1	2.15	0.46
1:D:65:VAL:HG12	1:D:66:ASN:H	1.79	0.46
1:A:283:ARG:O	1:A:357:HIS:ND1	2.49	0.46
1:C:91:LYS:HD2	1:C:91:LYS:HA	1.80	0.46
1:D:199:ARG:HD3	1:D:367:VAL:HG11	1.98	0.46
1:A:44:LEU:HD13	1:A:222:PHE:CE2	2.51	0.46
1:D:181:LYS:O	1:D:185:ILE:HG12	2.16	0.45
1:C:276:ILE:HD11	2:G:5:PHE:CZ	2.51	0.45
1:D:127:ARG:HA	1:D:149:HIS:ND1	2.32	0.45
1:D:103:ILE:HB	1:D:179:LEU:HD21	1.98	0.45
1:B:366:ALA:HA	1:B:372:ILE:HD11	2.00	0.44
1:B:62:ILE:HD11	1:B:68:PHE:CE2	2.53	0.44
1:D:372:ILE:HA	1:D:375:VAL:HG22	2.00	0.44
1:D:314:GLU:CD	1:D:317:ARG:HH21	2.21	0.44
1:B:134:VAL:HA	1:B:137:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:GLU:O	1:D:148:GLU:HG2	2.18	0.43
1:A:393:LEU:HD12	1:A:393:LEU:HA	1.77	0.43
1:D:45:LEU:HD23	1:D:245:ILE:HB	2.01	0.43
1:B:364:THR:HG22	1:B:375:VAL:HG21	2.01	0.43
1:C:266:LEU:HD23	1:C:312:PHE:CE1	2.54	0.43
1:A:54:SER:O	1:A:58:LYS:HG3	2.19	0.42
1:B:370:GLU:OE2	1:B:373:ARG:NH1	2.51	0.42
1:C:287:VAL:O	1:C:359:CYS:HA	2.19	0.42
1:D:204:THR:O	1:D:226:GLY:HA3	2.18	0.42
1:C:259:GLU:OE1	1:C:259:GLU:N	2.52	0.42
1:D:295:ASP:O	1:D:299:GLU:HG3	2.20	0.42
1:D:143:PRO:HG2	1:D:145:GLU:HG2	2.01	0.42
1:A:293:LYS:HD3	1:A:296:LEU:HD12	2.02	0.41
1:C:92:VAL:HG22	1:C:192:PRO:HD3	2.01	0.41
1:D:92:VAL:HG13	1:D:190:TYR:HD2	1.84	0.41
1:D:304:GLY:HA2	1:D:307:LYS:NZ	2.35	0.41
1:D:293:LYS:HG2	3:D:401:GDP:C6	2.55	0.41
1:D:126:PHE:CE2	1:D:149:HIS:HE1	2.39	0.41
1:C:391:TYR:O	5:C:501:HOH:O	2.22	0.41
1:C:273:PHE:HE1	1:C:287:VAL:HG11	1.85	0.41
1:C:286:SER:HA	1:C:357:HIS:HB2	2.01	0.41
1:D:54:SER:O	1:D:58:LYS:HG3	2.20	0.41
1:C:99:LEU:HD11	1:C:182:ILE:HG12	2.01	0.41
2:G:3:ILE:HG22	2:G:14:CYS:HB3	2.02	0.41
1:D:308:ILE:HB	1:D:315:PHE:CD2	2.56	0.40
1:D:309:GLU:HG3	1:D:315:PHE:HD2	1.85	0.40
1:C:61:ARG:HA	1:C:65:VAL:HG23	2.03	0.40
1:C:108:ALA:HB2	1:C:135:MET:HE1	2.03	0.40
1:D:145:GLU:O	1:D:149:HIS:CD2	2.73	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	332/348 (95%)	325 (98%)	6 (2%)	1 (0%)	41	30
1	B	318/348 (91%)	311 (98%)	6 (2%)	1 (0%)	41	30
1	C	326/348 (94%)	318 (98%)	7 (2%)	1 (0%)	41	30
1	D	311/348 (89%)	299 (96%)	11 (4%)	1 (0%)	41	30
2	E	14/17 (82%)	13 (93%)	1 (7%)	0	100	100
2	F	14/17 (82%)	14 (100%)	0	0	100	100
2	G	14/17 (82%)	14 (100%)	0	0	100	100
2	H	14/17 (82%)	13 (93%)	0	1 (7%)	1	0
All	All	1343/1460 (92%)	1307 (97%)	31 (2%)	5 (0%)	34	22

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	15	GLY
1	B	65	VAL
1	D	303	ALA
1	A	65	VAL
1	C	65	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	304/312 (97%)	303 (100%)	1 (0%)	92	92
1	B	292/312 (94%)	290 (99%)	2 (1%)	84	82
1	C	299/312 (96%)	295 (99%)	4 (1%)	69	65
1	D	287/312 (92%)	284 (99%)	3 (1%)	76	74
2	E	12/12 (100%)	12 (100%)	0	100	100
2	F	12/12 (100%)	12 (100%)	0	100	100
2	G	12/12 (100%)	12 (100%)	0	100	100
2	H	12/12 (100%)	12 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1230/1296 (95%)	1220 (99%)	10 (1%)	81	80

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	228	ARG
1	B	223	ASP
1	B	333	ARG
1	C	223	ASP
1	C	228	ARG
1	C	248	VAL
1	C	357	HIS
1	D	213	GLN
1	D	232	ARG
1	D	307	LYS

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	$\# Z > 2$
2	DTY	G	1	2	11,12,13	0.38	0	12,15,17	0.28	0
2	DTY	F	1	2	11,12,13	0.43	0	12,15,17	0.29	0
2	DTY	H	1	2	11,12,13	0.48	0	12,15,17	0.17	0
2	DTY	E	1	2	11,12,13	0.38	0	12,15,17	0.51	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DTY	G	1	2	-	0/5/6/8	0/1/1/1
2	DTY	F	1	2	-	0/5/6/8	0/1/1/1
2	DTY	H	1	2	-	0/5/6/8	0/1/1/1
2	DTY	E	1	2	-	0/5/6/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\# Z > 2$
3	GDP	C	401	-	24,30,30	4.64	14 (58%)	31,47,47	3.02	10 (32%)
3	GDP	B	401	-	24,30,30	4.65	14 (58%)	31,47,47	3.02	9 (29%)
3	GDP	D	401	-	24,30,30	4.72	16 (66%)	31,47,47	3.02	7 (22%)
3	GDP	A	401	-	24,30,30	4.57	14 (58%)	31,47,47	2.88	8 (25%)

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
3	GDP	C	401	-	-	2/12/32/32	0/3/3/3
3	GDP	B	401	-	-	3/12/32/32	0/3/3/3
3	GDP	D	401	-	-	2/12/32/32	0/3/3/3
3	GDP	A	401	-	-	2/12/32/32	0/3/3/3

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	GDP	C2'-C3'	-10.51	1.24	1.53
3	D	401	GDP	C2'-C3'	-10.51	1.24	1.53
3	B	401	GDP	C2'-C3'	-10.28	1.25	1.53
3	A	401	GDP	C2'-C3'	-10.28	1.25	1.53
3	B	401	GDP	O4'-C1'	-8.24	1.29	1.41
3	D	401	GDP	O4'-C1'	-8.23	1.29	1.41
3	A	401	GDP	O4'-C1'	-7.95	1.30	1.41
3	C	401	GDP	O4'-C1'	-7.88	1.30	1.41
3	D	401	GDP	C5-C6	7.63	1.54	1.41
3	B	401	GDP	C5-C6	7.44	1.54	1.41
3	D	401	GDP	C4-N3	7.29	1.47	1.35
3	A	401	GDP	C4-N3	7.27	1.47	1.35
3	B	401	GDP	C4-N3	7.22	1.47	1.35
3	C	401	GDP	C2-N2	7.17	1.48	1.33
3	C	401	GDP	C4-N3	7.15	1.46	1.35
3	A	401	GDP	C5-C6	7.14	1.53	1.41
3	C	401	GDP	C5-C6	7.14	1.53	1.41
3	D	401	GDP	C2'-C1'	7.10	1.64	1.53
3	D	401	GDP	C2-N2	7.05	1.48	1.33
3	B	401	GDP	C2-N2	7.03	1.48	1.33
3	A	401	GDP	C2-N2	6.95	1.47	1.33
3	C	401	GDP	C2'-C1'	6.80	1.64	1.53
3	B	401	GDP	C2'-C1'	6.62	1.63	1.53
3	A	401	GDP	C2'-C1'	6.53	1.63	1.53
3	B	401	GDP	C6-N1	5.43	1.42	1.33
3	C	401	GDP	C6-N1	5.41	1.42	1.33
3	D	401	GDP	C6-N1	5.33	1.42	1.33
3	A	401	GDP	C6-N1	5.21	1.42	1.33
3	D	401	GDP	C2-N1	4.86	1.44	1.35
3	C	401	GDP	C2-N1	4.85	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	GDP	C2-N1	4.80	1.43	1.35
3	C	401	GDP	O6-C6	-4.78	1.12	1.24
3	D	401	GDP	O6-C6	-4.72	1.12	1.24
3	D	401	GDP	O3'-C3'	4.69	1.54	1.43
3	B	401	GDP	O3'-C3'	4.67	1.54	1.43
3	A	401	GDP	O6-C6	-4.58	1.13	1.24
3	A	401	GDP	C2-N1	4.55	1.43	1.35
3	A	401	GDP	O3'-C3'	4.55	1.53	1.43
3	B	401	GDP	O6-C6	-4.54	1.13	1.24
3	C	401	GDP	O3'-C3'	4.35	1.53	1.43
3	B	401	GDP	C5'-C4'	-3.98	1.39	1.51
3	C	401	GDP	C5'-C4'	-3.83	1.39	1.51
3	A	401	GDP	C5'-C4'	-3.83	1.39	1.51
3	D	401	GDP	C5'-C4'	-3.73	1.40	1.51
3	D	401	GDP	C3'-C4'	3.19	1.61	1.53
3	B	401	GDP	C3'-C4'	3.10	1.60	1.53
3	A	401	GDP	C3'-C4'	3.09	1.60	1.53
3	C	401	GDP	C3'-C4'	3.07	1.60	1.53
3	D	401	GDP	PA-O5'	2.60	1.69	1.59
3	C	401	GDP	C5-C4	-2.45	1.34	1.40
3	A	401	GDP	PA-O5'	2.36	1.68	1.59
3	C	401	GDP	PA-O5'	2.35	1.68	1.59
3	D	401	GDP	C5-C4	-2.34	1.34	1.40
3	B	401	GDP	PA-O5'	2.31	1.68	1.59
3	B	401	GDP	C5-C4	-2.29	1.34	1.40
3	A	401	GDP	C5-C4	-2.24	1.35	1.40
3	D	401	GDP	O2'-C2'	2.08	1.47	1.43
3	D	401	GDP	C2-N3	2.04	1.44	1.34

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	GDP	C1'-N9-C4	14.04	151.30	126.64
3	B	401	GDP	C1'-N9-C4	13.38	150.16	126.64
3	C	401	GDP	C1'-N9-C4	13.18	149.80	126.64
3	A	401	GDP	C1'-N9-C4	12.59	148.75	126.64
3	C	401	GDP	N3-C2-N1	-4.89	120.70	127.22
3	B	401	GDP	N3-C2-N1	-4.72	120.93	127.22
3	A	401	GDP	N3-C2-N1	-4.70	120.96	127.22
3	D	401	GDP	N3-C2-N1	-4.62	121.05	127.22
3	A	401	GDP	C5-C6-N1	-4.52	117.25	123.43
3	B	401	GDP	C5-C6-N1	-4.35	117.48	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	GDP	C5-C6-N1	-4.07	117.87	123.43
3	D	401	GDP	C5-C6-N1	-4.06	117.88	123.43
3	A	401	GDP	C2-N1-C6	3.71	121.83	115.93
3	B	401	GDP	C2-N1-C6	3.45	121.41	115.93
3	C	401	GDP	C2-N1-C6	3.31	121.19	115.93
3	C	401	GDP	N2-C2-N1	3.30	122.39	117.25
3	C	401	GDP	PA-O3A-PB	-3.25	121.69	132.83
3	D	401	GDP	C2-N1-C6	3.13	120.90	115.93
3	B	401	GDP	N2-C2-N1	3.07	122.03	117.25
3	B	401	GDP	C4-C5-N7	-2.89	106.38	109.40
3	D	401	GDP	C4-C5-N7	-2.85	106.43	109.40
3	D	401	GDP	N2-C2-N1	2.85	121.68	117.25
3	A	401	GDP	C4-C5-N7	-2.68	106.60	109.40
3	D	401	GDP	PA-O3A-PB	-2.45	124.41	132.83
3	C	401	GDP	C4-C5-N7	-2.43	106.87	109.40
3	B	401	GDP	PA-O3A-PB	-2.40	124.59	132.83
3	A	401	GDP	O3'-C3'-C4'	-2.37	104.20	111.05
3	A	401	GDP	N2-C2-N1	2.35	120.90	117.25
3	C	401	GDP	C2'-C3'-C4'	2.33	107.17	102.64
3	C	401	GDP	C4-C5-C6	-2.32	118.58	120.80
3	A	401	GDP	PA-O3A-PB	-2.25	125.10	132.83
3	B	401	GDP	C2'-C3'-C4'	2.13	106.78	102.64
3	C	401	GDP	O3'-C3'-C4'	-2.09	104.99	111.05
3	B	401	GDP	C4-C5-C6	-2.08	118.81	120.80

There are no chirality outliers.

All (9) torsion outliers are listed below:

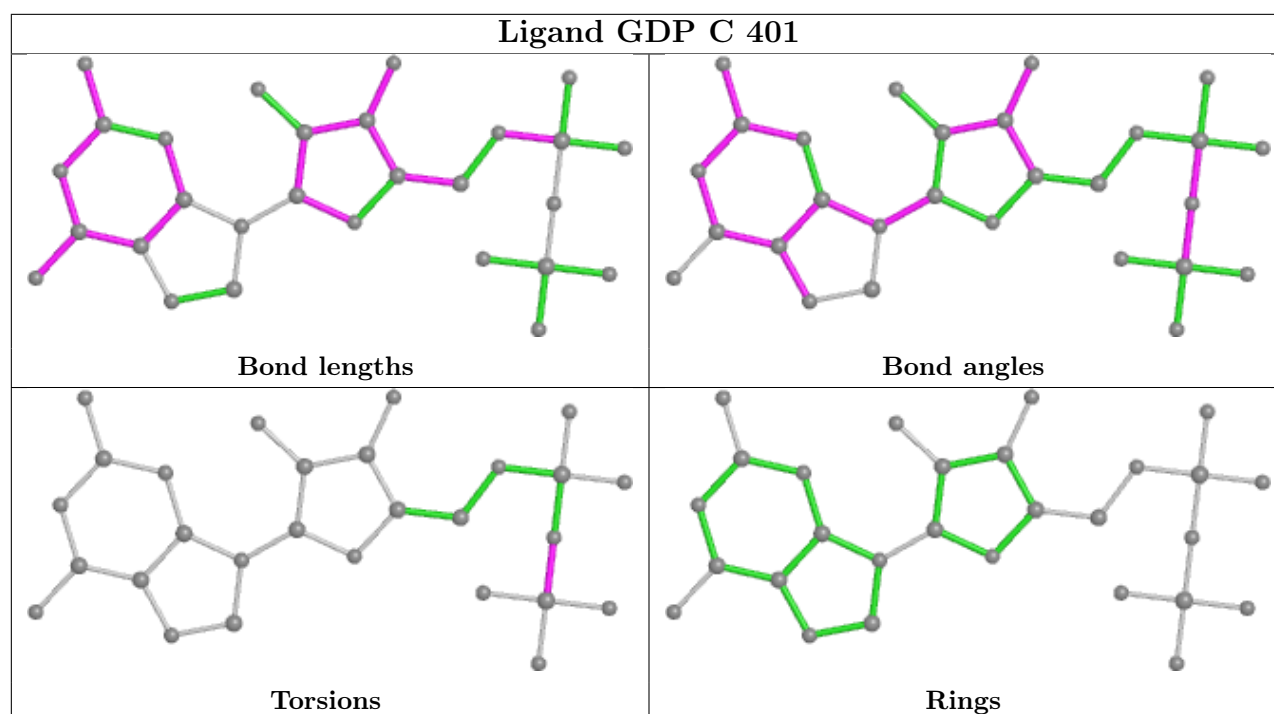
Mol	Chain	Res	Type	Atoms
3	B	401	GDP	PA-O3A-PB-O3B
3	D	401	GDP	PA-O3A-PB-O2B
3	D	401	GDP	PA-O3A-PB-O3B
3	C	401	GDP	PA-O3A-PB-O1B
3	C	401	GDP	PA-O3A-PB-O2B
3	B	401	GDP	PA-O3A-PB-O1B
3	A	401	GDP	PA-O3A-PB-O2B
3	A	401	GDP	PA-O3A-PB-O3B
3	B	401	GDP	PA-O3A-PB-O2B

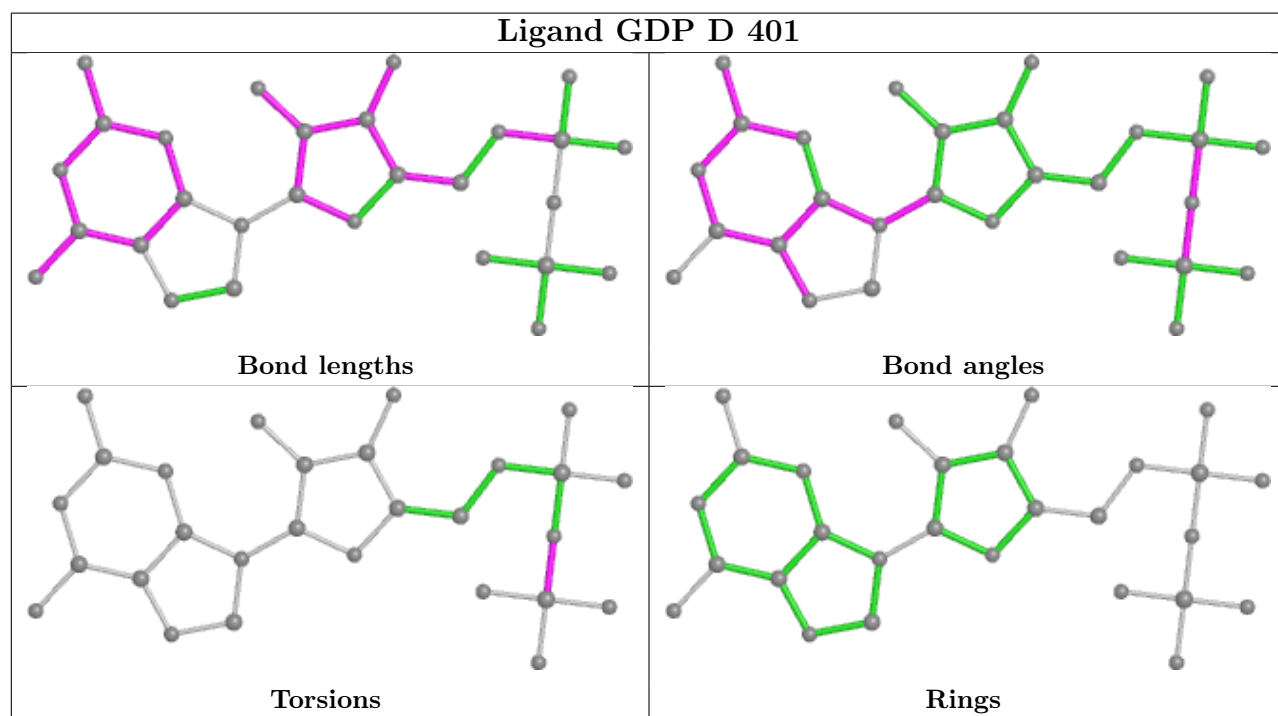
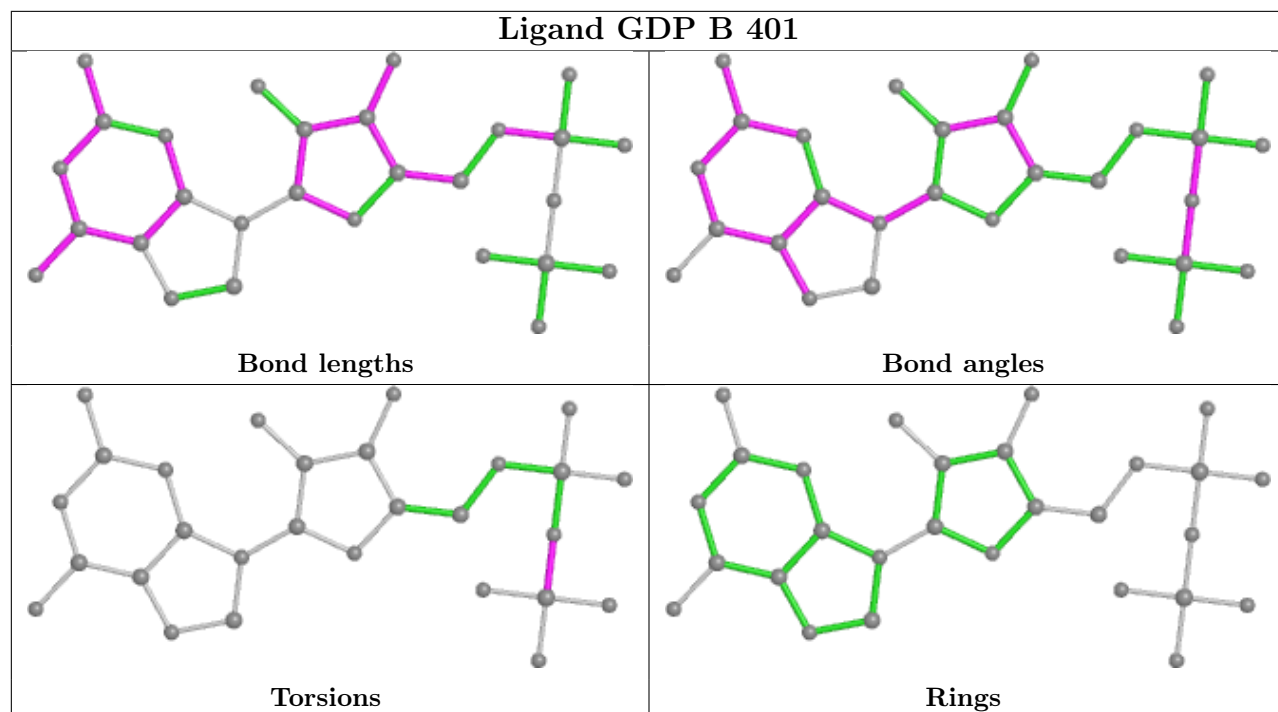
There are no ring outliers.

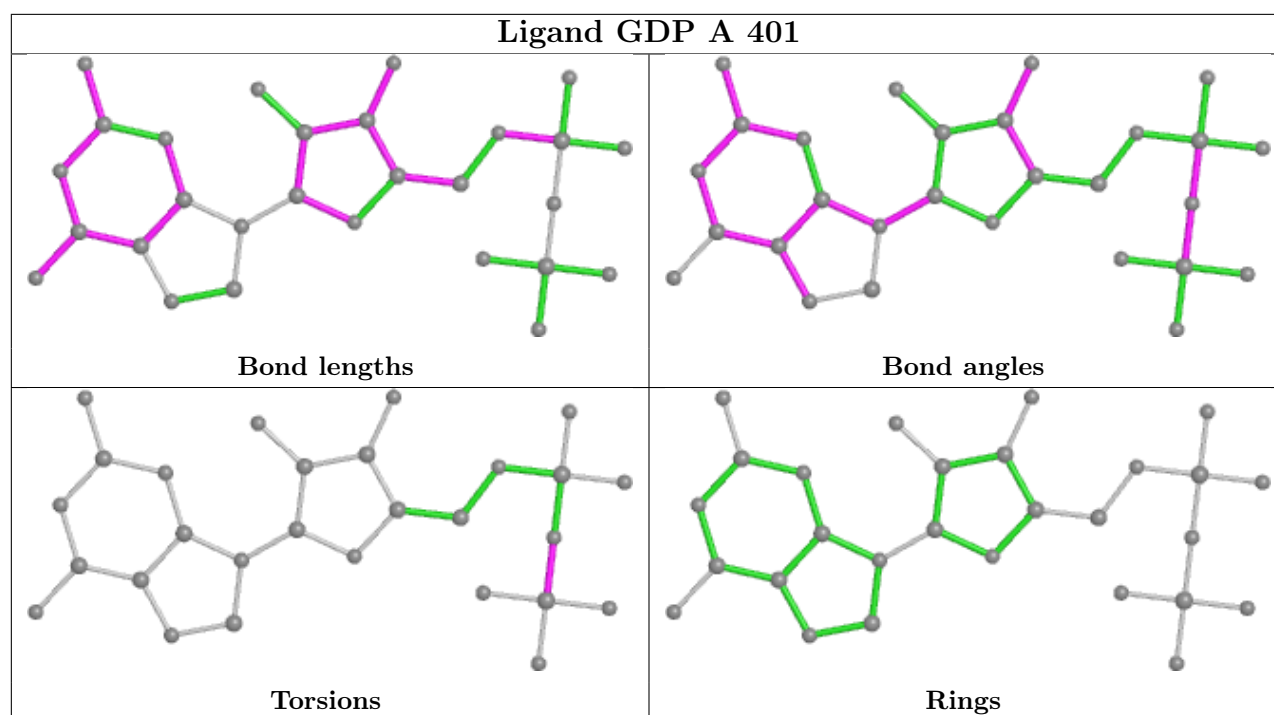
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	401	GDP	1	0
3	B	401	GDP	1	0
3	D	401	GDP	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 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 ⓘ

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, 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	338/348 (97%)	0.15	7 (2%) 63 72	5, 19, 42, 64	0
1	B	324/348 (93%)	0.26	13 (4%) 38 48	7, 24, 50, 68	0
1	C	332/348 (95%)	0.22	10 (3%) 50 59	10, 25, 50, 83	0
1	D	317/348 (91%)	1.03	54 (17%) 1 2	19, 44, 69, 91	0
2	E	14/17 (82%)	0.22	1 (7%) 16 24	5, 9, 25, 39	0
2	F	14/17 (82%)	0.10	1 (7%) 16 24	8, 12, 24, 48	0
2	G	14/17 (82%)	0.28	1 (7%) 16 24	13, 19, 45, 53	0
2	H	14/17 (82%)	0.18	1 (7%) 16 24	18, 23, 37, 52	0
All	All	1367/1460 (93%)	0.40	88 (6%) 19 28	5, 26, 59, 91	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	358	TYR	9.1
1	D	39	ALA	8.2
1	A	394	LEU	8.2
1	D	328	PRO	7.4
1	D	384	GLN	7.0
1	B	39	ALA	6.9
1	B	358	TYR	5.7
1	D	222	PHE	5.0
1	C	328	PRO	4.8
1	D	66	ASN	4.7
1	A	356	ARG	4.1
1	D	214	VAL	4.0
1	D	317	ARG	3.9
1	C	326	PRO	3.8
1	D	316	ALA	3.8
1	B	387	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	148	GLU	3.5
2	H	15	GLY	3.5
1	D	215	ASP	3.5
1	B	384	GLN	3.4
1	D	329	GLY	3.4
1	D	219	PHE	3.3
1	D	194	ASP	3.3
1	D	359	CYS	3.3
1	B	216	LYS	3.3
1	D	185	ILE	3.2
1	C	358	TYR	3.2
1	B	215	ASP	3.2
1	D	90	THR	3.2
1	D	217	VAL	3.2
1	D	204	THR	3.1
1	D	327	GLU	3.1
1	D	189	ASP	3.1
1	D	203	LEU	3.1
1	A	70	GLY	3.1
1	D	323	ASP	2.9
1	D	205	SER	2.9
1	D	314	GLU	2.9
1	D	67	GLY	2.9
1	D	99	LEU	2.8
1	B	204	THR	2.7
1	C	327	GLU	2.7
1	D	190	TYR	2.7
1	B	40	THR	2.7
1	D	159	VAL	2.7
1	D	141	ASP	2.6
1	D	383	ILE	2.6
1	D	92	VAL	2.6
1	D	186	LYS	2.6
1	D	319	THR	2.5
1	D	113	LEU	2.5
1	C	323	ASP	2.5
1	B	386	MET	2.5
1	D	334	VAL	2.5
1	C	135	MET	2.5
1	D	178	PHE	2.5
1	B	352	SER	2.5
2	F	15	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	197	LEU	2.4
1	D	40	THR	2.4
1	A	352	SER	2.4
1	A	38	ARG	2.4
1	B	206	GLY	2.4
2	G	15	GLY	2.4
1	D	192	PRO	2.3
1	D	381	ASP	2.3
2	E	15	GLY	2.3
1	B	68	PHE	2.3
1	D	65	VAL	2.3
1	D	179	LEU	2.3
1	D	63	LEU	2.3
1	D	332	PRO	2.2
1	C	329	GLY	2.2
1	D	119	LEU	2.2
1	B	322	GLU	2.2
1	C	38	ARG	2.2
1	D	41	HIS	2.2
1	D	183	ASP	2.2
1	D	376	PHE	2.1
1	C	216	LYS	2.1
1	A	358	TYR	2.1
1	C	204	THR	2.1
1	D	382	ILE	2.1
1	D	122	PRO	2.0
1	D	335	THR	2.0
1	A	114	VAL	2.0
1	D	191	VAL	2.0
1	D	288	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	DTY	E	1	12/13	0.93	0.14	11,15,24,33	0
2	DTY	F	1	12/13	0.94	0.11	11,16,19,36	0
2	DTY	G	1	12/13	0.94	0.10	19,24,27,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	DTY	H	1	12/13	0.95	0.09	15,28,36,44	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

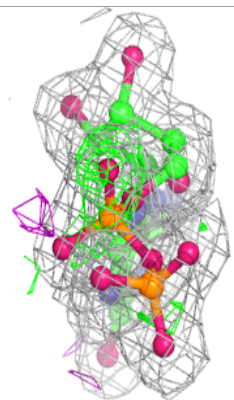
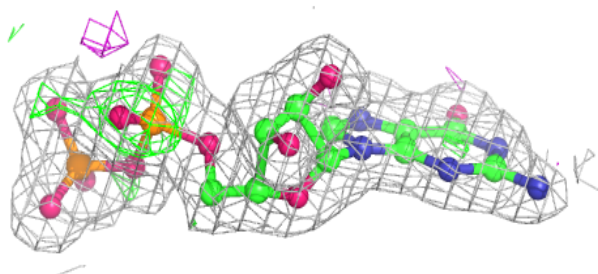
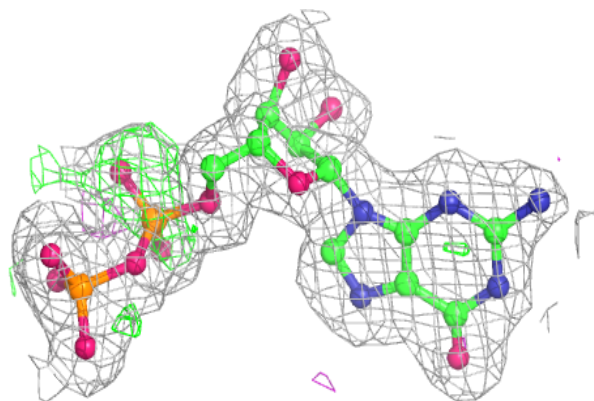
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GDP	C	401	28/28	0.94	0.15	7,10,27,62	0
3	GDP	D	401	28/28	0.96	0.11	17,30,41,46	0
3	GDP	A	401	28/28	0.97	0.12	2,5,8,12	0
3	GDP	B	401	28/28	0.98	0.10	5,9,17,21	0
4	CL	D	402	1/1	0.98	0.05	31,31,31,31	0
4	CL	B	402	1/1	0.99	0.04	14,14,14,14	0
4	CL	C	402	1/1	0.99	0.05	19,19,19,19	0
4	CL	A	402	1/1	0.99	0.05	12,12,12,12	0

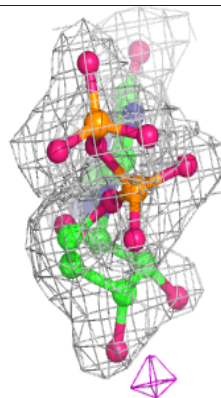
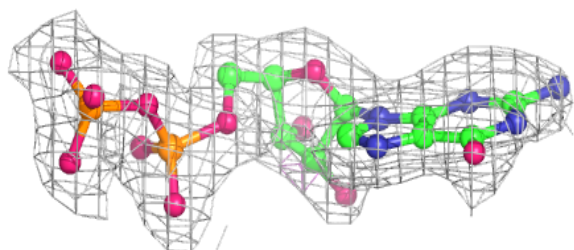
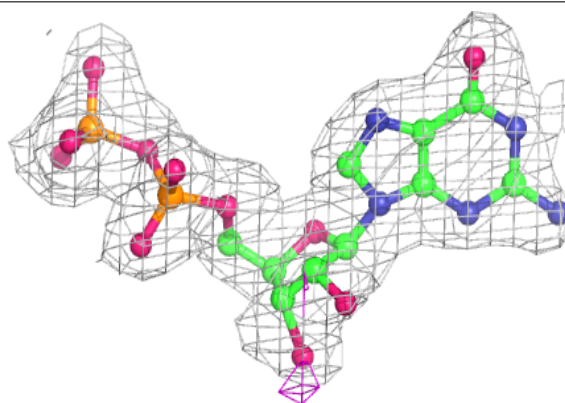
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP 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)

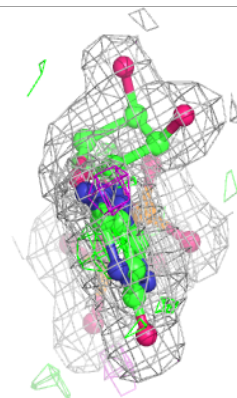
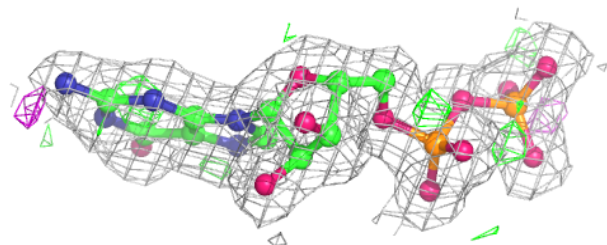
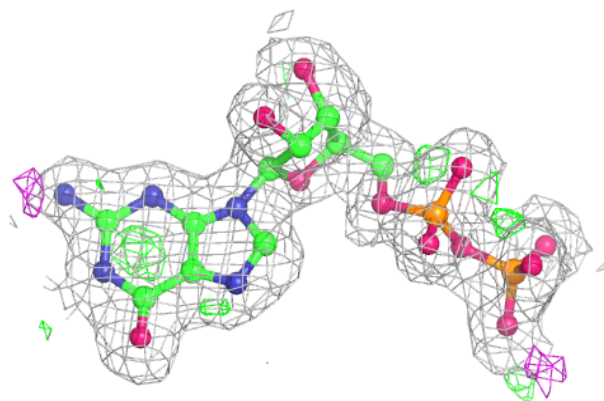
**Electron density around GDP D 401:**

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

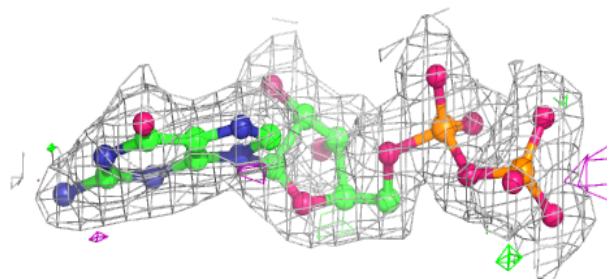
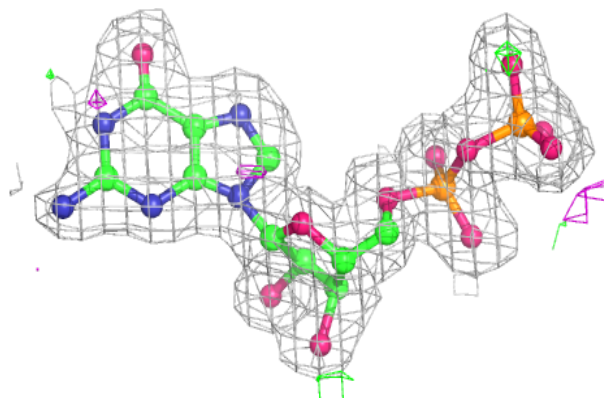


Electron density around GDP A 401:

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

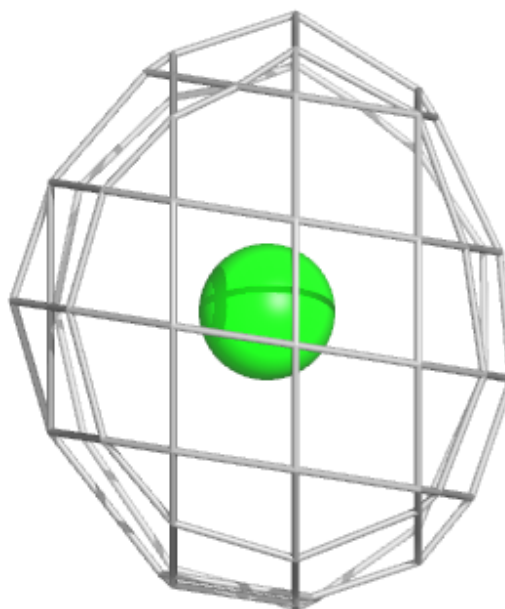
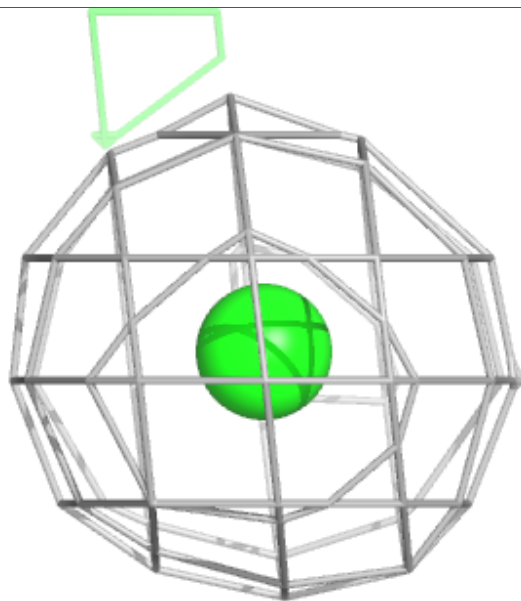
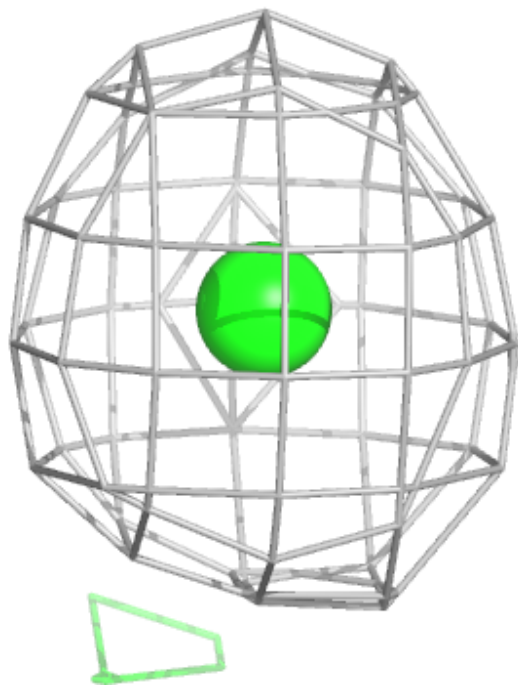
**Electron density around GDP B 401:**

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



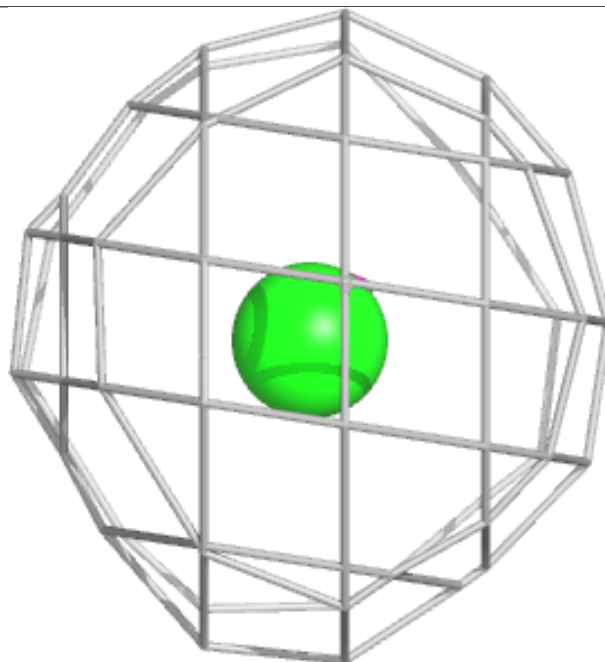
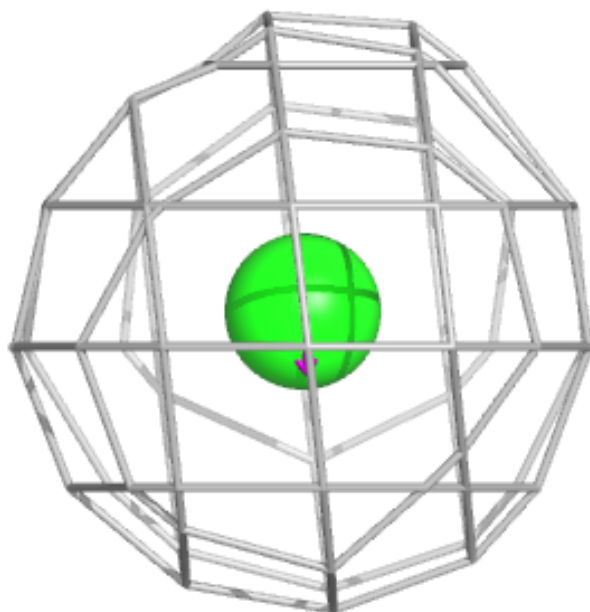
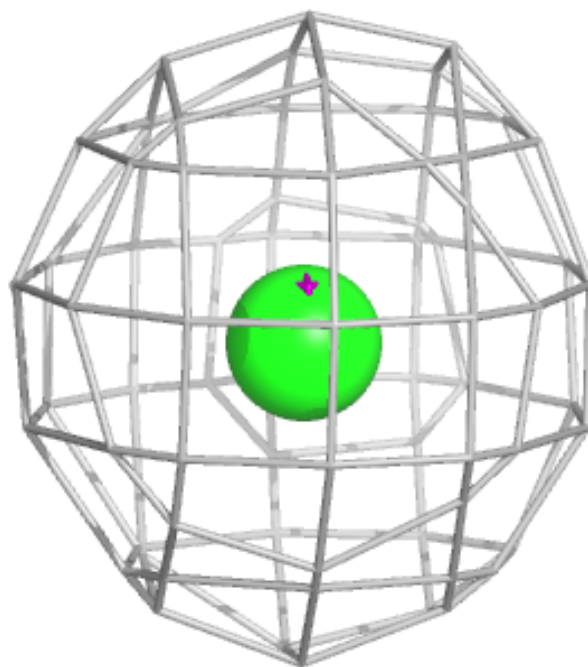
Electron density around CL D 402:

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



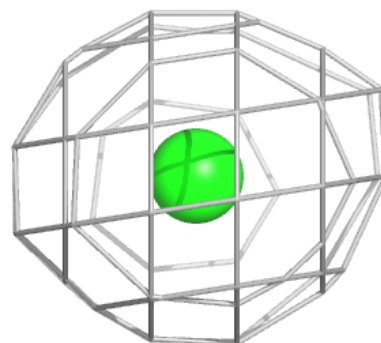
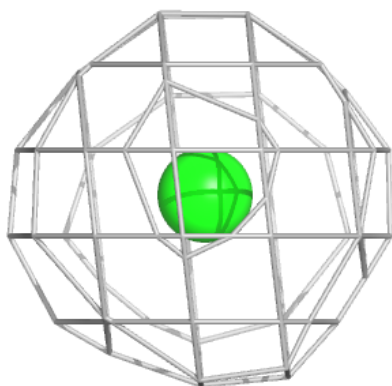
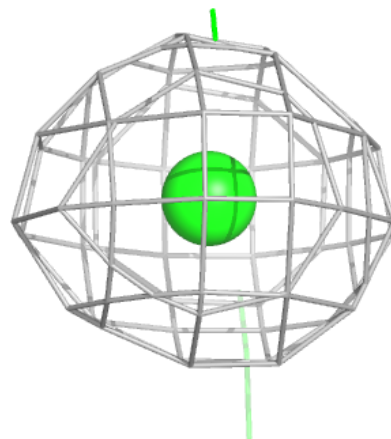
Electron density around CL B 402:

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



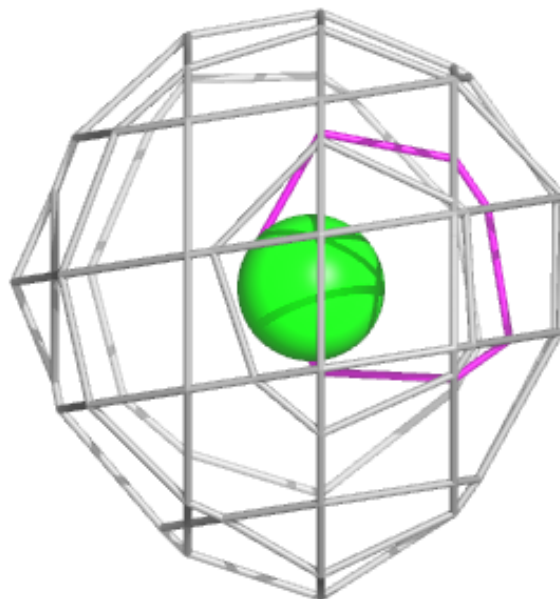
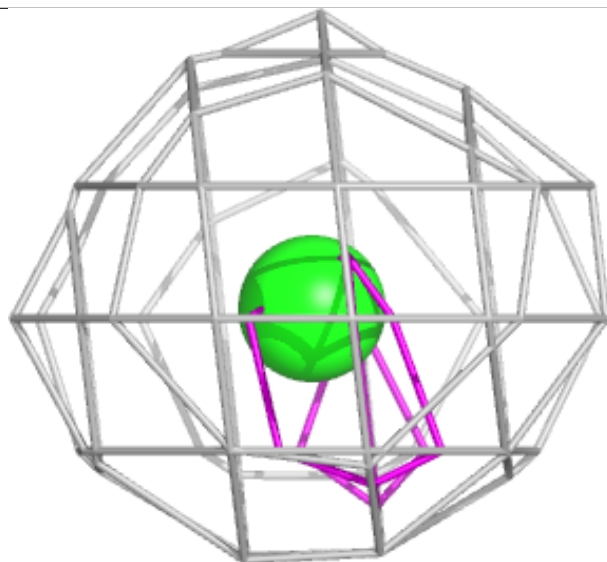
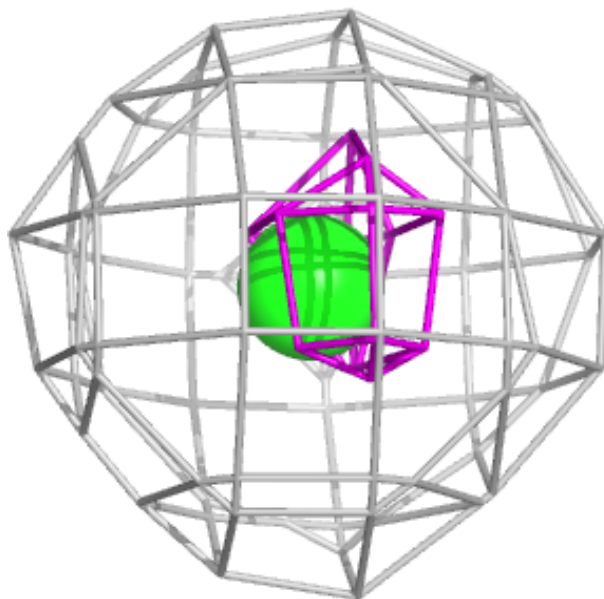
Electron density around CL C 402:

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



Electron density around CL 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.