



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:08 PM UTC

PDB ID : 7E5E / pdb_00007e5e
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

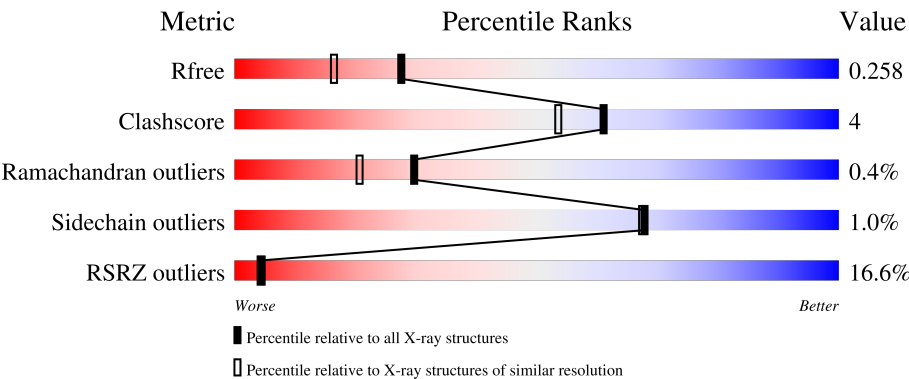
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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.



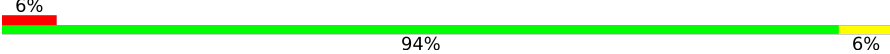
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	7% 90% 7% .
1	B	348	10% 84% 9% 7%
1	C	348	10% 84% 11% 5%
1	D	348	36% 76% 15% 9%
2	E	17	6% 100%

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Mol	Chain	Length	Quality of chain
2	F	17	
2	G	17	
2	H	17	

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			

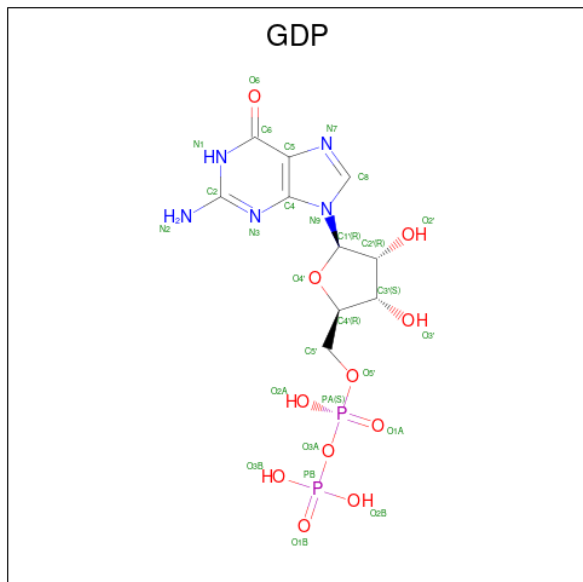
There are 8 discrepancies between the modelled and reference sequences:

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			

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	C	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	B	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		

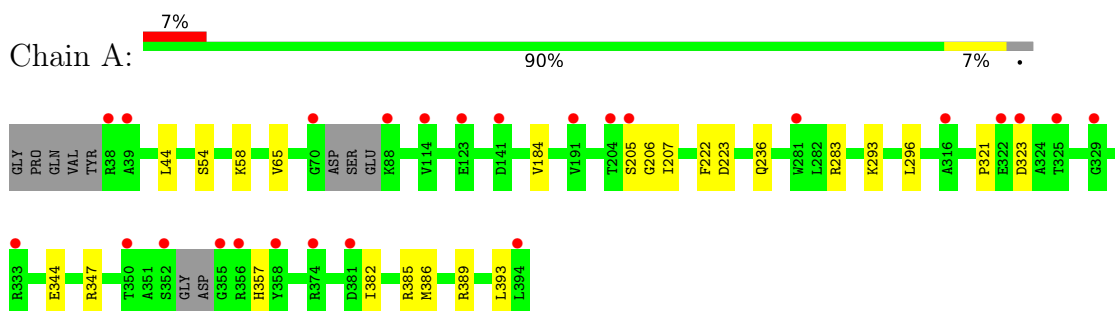
- Molecule 5 is water.

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

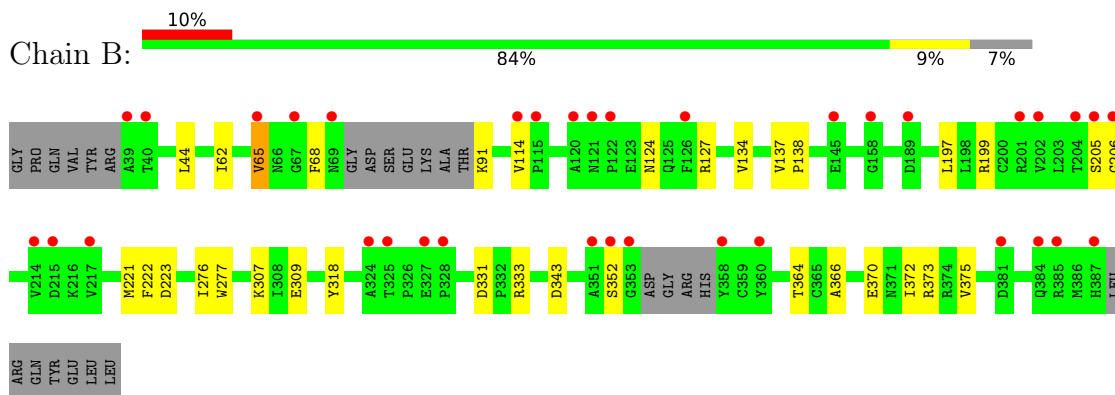
3 Residue-property plots [i](#)

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.

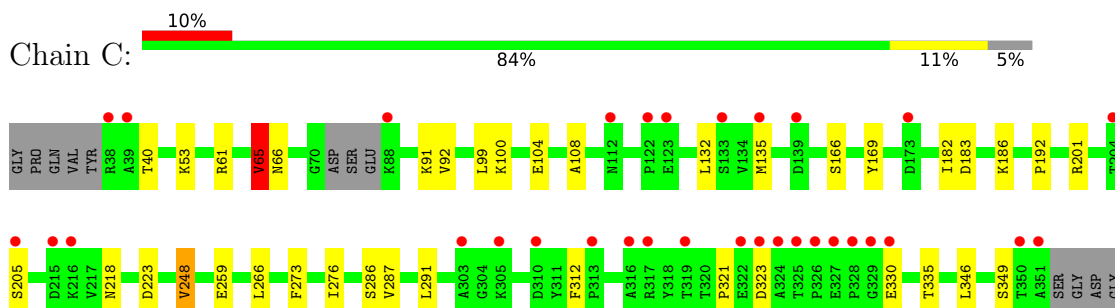
- Molecule 1: Isoform Gnas-2 of Guanine nucleotide-binding protein G(s) subunit alpha isoforms short



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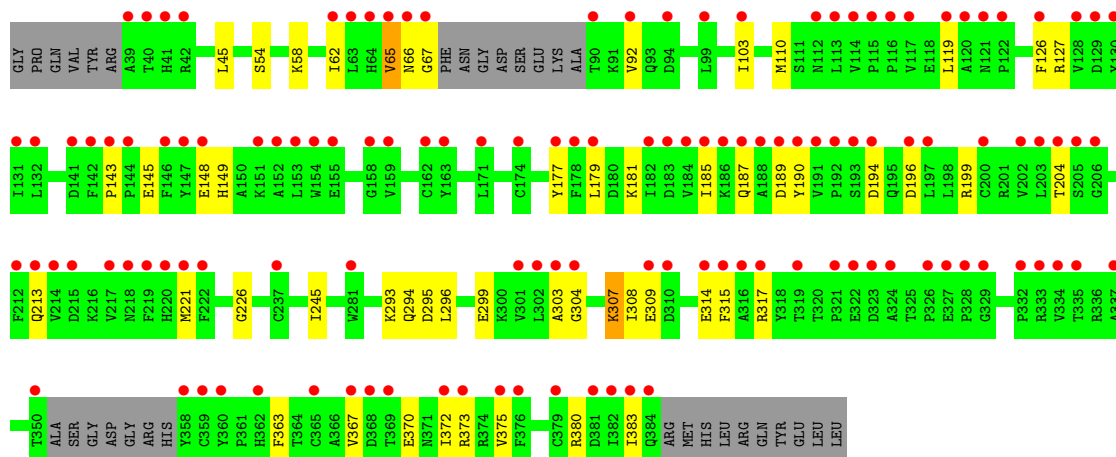
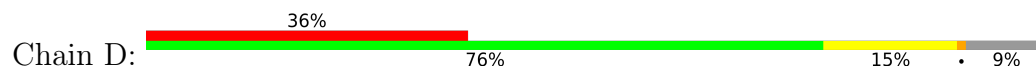


- Molecule 1: Isoform Gnas-2 of Guanine nucleotide-binding protein G(s) subunit alpha isoforms short





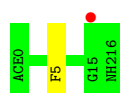
- Molecule 1: Isoform Gnas-2 of Guanine nucleotide-binding protein G(s) subunit alpha isoforms short



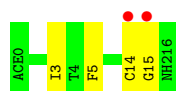
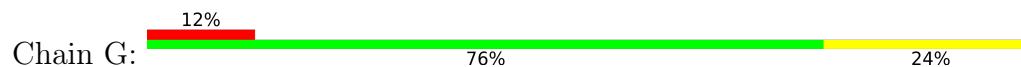
- Molecule 2: GD20



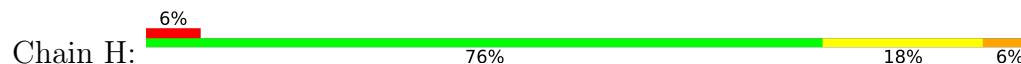
- Molecule 2: GD20

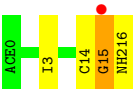


- Molecule 2: GD20



- 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) 81.0 (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 0.217 , 0.258	Depositor DCC
R_{free} test set	4044 reflections (3.96%)	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)	0.32 , 35.0	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: GDP, DTY, NH2, CL, 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	0.18	0/2836	0.39	0/3833
1	B	0.17	0/2711	0.37	0/3668
1	C	0.17	0/2789	0.36	0/3772
1	D	0.13	0/2653	0.34	0/3592
2	E	0.19	0/121	0.45	0/164
2	F	0.18	0/121	0.35	0/164
2	G	0.15	0/121	0.33	0/164
2	H	0.17	0/121	0.33	0/164
All	All	0.16	0/11473	0.36	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	14	0
1	B	2655	0	2604	18	0
1	C	2731	0	2685	27	0
1	D	2599	0	2554	34	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	2	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	94	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 (94) 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: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:C:108:ALA:HB2	1:C:135:MET:HE1	1.84	0.58
1:D:380:ARG:HA	1:D:383:ILE:HD12	1.87	0.57
1:D:370:GLU:CD	1:D:373:ARG:HH21	2.13	0.56
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:VAL:HG13	1:C:291:LEU:HA	1.91	0.52
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:B:91:LYS:HD3	1:B:197:LEU:HD22	1.91	0.52
1:C:104:GLU:HB2	1:C:135:MET:HE2	1.92	0.51
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:D:314:GLU:CD	1:D:317:ARG:HH21	2.21	0.48
1:C:53:LYS:NZ	3:C:401:GDP:O1B	2.45	0.48
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:VAL:HA	1:B:137:VAL:HG13	1.99	0.44
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:C:132:LEU:HA	1:C:135:MET:HE3	2.00	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:110:MET:HE1	1:D:119:LEU:HD23	2.00	0.42
1:D:204:THR:O	1:D:226:GLY:HA3	2.18	0.42
1:C:183:ASP:OD1	1:C:186:LYS:NZ	2.43	0.42
1:D:309:GLU:H	1:D:309:GLU:CD	2.27	0.42
1:B:318:TYR:OH	1:B:343:ASP:OD2	2.30	0.42
1:C:259:GLU:OE1	1:C:259:GLU:N	2.52	0.42
1:C:330:GLU:OE1	1:C:335:THR:OG1	2.36	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:A:382:ILE:HG22	1:A:386:MET:HE3	2.02	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:D:221:MET:HE3	1:D:221:MET:HB2	1.86	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:177:TYR:OH	1:D:196:ASP:OD1	2.36	0.40
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:B:221:MET:HE3	1:B:221:MET:HB2	1.95	0.40
1:C:61:ARG:HA	1:C:65:VAL:HG23	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%)	36	28
1	B	318/348 (91%)	311 (98%)	6 (2%)	1 (0%)	36	28
1	C	326/348 (94%)	318 (98%)	7 (2%)	1 (0%)	36	28
1	D	311/348 (89%)	299 (96%)	11 (4%)	1 (0%)	36	28
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%)	30	21

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%)	86	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	292/312 (94%)	289 (99%)	3 (1%)	68	67
1	C	299/312 (96%)	295 (99%)	4 (1%)	61	58
1	D	287/312 (92%)	283 (99%)	4 (1%)	59	56
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
All	All	1230/1296 (95%)	1218 (99%)	12 (1%)	68	67

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	184	VAL
1	B	65	VAL
1	B	114	VAL
1	B	223	ASP
1	C	65	VAL
1	C	205	SER
1	C	223	ASP
1	C	248	VAL
1	D	65	VAL
1	D	194	ASP
1	D	213	GLN
1	D	307	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	227	GLN
1	A	267	GLN
1	A	294	GLN
1	B	64	HIS
1	B	213	GLN
1	B	227	GLN
1	B	294	GLN
1	C	93	GLN
1	C	213	GLN
1	C	218	ASN

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Mol	Chain	Res	Type
1	C	294	GLN
1	C	384	GLN
1	D	267	GLN
1	D	362	HIS
2	H	11	ASN

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	0.40	0	10,15,17	0.18	0
2	DTY	H	1	2	11,12,13	0.49	0	10,15,17	0.20	0
2	DTY	F	1	2	11,12,13	0.46	0	10,15,17	0.22	0
2	DTY	E	1	2	11,12,13	0.40	0	10,15,17	0.25	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	H	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	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 oligosaccharides 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	A	401	-	29,30,30	3.64	16 (55%)	45,47,47	2.26	12 (26%)
3	GDP	C	401	-	29,30,30	3.65	16 (55%)	45,47,47	2.35	13 (28%)
3	GDP	D	401	-	29,30,30	3.72	16 (55%)	45,47,47	2.37	12 (26%)
3	GDP	B	401	-	29,30,30	3.66	16 (55%)	45,47,47	2.35	13 (28%)

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	A	401	-	-	2/16/32/32	0/3/3/3
3	GDP	C	401	-	-	2/16/32/32	0/3/3/3
3	GDP	D	401	-	-	2/16/32/32	0/3/3/3
3	GDP	B	401	-	-	3/16/32/32	0/3/3/3

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	GDP	C2'-C3'	-10.63	1.24	1.53
3	D	401	GDP	C2'-C3'	-10.62	1.24	1.53
3	B	401	GDP	C2'-C3'	-10.39	1.25	1.53
3	A	401	GDP	C2'-C3'	-10.39	1.25	1.53
3	C	401	GDP	C2-N2	6.01	1.48	1.34
3	D	401	GDP	C2-N2	5.90	1.48	1.34
3	B	401	GDP	C2-N2	5.89	1.48	1.34
3	A	401	GDP	C2-N2	5.82	1.47	1.34
3	C	401	GDP	O6-C6	-5.81	1.12	1.23
3	D	401	GDP	O6-C6	-5.73	1.12	1.23
3	D	401	GDP	C4-N3	5.62	1.47	1.34
3	A	401	GDP	C4-N3	5.60	1.47	1.34
3	B	401	GDP	C4-N3	5.56	1.47	1.34
3	A	401	GDP	O6-C6	-5.55	1.13	1.23
3	C	401	GDP	C4-N3	5.51	1.46	1.34
3	B	401	GDP	O6-C6	-5.50	1.13	1.23
3	B	401	GDP	O4'-C1'	-5.38	1.29	1.42
3	D	401	GDP	O4'-C1'	-5.37	1.29	1.42
3	A	401	GDP	O4'-C1'	-5.20	1.30	1.42
3	C	401	GDP	O4'-C1'	-5.16	1.30	1.42
3	D	401	GDP	PA-O3A	4.58	1.64	1.59
3	D	401	GDP	C2-N3	4.58	1.44	1.33
3	A	401	GDP	C2-N3	4.50	1.44	1.33
3	D	401	GDP	O3'-C3'	4.46	1.54	1.43
3	B	401	GDP	O3'-C3'	4.45	1.54	1.43
3	B	401	GDP	C2-N3	4.44	1.43	1.33
3	C	401	GDP	C2-N3	4.36	1.43	1.33
3	A	401	GDP	O3'-C3'	4.33	1.53	1.43
3	A	401	GDP	PA-O3A	4.21	1.64	1.59
3	C	401	GDP	O3'-C3'	4.14	1.53	1.43
3	B	401	GDP	C5'-C4'	-4.11	1.39	1.51
3	C	401	GDP	C5'-C4'	-3.96	1.39	1.51
3	A	401	GDP	C5'-C4'	-3.96	1.39	1.51
3	B	401	GDP	PA-O3A	3.88	1.63	1.59
3	D	401	GDP	C5'-C4'	-3.86	1.40	1.51
3	A	401	GDP	C4-N9	-3.76	1.28	1.38
3	C	401	GDP	C4-N9	-3.71	1.28	1.38
3	B	401	GDP	C4-N9	-3.64	1.28	1.38
3	C	401	GDP	PA-O3A	3.58	1.63	1.59
3	D	401	GDP	C2'-C1'	3.52	1.64	1.53
3	D	401	GDP	C4-N9	-3.40	1.29	1.38
3	C	401	GDP	C2'-C1'	3.37	1.64	1.53
3	B	401	GDP	C2'-C1'	3.29	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	GDP	C2'-C1'	3.24	1.63	1.53
3	D	401	GDP	C3'-C4'	3.22	1.61	1.53
3	B	401	GDP	C3'-C4'	3.13	1.60	1.53
3	A	401	GDP	C3'-C4'	3.11	1.60	1.53
3	C	401	GDP	C3'-C4'	3.09	1.60	1.53
3	D	401	GDP	C5-N7	-3.07	1.32	1.39
3	A	401	GDP	C5-N7	-3.02	1.33	1.39
3	B	401	GDP	C5-N7	-2.99	1.33	1.39
3	C	401	GDP	C5-N7	-2.89	1.33	1.39
3	D	401	GDP	C5-C6	2.71	1.54	1.44
3	D	401	GDP	PA-O5'	2.66	1.69	1.59
3	D	401	GDP	C2-N1	2.64	1.44	1.37
3	C	401	GDP	C2-N1	2.63	1.44	1.37
3	B	401	GDP	C5-C6	2.62	1.54	1.44
3	B	401	GDP	C2-N1	2.60	1.43	1.37
3	A	401	GDP	C5-C6	2.48	1.53	1.44
3	C	401	GDP	C5-C6	2.48	1.53	1.44
3	A	401	GDP	C2-N1	2.41	1.43	1.37
3	A	401	GDP	PA-O5'	2.41	1.68	1.59
3	C	401	GDP	PA-O5'	2.41	1.68	1.59
3	B	401	GDP	PA-O5'	2.36	1.68	1.59

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	GDP	C1'-N9-C8	-9.24	100.49	126.73
3	B	401	GDP	C1'-N9-C8	-8.96	101.27	126.73
3	C	401	GDP	C1'-N9-C8	-8.76	101.85	126.73
3	A	401	GDP	C1'-N9-C8	-8.48	102.63	126.73
3	D	401	GDP	C1'-N9-C4	8.40	151.31	126.49
3	B	401	GDP	C1'-N9-C4	8.01	150.16	126.49
3	C	401	GDP	C1'-N9-C4	7.89	149.80	126.49
3	A	401	GDP	C1'-N9-C4	7.54	148.75	126.49
3	B	401	GDP	N9-C8-N7	-3.61	106.71	113.40
3	D	401	GDP	N9-C8-N7	-3.56	106.81	113.40
3	A	401	GDP	N9-C8-N7	-3.51	106.89	113.40
3	C	401	GDP	N9-C8-N7	-3.47	106.97	113.40
3	D	401	GDP	C2-N3-C4	3.00	117.47	112.30
3	D	401	GDP	C5-C4-N3	-2.96	123.68	128.39
3	A	401	GDP	C4'-O4'-C1'	-2.92	103.01	109.47
3	C	401	GDP	C2-N3-C4	2.90	117.29	112.30
3	D	401	GDP	C4'-O4'-C1'	-2.84	103.19	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	GDP	C2-N3-C4	2.81	117.14	112.30
3	B	401	GDP	C4-C5-N7	-2.71	106.38	110.67
3	D	401	GDP	C4-C5-N7	-2.68	106.42	110.67
3	C	401	GDP	C4'-O4'-C1'	-2.67	103.57	109.47
3	C	401	GDP	N2-C2-N1	2.67	122.39	116.76
3	B	401	GDP	C5-C4-N3	-2.61	124.23	128.39
3	D	401	GDP	C5-C4-N9	2.57	110.26	105.66
3	A	401	GDP	C4-C5-N7	-2.56	106.61	110.67
3	C	401	GDP	C5-C4-N9	2.55	110.23	105.66
3	A	401	GDP	C2-N3-C4	2.55	116.69	112.30
3	B	401	GDP	C5-C4-N9	2.54	110.20	105.66
3	B	401	GDP	C4'-O4'-C1'	-2.52	103.90	109.47
3	C	401	GDP	C5-C4-N3	-2.52	124.38	128.39
3	A	401	GDP	C5-C4-N3	-2.52	124.38	128.39
3	B	401	GDP	N2-C2-N1	2.50	122.03	116.76
3	B	401	GDP	C6-C5-N7	2.48	134.81	130.29
3	A	401	GDP	C5-C4-N9	2.46	110.06	105.66
3	C	401	GDP	C4-C5-N7	-2.40	106.86	110.67
3	A	401	GDP	O3'-C3'-C4'	-2.39	104.20	111.08
3	C	401	GDP	C2'-C3'-C4'	2.36	107.17	102.61
3	C	401	GDP	C6-C5-N7	2.35	134.56	130.29
3	D	401	GDP	C6-C5-N7	2.34	134.56	130.29
3	D	401	GDP	N2-C2-N1	2.33	121.68	116.76
3	D	401	GDP	C2-N1-C6	-2.32	120.90	125.11
3	A	401	GDP	C6-C5-N7	2.32	134.51	130.29
3	D	401	GDP	C8-N7-C5	2.31	108.38	104.26
3	B	401	GDP	C8-N7-C5	2.24	108.25	104.26
3	A	401	GDP	C2'-C1'-N9	2.24	119.47	113.25
3	C	401	GDP	C2-N1-C6	-2.16	121.19	125.11
3	B	401	GDP	C2'-C3'-C4'	2.16	106.78	102.61
3	C	401	GDP	O3'-C3'-C4'	-2.12	104.99	111.08
3	A	401	GDP	C8-N7-C5	2.06	107.94	104.26
3	B	401	GDP	C2-N1-C6	-2.04	121.41	125.11

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

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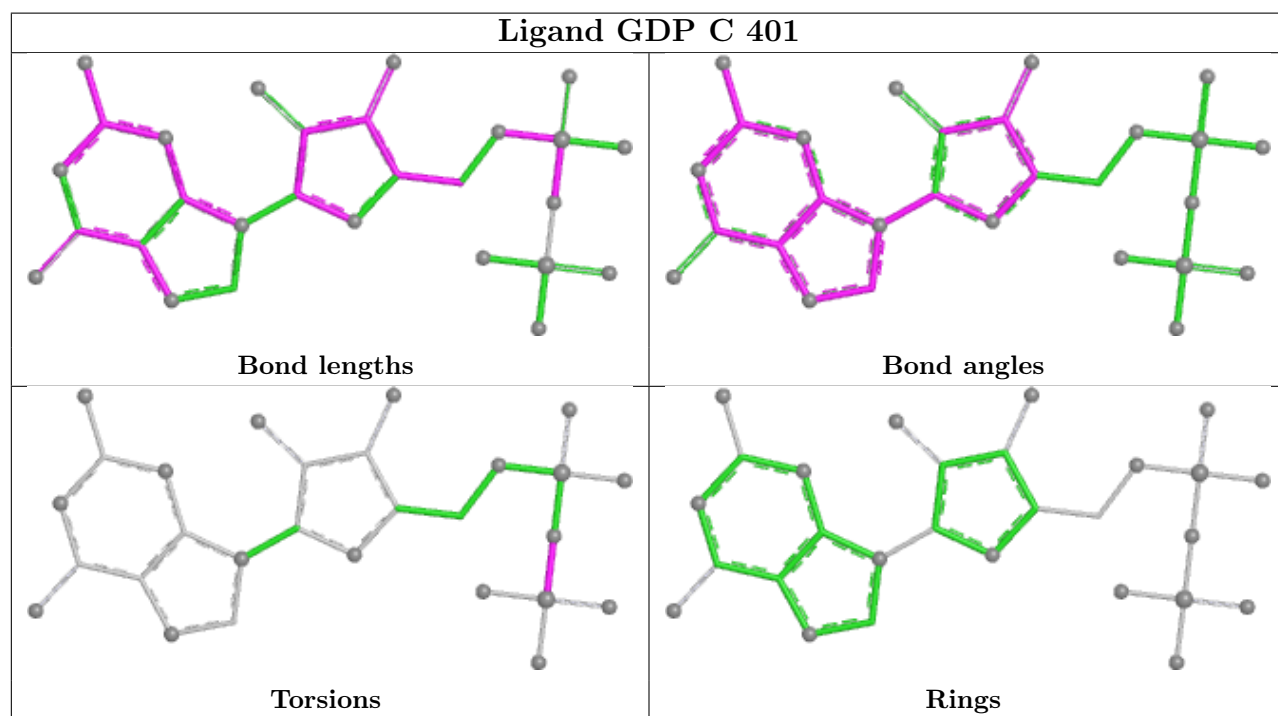
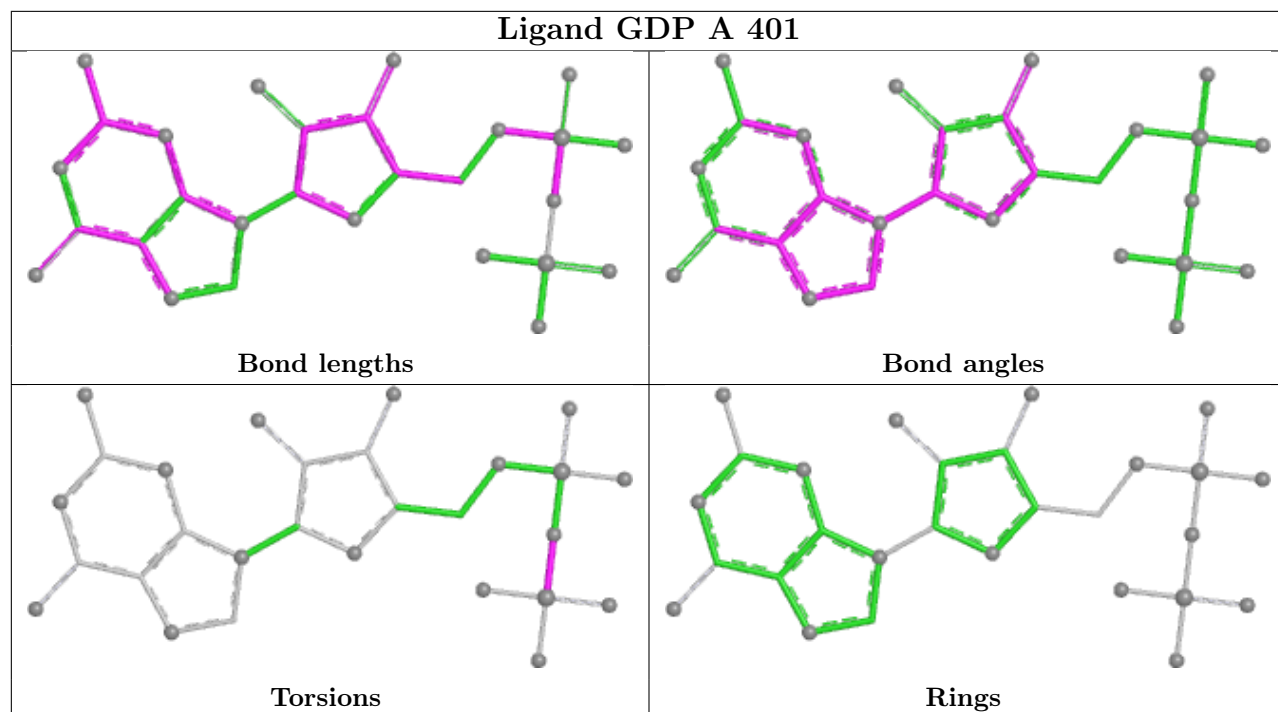
Mol	Chain	Res	Type	Atoms
3	C	401	GDP	PA-O3A-PB-O2B
3	B	401	GDP	PA-O3A-PB-O1B
3	A	401	GDP	PA-O3A-PB-O2B
3	A	401	GDP	PA-O3A-PB-O3B
3	B	401	GDP	PA-O3A-PB-O2B

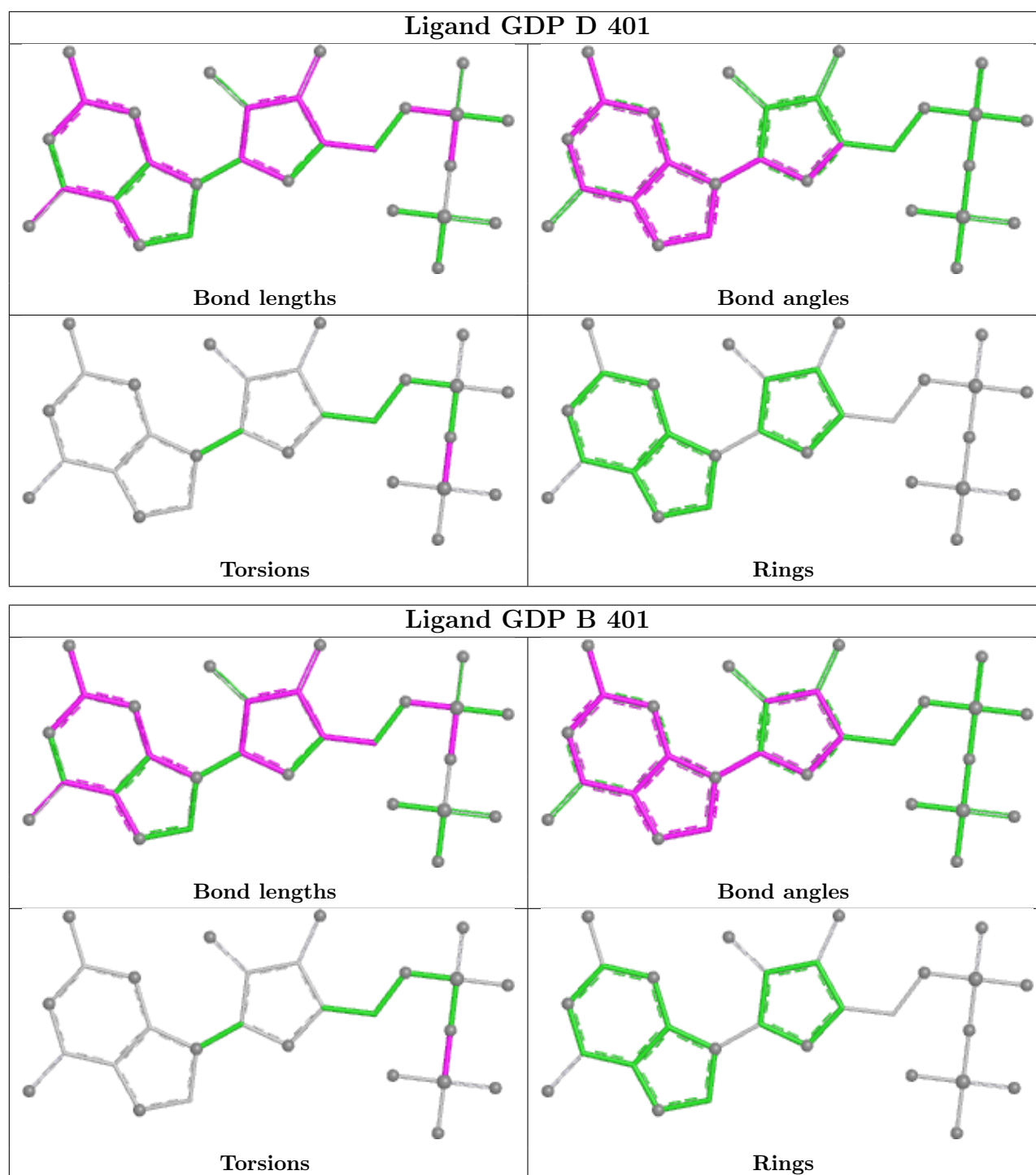
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	401	GDP	2	0
3	D	401	GDP	1	0
3	B	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%)	0.44	25 (7%) 20 23	5, 19, 42, 64	0
1	B	324/348 (93%)	0.68	35 (10%) 11 12	7, 24, 50, 68	0
1	C	332/348 (95%)	0.63	35 (10%) 11 13	10, 25, 50, 83	0
1	D	317/348 (91%)	1.81	127 (40%) 0 0	19, 44, 69, 91	0
2	E	14/17 (82%)	-0.02	1 (7%) 22 25	5, 9, 25, 39	0
2	F	14/17 (82%)	0.20	1 (7%) 22 25	8, 12, 24, 48	0
2	G	14/17 (82%)	0.54	2 (14%) 6 7	13, 19, 45, 53	0
2	H	14/17 (82%)	0.60	1 (7%) 22 25	18, 23, 37, 52	0
All	All	1367/1460 (93%)	0.86	227 (16%) 4 4	5, 26, 59, 91	0

All (227) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	222	PHE	6.2
1	B	39	ALA	6.2
1	D	384	GLN	5.8
1	D	328	PRO	5.7
1	D	214	VAL	5.6
1	B	358	TYR	5.5
1	D	358	TYR	5.4
1	D	317	ARG	5.2
1	D	193	SER	5.0
1	D	329	GLY	5.0
1	D	182	ILE	4.9
1	D	99	LEU	4.7
1	C	326	PRO	4.6
1	D	205	SER	4.5
1	D	324	ALA	4.5
1	B	353	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
2	G	15	GLY	4.3
1	D	122	PRO	4.3
2	F	15	GLY	4.3
1	C	328	PRO	4.3
1	D	316	ALA	4.2
1	D	196	ASP	4.2
1	D	39	ALA	4.2
1	D	217	VAL	4.1
1	B	206	GLY	4.1
1	D	197	LEU	4.1
1	D	204	THR	4.1
1	D	159	VAL	4.0
1	D	178	PHE	4.0
1	D	90	THR	3.9
1	D	219	PHE	3.9
1	D	65	VAL	3.8
1	A	394	LEU	3.8
1	D	203	LEU	3.7
1	D	40	THR	3.7
1	C	358	TYR	3.7
1	D	154	TRP	3.7
1	D	303	ALA	3.7
1	B	384	GLN	3.7
1	D	191	VAL	3.7
1	D	382	ILE	3.6
1	D	92	VAL	3.6
1	D	314	GLU	3.6
1	D	119	LEU	3.6
1	D	141	ASP	3.6
1	B	351	ALA	3.6
1	B	40	THR	3.6
1	D	179	LEU	3.6
2	H	15	GLY	3.5
1	B	204	THR	3.5
1	B	114	VAL	3.5
1	D	189	ASP	3.5
1	D	381	ASP	3.5
1	D	186	LYS	3.5
1	C	327	GLU	3.4
1	D	215	ASP	3.4
1	D	115	PRO	3.4
1	D	113	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	117	VAL	3.3
1	A	39	ALA	3.3
1	D	126	PHE	3.3
1	D	327	GLU	3.3
1	D	202	VAL	3.3
1	D	281	TRP	3.3
2	E	15	GLY	3.3
1	A	325	THR	3.3
1	B	387	HIS	3.2
1	B	120	ALA	3.2
1	C	325	THR	3.2
1	D	379	CYS	3.2
1	A	356	ARG	3.2
1	C	324	ALA	3.2
1	D	185	ILE	3.2
1	D	375	VAL	3.2
1	D	121	ASN	3.1
1	D	152	ALA	3.1
1	A	358	TYR	3.1
1	B	328	PRO	3.1
1	D	332	PRO	3.1
1	C	323	ASP	3.1
1	D	131	ILE	3.1
1	D	376	PHE	3.1
1	B	205	SER	3.0
1	D	192	PRO	3.0
1	C	133	SER	3.0
1	D	158	GLY	3.0
1	D	177	TYR	3.0
1	C	351	ALA	3.0
1	C	329	GLY	2.9
1	D	116	PRO	2.9
1	B	327	GLU	2.9
1	D	359	CYS	2.9
1	D	147	TYR	2.9
1	C	316	ALA	2.9
2	G	14	CYS	2.9
1	D	151	LYS	2.9
1	C	303	ALA	2.9
1	D	171	LEU	2.9
1	D	326	PRO	2.8
1	D	333	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	39	ALA	2.8
1	D	67	GLY	2.8
1	B	325	THR	2.8
1	A	323	ASP	2.8
1	B	385	ARG	2.8
1	D	41	HIS	2.8
1	D	218	ASN	2.8
1	A	88	LYS	2.8
1	D	372	ILE	2.8
1	D	302	LEU	2.7
1	C	215	ASP	2.7
1	D	103	ILE	2.7
1	B	352	SER	2.7
1	B	214	VAL	2.7
1	D	301	VAL	2.7
1	D	190	TYR	2.7
1	A	352	SER	2.7
1	C	205	SER	2.7
1	D	66	ASN	2.7
1	D	128	VAL	2.7
1	D	184	VAL	2.7
1	D	188	ALA	2.7
1	D	163	TYR	2.7
1	A	38	ARG	2.7
1	D	383	ILE	2.7
1	B	65	VAL	2.7
1	D	360	TYR	2.6
1	D	221	MET	2.6
1	B	215	ASP	2.6
1	D	304	GLY	2.6
1	A	114	VAL	2.6
1	A	322	GLU	2.6
1	D	112	ASN	2.6
1	D	200	CYS	2.6
1	D	146	PHE	2.6
1	D	315	PHE	2.6
1	B	201	ARG	2.6
1	D	323	ASP	2.6
1	D	206	GLY	2.6
1	B	202	VAL	2.6
1	B	69	ASN	2.6
1	D	130	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	355	GLY	2.5
1	B	217	VAL	2.5
1	D	319	THR	2.5
1	C	216	LYS	2.5
1	A	204	THR	2.5
1	D	213	GLN	2.5
1	C	123	GLU	2.5
1	D	129	ASP	2.5
1	D	368	ASP	2.5
1	D	174	CYS	2.5
1	B	126	PHE	2.5
1	D	334	VAL	2.5
1	C	313	PRO	2.5
1	A	70	GLY	2.4
1	A	316	ALA	2.4
1	D	120	ALA	2.4
1	B	381	ASP	2.4
1	D	373	ARG	2.4
1	D	237	CYS	2.4
1	D	335	THR	2.4
1	D	63	LEU	2.4
1	D	309	GLU	2.4
1	D	94	ASP	2.3
1	D	194	ASP	2.3
1	B	145	GLU	2.3
1	D	322	GLU	2.3
1	D	62	ILE	2.3
1	B	122	PRO	2.3
1	C	350	THR	2.3
1	D	64	HIS	2.3
1	D	155	GLU	2.3
1	C	387	HIS	2.3
1	B	115	PRO	2.3
1	D	143	PRO	2.3
1	C	310	ASP	2.3
1	D	114	VAL	2.3
1	D	365	CYS	2.3
1	A	329	GLY	2.2
1	B	360	TYR	2.2
1	D	183	ASP	2.2
1	D	369	THR	2.2
1	D	144	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	310	ASP	2.2
1	D	148	GLU	2.2
1	C	388	LEU	2.2
1	D	187	GLN	2.2
1	B	67	GLY	2.2
1	B	189	ASP	2.2
1	C	139	ASP	2.2
1	C	122	PRO	2.2
1	C	38	ARG	2.2
1	D	367	VAL	2.2
1	A	381	ASP	2.2
1	D	162	CYS	2.2
1	C	305	LYS	2.2
1	A	141	ASP	2.1
1	C	204	THR	2.1
1	D	321	PRO	2.1
1	C	135	MET	2.1
1	C	322	GLU	2.1
1	C	330	GLU	2.1
1	D	212	PHE	2.1
1	C	173	ASP	2.1
1	A	205	SER	2.1
1	A	281	TRP	2.1
1	A	191	VAL	2.1
1	A	123	GLU	2.1
1	D	132	LEU	2.1
1	D	337	ALA	2.1
1	A	333	ARG	2.1
1	A	374	ARG	2.1
1	C	88	LYS	2.1
1	C	319	THR	2.1
1	D	350	THR	2.1
1	B	158	GLY	2.1
1	D	220	HIS	2.1
1	C	112	ASN	2.1
1	D	153	LEU	2.1
1	B	324	ALA	2.1
1	A	350	THR	2.0
1	C	317	ARG	2.0
1	D	142	PHE	2.0
1	D	362	HIS	2.0
1	B	121	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	42	ARG	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	0.90	0.09	11,15,24,33	0
2	DTY	F	1	12/13	0.91	0.09	11,16,19,36	0
2	DTY	G	1	12/13	0.91	0.08	19,24,27,31	0
2	DTY	H	1	12/13	0.91	0.08	15,28,36,44	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

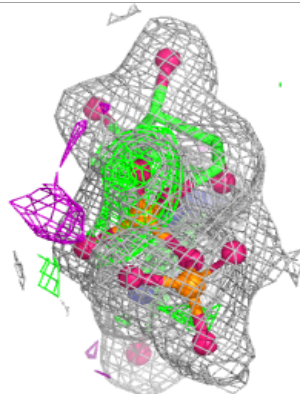
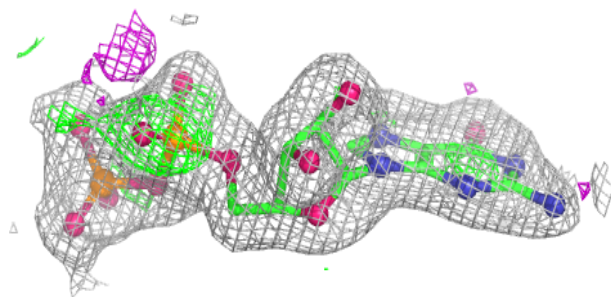
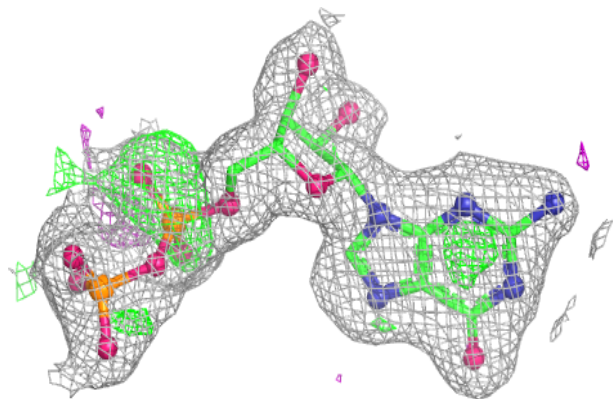
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GDP	C	401	28/28	0.94	0.10	7,10,27,62	0
3	GDP	D	401	28/28	0.94	0.10	17,30,41,46	0
3	GDP	A	401	28/28	0.97	0.06	2,5,8,12	0
3	GDP	B	401	28/28	0.97	0.06	5,9,17,21	0
4	CL	D	402	1/1	0.97	0.05	31,31,31,31	0
4	CL	C	402	1/1	0.98	0.05	19,19,19,19	0
4	CL	A	402	1/1	0.99	0.06	12,12,12,12	0
4	CL	B	402	1/1	0.99	0.05	14,14,14,14	0

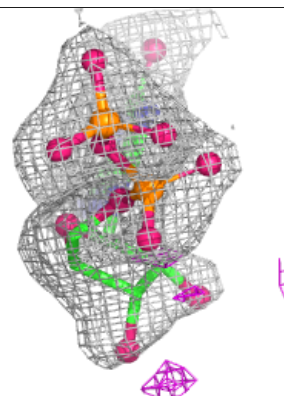
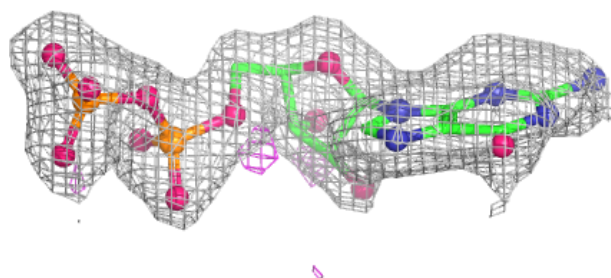
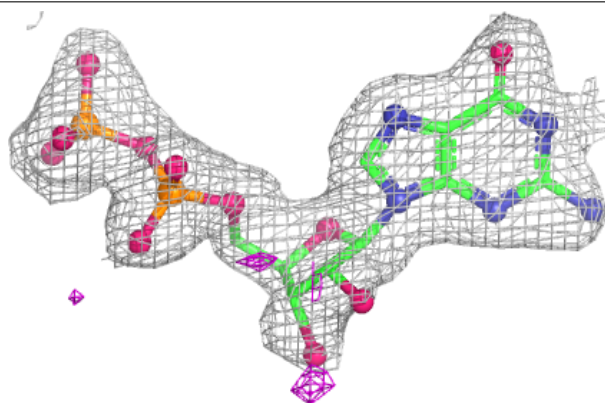
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

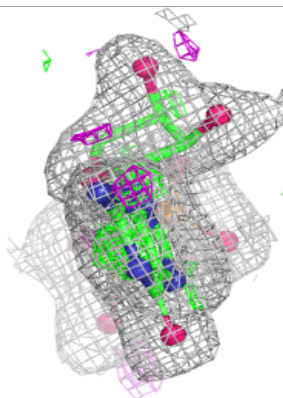
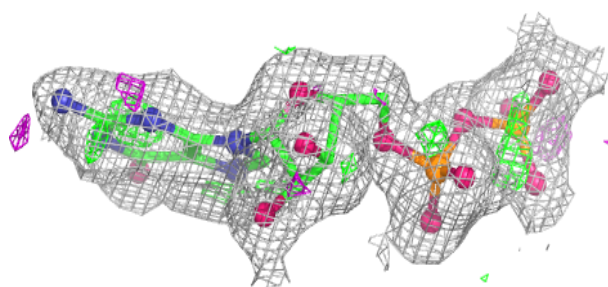
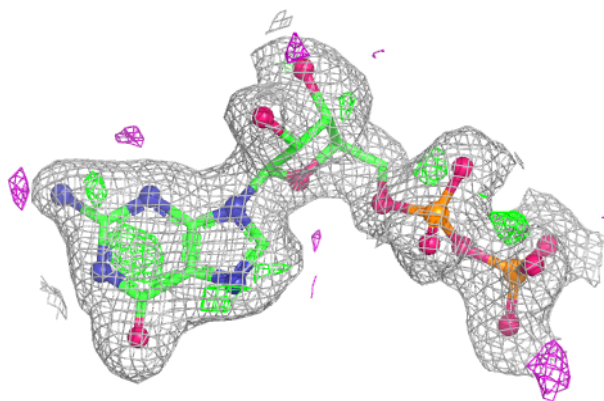
**Electron density around GDP D 401:**

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

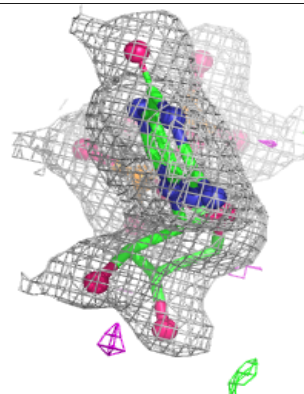
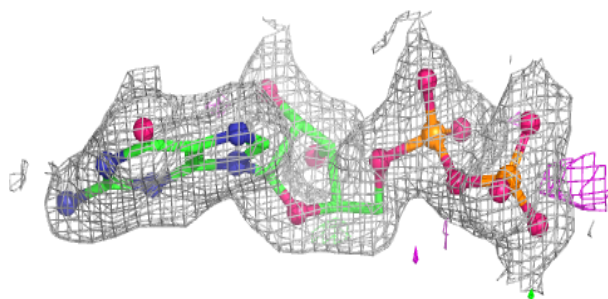
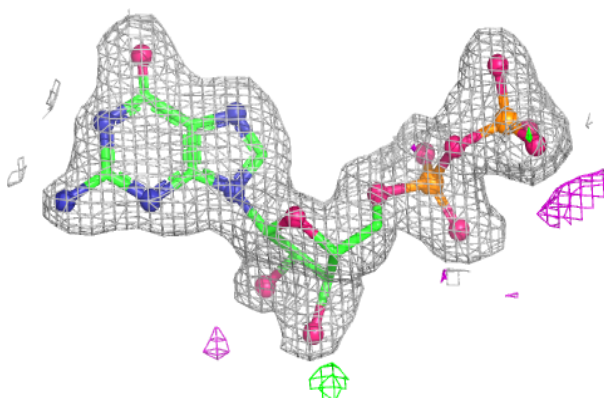


Electron density around GDP A 401:

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

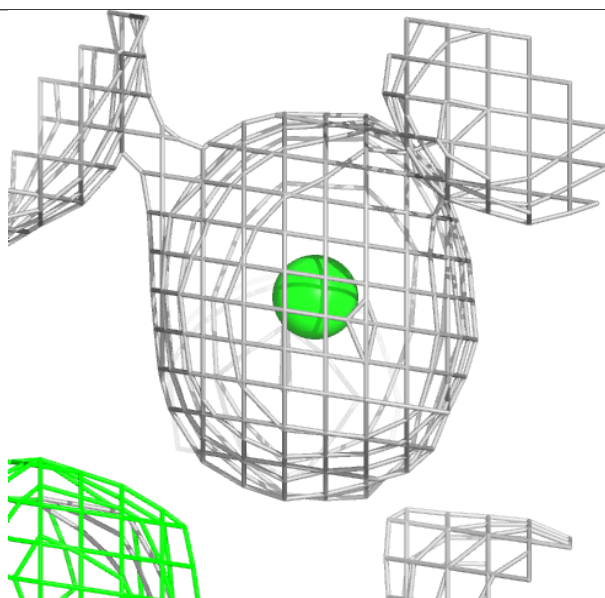
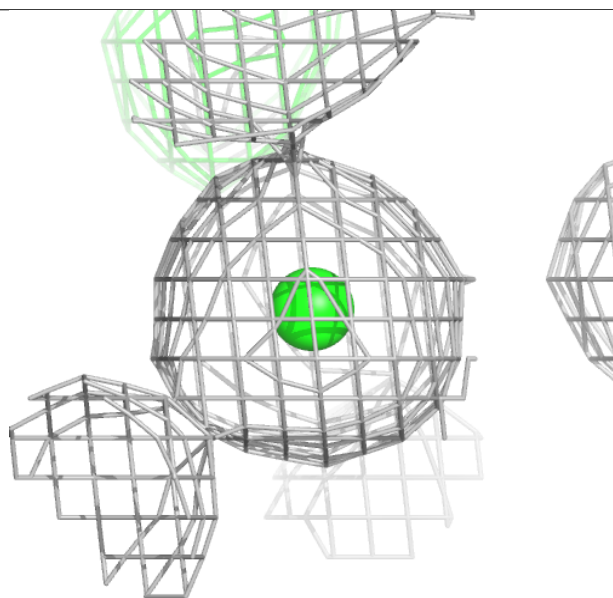
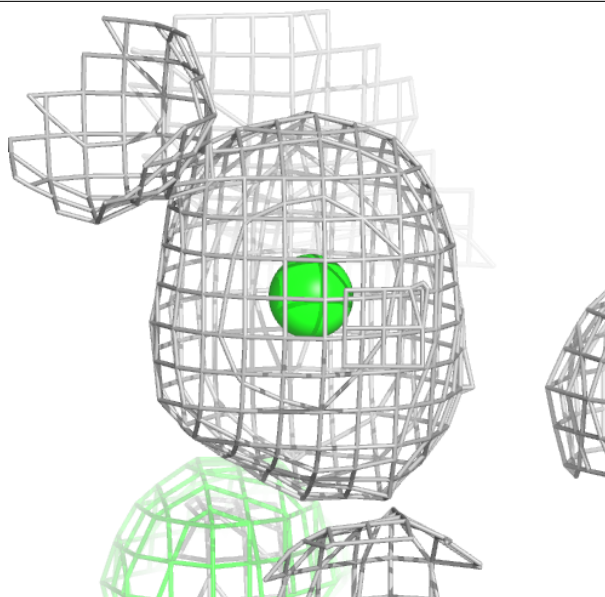
**Electron density around GDP B 401:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



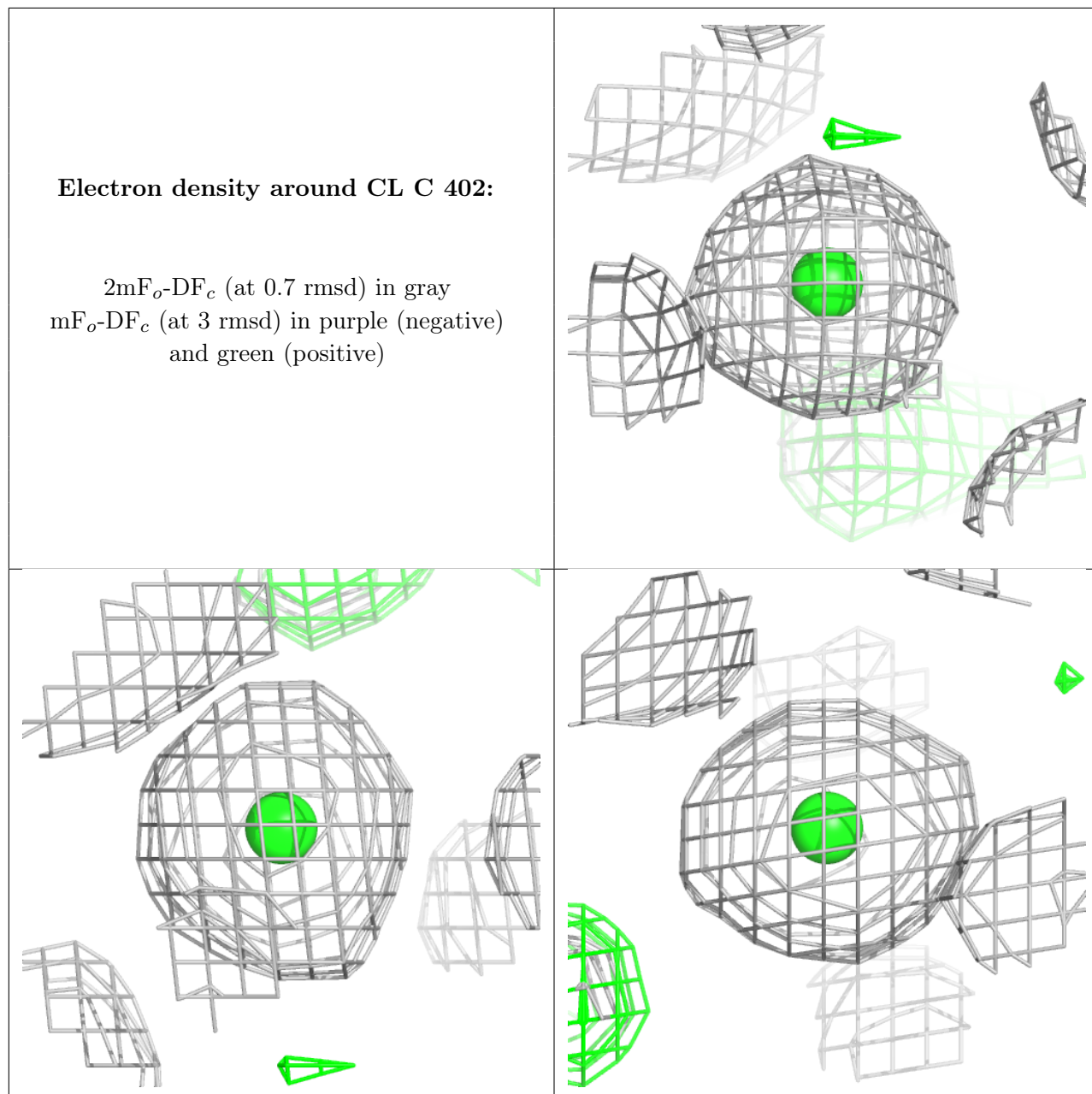
Electron density around CL D 402:

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



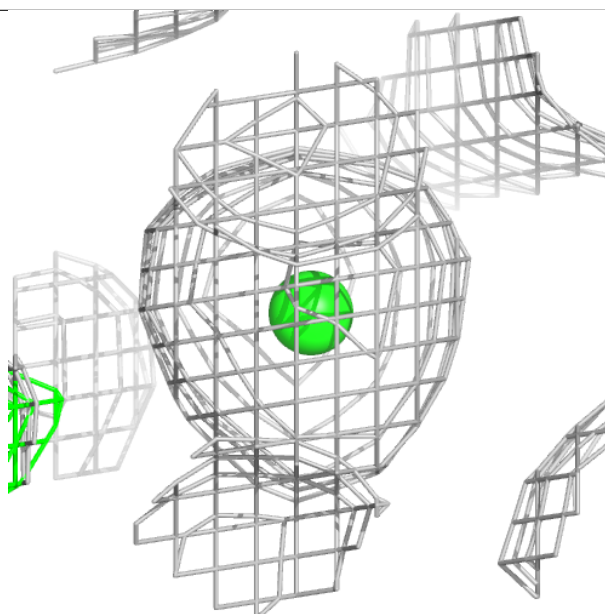
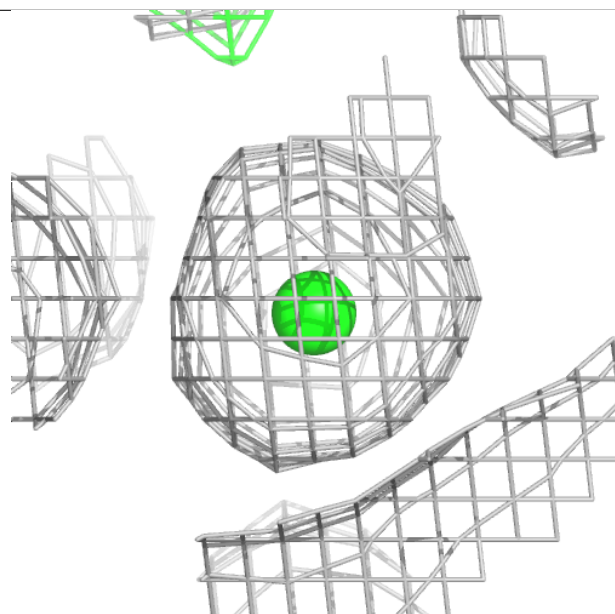
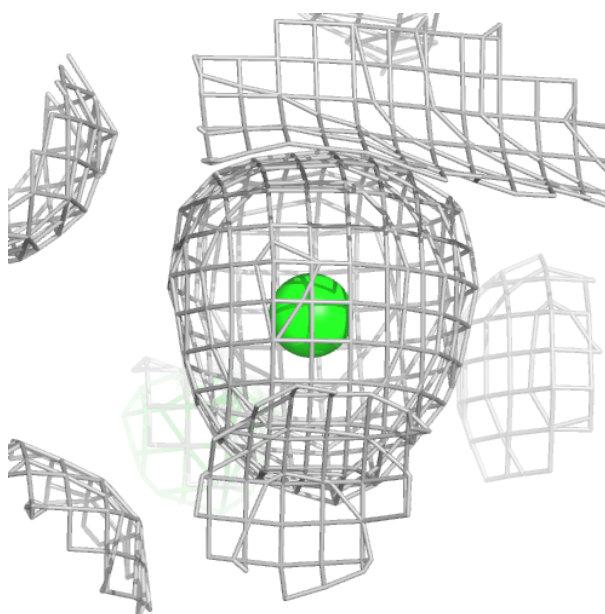
Electron density around CL C 402:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



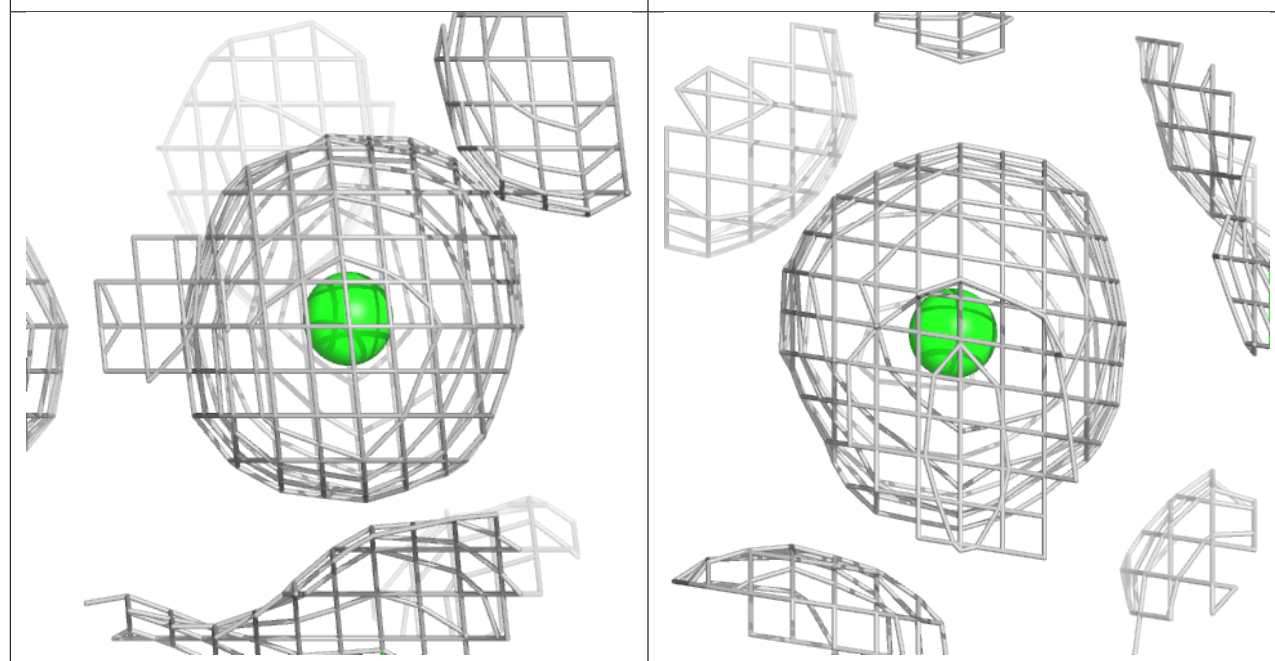
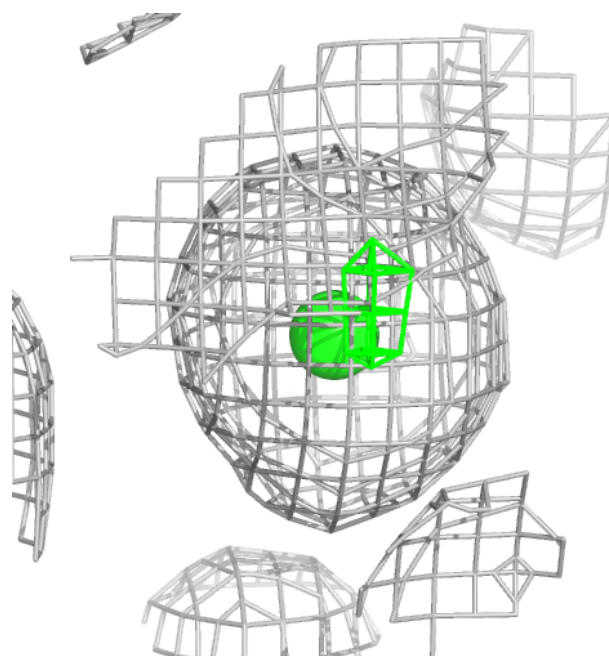
Electron density around CL A 402:

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



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)



6.5 Other polymers ⓘ

There are no such residues in this entry.