Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:17 am BST

PDB ID	:	4G5R
Title	:	Structure of LGN GL4/Galphai3 complex
Authors	:	Jia, M.; Li, J.; Zhu, J.; Wen, W.; Zhang, M.; Wang, W.
Deposited on	:	2012-07-18
Resolution	:	3.48 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

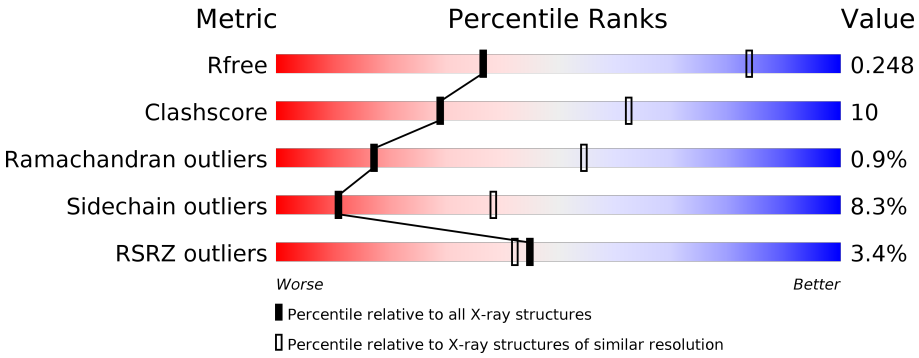
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.48 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	1379 (3.56-3.40)
Clashscore	141614	1461 (3.56-3.40)
Ramachandran outliers	138981	1424 (3.56-3.40)
Sidechain outliers	138945	1425 (3.56-3.40)
RSRZ outliers	127900	1289 (3.56-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	330	2% 75% 20%
1	B	330	5% 71% 22% 5%
1	C	330	3% 73% 21%
1	D	330	4% 72% 20%
2	E	25	48% 28% 16%
2	F	25	60% 12% 16% 12%

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Mol	Chain	Length	Quality of chain
2	G	25	64% 20% 12%
2	Z	25	8% 56% 20% 8% 16%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10601 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.

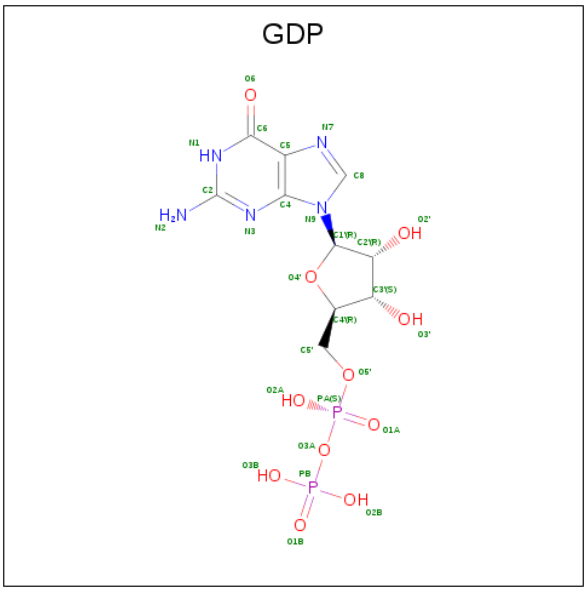
- Molecule 1 is a protein called Guanine nucleotide-binding protein G(k) subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2432	1547	398	472	15			
1	B	313	Total	C	N	O	S	0	0	0
			2412	1534	397	467	14			
1	C	317	Total	C	N	O	S	0	0	0
			2426	1541	403	467	15			
1	D	317	Total	C	N	O	S	0	0	0
			2426	1542	401	468	15			

- Molecule 2 is a protein called G-protein-signaling modulator 2.

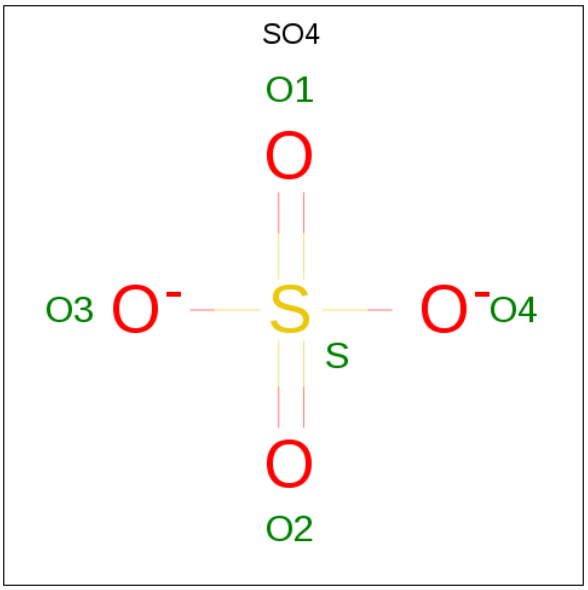
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	21	Total	C	N	O	S	0	0	0
			179	114	33	31	1			
2	F	22	Total	C	N	O	S	0	0	0
			184	117	34	32	1			
2	G	22	Total	C	N	O	S	0	0	0
			184	116	34	33	1			
2	Z	21	Total	C	N	O	S	0	0	0
			179	114	33	31	1			

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



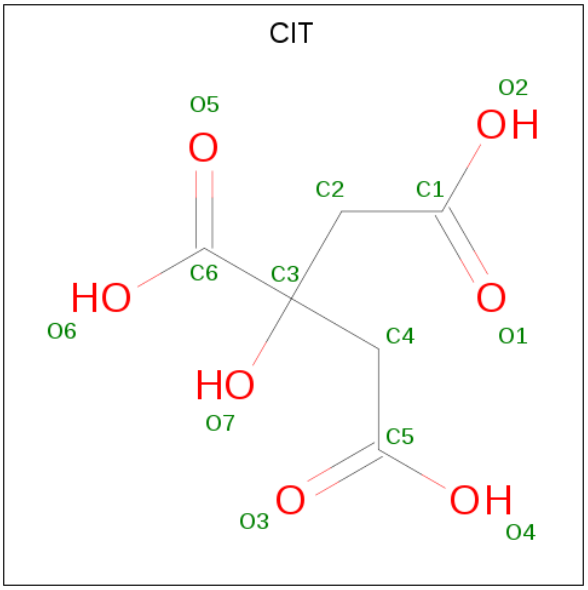
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	C	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



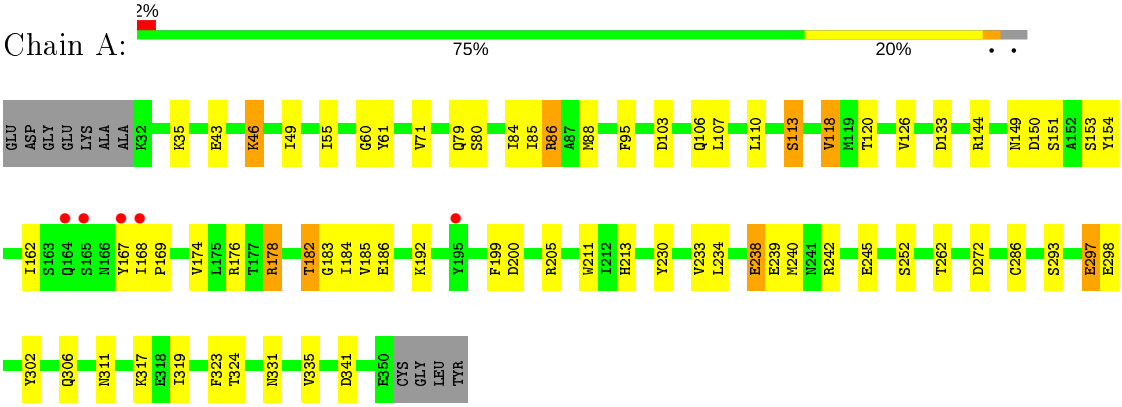
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 13 6 7	0	0
5	B	1	Total C O 13 6 7	0	0
5	C	1	Total C O 13 6 7	0	0
5	C	1	Total C O 13 6 7	0	0

3 Residue-property plots (i)

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

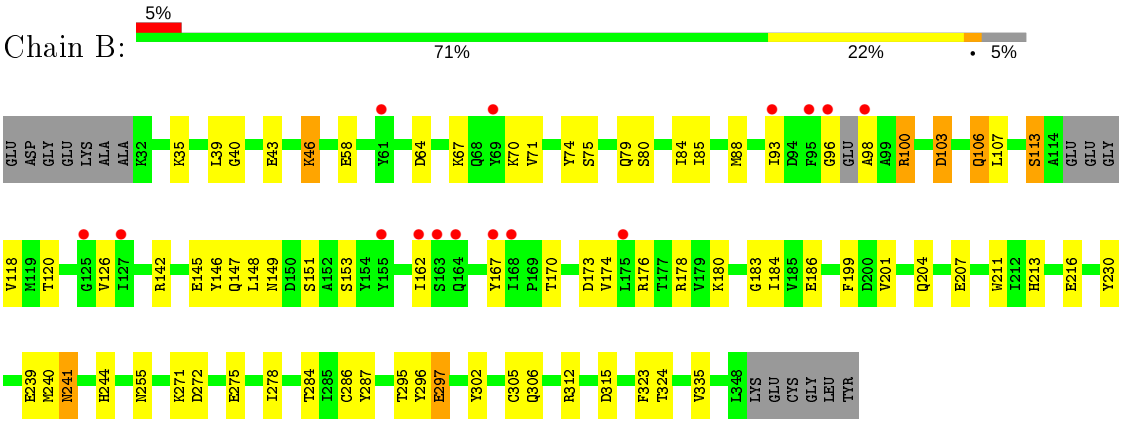
- Molecule 1: Guanine nucleotide-binding protein G(k) subunit alpha

Chain A:



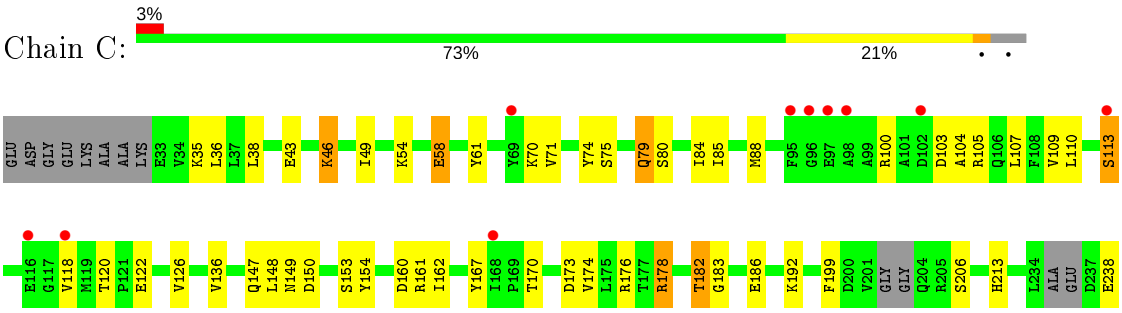
- Molecule 1: Guanine nucleotide-binding protein G(k) subunit alpha

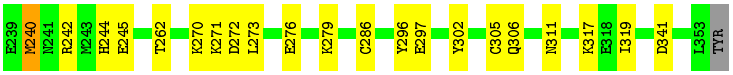
Chain B:



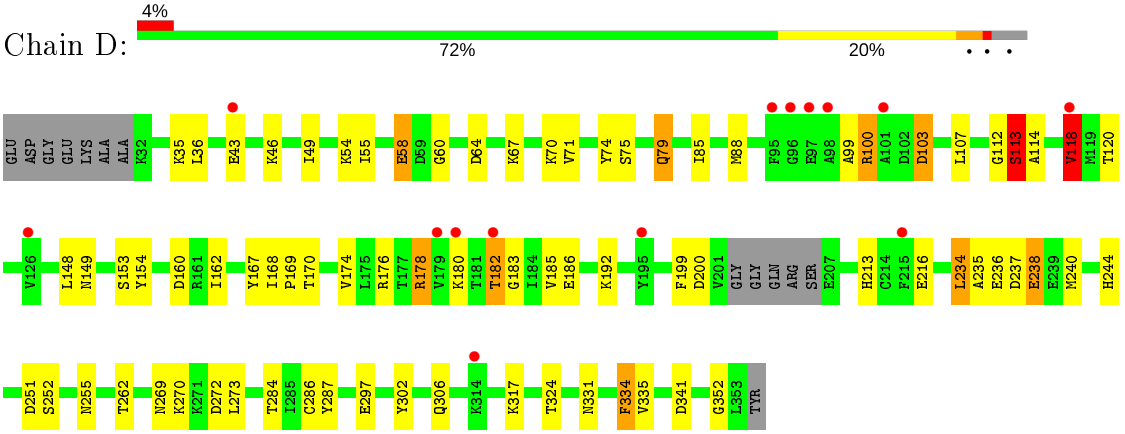
- Molecule 1: Guanine nucleotide-binding protein G(k) subunit alpha

Chain C:

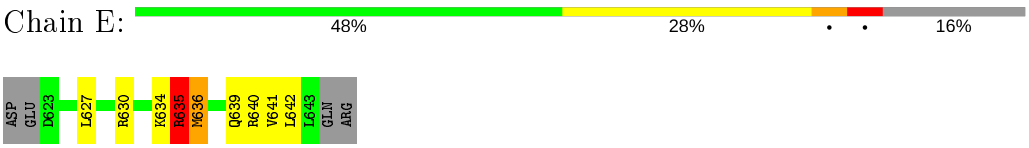




• Molecule 1: Guanine nucleotide-binding protein G(k) subunit alpha



• Molecule 2: G-protein-signaling modulator 2



• Molecule 2: G-protein-signaling modulator 2

• Molecule 2: G-protein-signaling modulator 2

• Molecule 2: G-protein-signaling modulator 2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	209.55Å 209.55Å 237.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.04 – 3.48 49.64 – 3.48	Depositor EDS
% Data completeness (in resolution range)	98.1 (48.04-3.48) 98.4 (49.64-3.48)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.79 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.6.0117, PHENIX 1.8_1063	Depositor
R, R_{free}	0.209 , 0.253 0.205 , 0.248	Depositor DCC
R_{free} test set	1967 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	95.4	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 68.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	10601	wwPDB-VP
Average B, all atoms (Å^2)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% 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: GDP, SO4, CIT

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	0/2477	0.47	0/3364
1	B	0.28	0/2455	0.47	0/3326
1	C	0.28	0/2468	0.47	0/3346
1	D	0.28	0/2468	0.47	0/3345
2	E	0.30	0/180	0.63	0/238
2	F	0.31	0/185	0.62	0/245
2	G	0.27	0/185	0.50	0/246
2	Z	0.30	0/180	0.66	0/238
All	All	0.28	0/10598	0.48	0/14348

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	2432	0	2260	45	0
1	B	2412	0	2266	54	0
1	C	2426	0	2271	47	0
1	D	2426	0	2282	48	0
2	E	179	0	187	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	184	0	189	10	0
2	G	184	0	184	6	0
2	Z	179	0	187	3	0
3	A	28	0	12	2	0
3	B	28	0	12	4	0
3	C	28	0	12	3	0
3	D	28	0	12	1	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
5	B	26	0	10	4	0
5	C	26	0	10	2	0
All	All	10601	0	9894	197	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 10.

All (197) 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:183:GLY:HA2	1:B:204:GLN:HG3	1.54	0.89
1:B:43:GLU:OE2	2:F:640:ARG:NH1	2.14	0.80
1:D:103:ASP:N	1:D:103:ASP:OD1	2.19	0.75
1:A:43:GLU:OE1	2:E:640:ARG:NH1	2.19	0.74
1:C:271:LYS:NZ	5:C:402:CIT:O3	2.23	0.70
1:A:35:LYS:NZ	1:A:213:HIS:O	2.25	0.69
1:D:43:GLU:OE1	2:Z:640:ARG:NH1	2.25	0.69
1:B:103:ASP:O	1:B:107:LEU:N	2.27	0.68
1:C:43:GLU:OE1	2:G:640:ARG:NH1	2.27	0.67
1:B:147:GLN:O	2:F:639:GLN:NE2	2.27	0.67
1:C:192:LYS:NZ	1:C:341:ASP:OD1	2.28	0.67
1:B:70:LYS:HG2	1:B:74:TYR:HE2	1.61	0.65
1:B:103:ASP:N	1:B:103:ASP:OD2	2.23	0.65
1:C:147:GLN:O	2:G:639:GLN:NE2	2.29	0.65
1:D:234:LEU:HD22	1:D:238:GLU:HG3	1.79	0.65
1:A:151:SER:HG	3:A:401:GDP:HO3'	1.45	0.63
1:D:103:ASP:O	1:D:107:LEU:N	2.32	0.63
1:D:262:THR:O	1:D:317:LYS:NZ	2.32	0.63
2:E:634:LYS:O	2:E:636:MET:N	2.29	0.63
1:A:103:ASP:HB3	1:A:126:VAL:HG13	1.81	0.62
1:B:241:ASN:OD1	1:B:244:HIS:ND1	2.28	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ARG:NH2	1:B:103:ASP:OD1	2.33	0.60
1:A:178:ARG:NH2	2:E:639:GLN:O	2.34	0.60
1:C:100:ARG:NH2	1:C:103:ASP:OD2	2.34	0.60
1:C:161:ARG:NH1	1:C:173:ASP:OD2	2.31	0.60
1:B:170:THR:HG23	1:B:173:ASP:H	1.67	0.59
1:B:184:ILE:HD11	1:B:211:TRP:HA	1.83	0.59
1:C:296:TYR:HB3	5:C:403:CIT:O2	2.02	0.59
1:C:279:LYS:HD3	1:D:334:PHE:HE1	1.68	0.58
1:D:192:LYS:NZ	1:D:341:ASP:OD1	2.35	0.58
1:B:43:GLU:OE2	1:B:178:ARG:NH1	2.38	0.57
1:D:235:ALA:O	1:D:238:GLU:HG2	2.04	0.57
1:C:162:ILE:HG22	1:C:167:TYR:CZ	2.39	0.57
1:A:55:ILE:HA	1:A:60:GLY:HA2	1.84	0.57
1:D:54:LYS:HA	1:D:58:GLU:OE1	2.05	0.56
1:A:230:TYR:O	1:A:286:CYS:HB2	2.05	0.56
1:C:178:ARG:HH11	1:C:178:ARG:HB3	1.70	0.56
1:B:271:LYS:NZ	5:B:403:CIT:O3	2.35	0.56
1:A:184:ILE:HD11	1:A:211:TRP:HA	1.88	0.56
1:B:96:GLY:O	1:B:98:ALA:N	2.39	0.56
1:D:270:LYS:HB3	1:D:273:LEU:HD12	1.88	0.56
1:B:103:ASP:HB2	1:B:126:VAL:HG13	1.88	0.55
1:B:142:ARG:NH1	1:B:145:GLU:OE1	2.38	0.55
1:C:262:THR:O	1:C:317:LYS:NZ	2.40	0.55
1:C:311:ASN:HB2	1:C:319:ILE:HD11	1.87	0.55
1:B:162:ILE:HG22	1:B:167:TYR:CZ	2.42	0.55
1:C:70:LYS:HG2	1:C:74:TYR:HE2	1.72	0.55
1:D:251:ASP:OD1	1:D:255:ASN:ND2	2.40	0.55
1:B:201:VAL:O	1:B:211:TRP:NE1	2.39	0.55
1:B:272:ASP:N	1:B:272:ASP:OD1	2.40	0.55
1:C:276:GLU:HA	1:C:279:LYS:HE3	1.89	0.54
2:F:634:LYS:O	2:F:636:MET:N	2.40	0.54
1:D:112:GLY:C	1:D:114:ALA:H	2.10	0.54
1:B:178:ARG:NH2	2:F:639:GLN:O	2.41	0.54
1:A:43:GLU:OE1	1:A:178:ARG:NH1	2.39	0.54
1:C:272:ASP:N	1:C:272:ASP:OD1	2.42	0.53
1:B:230:TYR:O	1:B:286:CYS:HB2	2.09	0.53
1:B:186:GLU:HG3	1:B:199:PHE:CE2	2.43	0.53
1:A:86:ARG:HH11	1:A:86:ARG:HG3	1.74	0.53
1:B:75:SER:O	1:B:79:GLN:HG3	2.09	0.53
1:A:335:VAL:HG22	5:B:402:CIT:O3	2.08	0.53
1:C:182:THR:OG1	1:C:183:GLY:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:ASP:O	1:C:107:LEU:N	2.33	0.53
1:A:162:ILE:HG22	1:A:167:TYR:CZ	2.43	0.52
1:A:297:GLU:HG3	1:B:323:PHE:CD1	2.44	0.52
1:B:93:ILE:HD11	1:B:142:ARG:NH2	2.24	0.52
1:B:151:SER:HB2	1:B:178:ARG:HD2	1.92	0.52
1:B:40:GLY:O	2:F:632:GLN:NE2	2.41	0.52
1:B:85:ILE:HA	1:B:88:MET:HG3	1.92	0.51
1:D:186:GLU:HG3	1:D:199:PHE:CE2	2.45	0.51
1:B:180:LYS:HB3	2:F:642:LEU:HD22	1.92	0.51
1:C:103:ASP:OD1	1:C:104:ALA:N	2.44	0.51
3:B:401:GDP:O3B	2:F:635:ARG:NH2	2.44	0.51
1:A:144:ARG:O	1:A:233:VAL:HG23	2.11	0.51
1:D:182:THR:OG1	1:D:183:GLY:N	2.43	0.51
1:A:79:GLN:HB2	2:E:639:GLN:HA	1.93	0.51
1:D:272:ASP:N	1:D:272:ASP:OD1	2.44	0.50
1:C:240:MET:HE3	1:C:245:GLU:HG3	1.93	0.50
3:C:401:GDP:O3B	2:G:635:ARG:NH2	2.44	0.50
1:D:112:GLY:O	1:D:114:ALA:N	2.42	0.50
1:D:213:HIS:ND1	1:D:216:GLU:OE1	2.38	0.50
1:D:70:LYS:HG2	1:D:74:TYR:HE2	1.77	0.50
1:A:113:SER:O	1:A:113:SER:OG	2.29	0.50
1:A:297:GLU:HG3	1:B:323:PHE:CG	2.47	0.50
1:A:176:ARG:NH1	3:A:401:GDP:O2'	2.42	0.50
1:B:296:TYR:HB3	5:B:402:CIT:O6	2.12	0.50
1:B:103:ASP:HA	1:B:106:GLN:HB3	1.93	0.49
1:C:38:LEU:HD23	1:C:46:LYS:HA	1.93	0.49
1:C:85:ILE:HA	1:C:88:MET:HG3	1.94	0.49
1:C:54:LYS:HA	1:C:58:GLU:OE1	2.11	0.49
1:A:272:ASP:OD1	1:A:272:ASP:N	2.43	0.49
1:A:262:THR:O	1:A:317:LYS:NZ	2.45	0.49
1:D:75:SER:O	1:D:79:GLN:HG3	2.12	0.49
1:C:75:SER:O	1:C:79:GLN:HG3	2.11	0.49
1:B:70:LYS:HG2	1:B:74:TYR:CE2	2.45	0.49
1:D:85:ILE:HA	1:D:88:MET:HG3	1.95	0.49
2:E:635:ARG:O	2:E:640:ARG:NH1	2.39	0.49
1:B:295:THR:HG22	5:B:402:CIT:O4	2.13	0.48
1:D:148:LEU:HD12	1:D:149:ASN:H	1.78	0.48
1:D:180:LYS:NZ	2:Z:637:ASP:HB3	2.28	0.48
1:A:182:THR:OG1	1:A:183:GLY:N	2.46	0.48
1:A:192:LYS:NZ	1:A:341:ASP:OD1	2.45	0.48
1:D:64:ASP:O	1:D:67:LYS:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:SER:HB3	2:G:629:LEU:HD11	1.96	0.48
1:C:244:HIS:HE1	1:C:286:CYS:O	1.96	0.48
1:A:85:ILE:HA	1:A:88:MET:HG3	1.96	0.48
1:C:35:LYS:NZ	1:C:213:HIS:O	2.44	0.47
2:F:635:ARG:HG2	2:F:640:ARG:CZ	2.44	0.47
2:E:627:LEU:HD13	2:E:630:ARG:HH21	1.78	0.47
1:C:46:LYS:HE2	1:C:46:LYS:HB2	1.63	0.47
1:B:35:LYS:NZ	1:B:216:GLU:O	2.37	0.47
1:C:80:SER:O	1:C:84:ILE:HG13	2.14	0.47
1:A:185:VAL:HB	1:A:200:ASP:HB3	1.96	0.47
3:C:401:GDP:PB	2:G:635:ARG:HH21	2.38	0.47
1:B:324:THR:HG22	1:B:335:VAL:HG21	1.97	0.47
1:D:324:THR:HG22	1:D:335:VAL:HG21	1.98	0.46
1:A:311:ASN:HB2	1:A:319:ILE:HD11	1.96	0.46
1:D:162:ILE:HG22	1:D:167:TYR:CE1	2.50	0.46
1:D:154:TYR:CD2	1:D:176:ARG:HG3	2.51	0.46
1:D:55:ILE:HA	1:D:60:GLY:HA2	1.99	0.46
1:A:149:ASN:HD21	1:A:151:SER:HB2	1.81	0.45
1:D:43:GLU:CD	1:D:178:ARG:HH12	2.19	0.45
1:D:235:ALA:O	1:D:237:ASP:N	2.49	0.45
1:C:176:ARG:NH1	3:C:401:GDP:O2'	2.47	0.45
1:D:113:SER:O	1:D:118:VAL:HG13	2.16	0.45
1:C:178:ARG:HB3	2:G:640:ARG:HG3	1.98	0.45
1:D:79:GLN:HB2	2:Z:639:GLN:HA	1.98	0.45
1:A:110:LEU:O	1:A:113:SER:HB3	2.16	0.45
1:B:80:SER:O	1:B:84:ILE:HG13	2.16	0.45
1:C:110:LEU:O	1:C:113:SER:HB3	2.16	0.45
1:B:46:LYS:HE2	1:B:46:LYS:HB2	1.60	0.45
1:B:302:TYR:O	1:B:306:GLN:HG2	2.16	0.45
1:B:113:SER:OG	1:B:113:SER:O	2.32	0.44
1:B:176:ARG:NH1	3:B:401:GDP:O2'	2.47	0.44
1:C:154:TYR:CD2	1:C:176:ARG:HG3	2.53	0.44
2:F:635:ARG:HG2	2:F:640:ARG:NH1	2.32	0.44
1:A:86:ARG:NH1	1:A:86:ARG:HG3	2.32	0.44
1:C:113:SER:OG	1:C:113:SER:O	2.32	0.43
1:B:64:ASP:O	1:B:67:LYS:HB2	2.18	0.43
1:C:122:GLU:O	1:C:126:VAL:HG23	2.19	0.43
1:A:103:ASP:O	1:A:107:LEU:N	2.47	0.43
1:B:176:ARG:HH22	3:B:401:GDP:HN22	1.67	0.43
1:D:168:ILE:HA	1:D:169:PRO:HD3	1.86	0.43
1:D:185:VAL:HB	1:D:200:ASP:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:627:LEU:HD13	2:E:630:ARG:NH2	2.34	0.43
1:D:114:ALA:HA	1:D:118:VAL:HG13	2.00	0.43
1:D:99:ALA:HB3	1:D:100:ARG:HH21	1.84	0.43
1:A:238:GLU:HB3	1:A:245:GLU:OE2	2.19	0.43
1:A:297:GLU:OE2	1:B:296:TYR:OH	2.29	0.43
1:A:293:SER:OG	1:A:298:GLU:OE1	2.32	0.43
1:D:170:THR:O	1:D:174:VAL:HG23	2.19	0.43
1:C:88:MET:SD	1:C:136:VAL:HG22	2.59	0.43
1:D:269:ASN:ND2	3:D:401:GDP:N7	2.66	0.43
1:C:302:TYR:O	1:C:306:GLN:HG2	2.18	0.42
1:D:35:LYS:NZ	1:D:216:GLU:O	2.35	0.42
1:A:149:ASN:OD1	1:A:150:ASP:N	2.52	0.42
1:C:162:ILE:HG22	1:C:167:TYR:CE1	2.55	0.42
1:A:186:GLU:HG3	1:A:199:PHE:CE2	2.54	0.42
1:B:170:THR:O	1:B:174:VAL:HG23	2.20	0.42
1:D:113:SER:OG	1:D:113:SER:O	2.37	0.42
1:A:154:TYR:CD2	1:A:176:ARG:HG3	2.54	0.42
1:C:170:THR:O	1:C:174:VAL:HG23	2.19	0.42
1:C:70:LYS:HG2	1:C:74:TYR:CE2	2.52	0.42
1:D:302:TYR:O	1:D:306:GLN:HG2	2.20	0.42
1:D:334:PHE:C	1:D:334:PHE:CD2	2.93	0.42
1:C:186:GLU:HG3	1:C:199:PHE:CE2	2.55	0.42
1:D:35:LYS:NZ	1:D:213:HIS:O	2.51	0.42
1:C:161:ARG:NH2	1:C:173:ASP:OD1	2.53	0.41
1:D:244:HIS:HE1	1:D:286:CYS:O	2.03	0.41
1:C:279:LYS:HD3	1:D:334:PHE:CE1	2.52	0.41
1:D:334:PHE:C	1:D:334:PHE:HD2	2.23	0.41
1:A:80:SER:O	1:A:84:ILE:HG13	2.20	0.41
1:B:284:THR:HA	1:B:287:TYR:O	2.19	0.41
1:B:93:ILE:HD11	1:B:142:ARG:HH21	1.84	0.41
1:A:323:PHE:CD1	1:B:297:GLU:HG3	2.56	0.41
1:D:100:ARG:HD2	1:D:100:ARG:N	2.36	0.41
1:D:284:THR:HA	1:D:287:TYR:O	2.21	0.41
1:C:148:LEU:HD12	1:C:149:ASN:H	1.84	0.41
1:C:149:ASN:OD1	1:C:150:ASP:N	2.53	0.41
1:B:39:LEU:HA	2:F:632:GLN:HE22	1.85	0.41
1:A:297:GLU:HG2	1:A:297:GLU:H	1.48	0.41
1:B:176:ARG:HH22	3:B:401:GDP:N2	2.18	0.41
1:A:324:THR:HG22	1:A:335:VAL:HG21	2.03	0.41
1:C:105:ARG:O	1:C:109:VAL:HG23	2.20	0.41
1:C:270:LYS:HB3	1:C:273:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:PHE:HB3	1:A:133:ASP:OD2	2.19	0.41
1:A:168:ILE:HA	1:A:169:PRO:HD3	1.87	0.41
1:A:61:TYR:CD1	1:A:174:VAL:HG11	2.56	0.41
1:A:46:LYS:HB2	1:A:46:LYS:HE2	1.61	0.41
1:C:61:TYR:CD1	1:C:174:VAL:HG11	2.57	0.40
1:A:302:TYR:O	1:A:306:GLN:HG2	2.21	0.40
1:B:255:ASN:ND2	1:B:312:ARG:HG3	2.37	0.40
1:B:146:TYR:CE2	1:B:148:LEU:HB2	2.56	0.40
1:B:213:HIS:ND1	1:B:216:GLU:OE1	2.40	0.40
1:B:275:GLU:O	1:B:278:ILE:HG22	2.22	0.40
1:A:323:PHE:CE1	1:B:297:GLU:HG3	2.56	0.40
1:D:162:ILE:HG22	1:D:167:TYR:CZ	2.57	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	317/330 (96%)	305 (96%)	10 (3%)	2 (1%)	25 63
1	B	307/330 (93%)	295 (96%)	12 (4%)	0	100 100
1	C	311/330 (94%)	298 (96%)	13 (4%)	0	100 100
1	D	313/330 (95%)	298 (95%)	11 (4%)	4 (1%)	12 45
2	E	19/25 (76%)	17 (90%)	0	2 (10%)	0 5
2	F	20/25 (80%)	17 (85%)	1 (5%)	2 (10%)	0 6
2	G	20/25 (80%)	18 (90%)	2 (10%)	0	100 100
2	Z	19/25 (76%)	17 (90%)	0	2 (10%)	0 5
All	All	1326/1420 (93%)	1265 (95%)	49 (4%)	12 (1%)	17 54

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	VAL
2	E	635	ARG
2	F	635	ARG
2	Z	635	ARG
1	A	205	ARG
1	D	113	SER
1	D	236	GLU
2	F	636	MET
2	Z	636	MET
1	D	352	GLY
2	E	636	MET
1	D	118	VAL

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	246/290 (85%)	227 (92%)	19 (8%)	13 42
1	B	248/290 (86%)	230 (93%)	18 (7%)	14 44
1	C	247/290 (85%)	229 (93%)	18 (7%)	14 44
1	D	248/290 (86%)	226 (91%)	22 (9%)	9 36
2	E	20/24 (83%)	17 (85%)	3 (15%)	3 15
2	F	20/24 (83%)	18 (90%)	2 (10%)	7 30
2	G	20/24 (83%)	17 (85%)	3 (15%)	3 15
2	Z	20/24 (83%)	16 (80%)	4 (20%)	1 5
All	All	1069/1256 (85%)	980 (92%)	89 (8%)	11 38

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LYS
1	A	49	ILE
1	A	71	VAL
1	A	86	ARG

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Mol	Chain	Res	Type
1	A	106	GLN
1	A	113	SER
1	A	118	VAL
1	A	120	THR
1	A	153	SER
1	A	178	ARG
1	A	182	THR
1	A	234	LEU
1	A	238	GLU
1	A	239	GLU
1	A	240	MET
1	A	242	ARG
1	A	252	SER
1	A	297	GLU
1	A	331	ASN
1	B	46	LYS
1	B	58	GLU
1	B	71	VAL
1	B	100	ARG
1	B	103	ASP
1	B	106	GLN
1	B	113	SER
1	B	118	VAL
1	B	120	THR
1	B	149	ASN
1	B	153	SER
1	B	207	GLU
1	B	239	GLU
1	B	240	MET
1	B	241	ASN
1	B	297	GLU
1	B	305	CYS
1	B	315	ASP
1	C	36	LEU
1	C	46	LYS
1	C	49	ILE
1	C	58	GLU
1	C	71	VAL
1	C	79	GLN
1	C	113	SER
1	C	118	VAL
1	C	120	THR

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Mol	Chain	Res	Type
1	C	153	SER
1	C	160	ASP
1	C	178	ARG
1	C	182	THR
1	C	238	GLU
1	C	240	MET
1	C	242	ARG
1	C	297	GLU
1	C	305	CYS
1	D	36	LEU
1	D	46	LYS
1	D	49	ILE
1	D	58	GLU
1	D	71	VAL
1	D	79	GLN
1	D	100	ARG
1	D	103	ASP
1	D	113	SER
1	D	118	VAL
1	D	120	THR
1	D	153	SER
1	D	160	ASP
1	D	178	ARG
1	D	182	THR
1	D	234	LEU
1	D	238	GLU
1	D	240	MET
1	D	252	SER
1	D	297	GLU
1	D	331	ASN
1	D	334	PHE
2	E	635	ARG
2	E	641	VAL
2	E	642	LEU
2	F	640	ARG
2	F	642	LEU
2	G	635	ARG
2	G	642	LEU
2	G	643	LEU
2	Z	635	ARG
2	Z	640	ARG
2	Z	641	VAL

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Mol	Chain	Res	Type
2	Z	642	LEU

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

Mol	Chain	Res	Type
1	A	79	GLN
1	D	255	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

11 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	CIT	B	403	-	3,12,12	1.39	0	3,17,17	2.42	2 (66%)
4	SO4	B	404	-	4,4,4	0.14	0	6,6,6	0.07	0
4	SO4	A	402	-	4,4,4	0.14	0	6,6,6	0.05	0
5	CIT	B	402	-	3,12,12	1.40	0	3,17,17	2.59	2 (66%)
3	GDP	A	401	-	24,30,30	1.14	2 (8%)	31,47,47	2.00	7 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GDP	C	401	-	24,30,30	1.15	2 (8%)	31,47,47	1.94	8 (25%)
3	GDP	D	401	-	24,30,30	1.13	2 (8%)	31,47,47	1.96	8 (25%)
5	CIT	C	402	-	3,12,12	1.41	0	3,17,17	2.27	2 (66%)
4	SO4	C	404	-	4,4,4	0.15	0	6,6,6	0.05	0
3	GDP	B	401	-	24,30,30	1.15	2 (8%)	31,47,47	1.94	8 (25%)
5	CIT	C	403	-	3,12,12	1.75	1 (33%)	3,17,17	3.95	2 (66%)

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
5	CIT	B	403	-	-	0/6/16/16	-
5	CIT	B	402	-	-	1/6/16/16	-
3	GDP	A	401	-	-	5/12/32/32	0/3/3/3
3	GDP	C	401	-	-	3/12/32/32	0/3/3/3
3	GDP	D	401	-	-	3/12/32/32	0/3/3/3
5	CIT	C	402	-	-	0/6/16/16	-
3	GDP	B	401	-	-	3/12/32/32	0/3/3/3
5	CIT	C	403	-	-	3/6/16/16	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	GDP	C6-C5	4.05	1.48	1.41
3	B	401	GDP	C6-C5	4.02	1.48	1.41
3	C	401	GDP	C6-C5	4.00	1.48	1.41
3	D	401	GDP	C6-C5	3.87	1.48	1.41
3	C	401	GDP	C5-C4	2.41	1.47	1.40
3	B	401	GDP	C5-C4	2.40	1.47	1.40
3	D	401	GDP	C5-C4	2.32	1.47	1.40
3	A	401	GDP	C5-C4	2.26	1.46	1.40
5	C	403	CIT	C2-C3	-2.24	1.51	1.54

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	403	CIT	C3-C2-C1	-6.35	104.82	114.98
3	A	401	GDP	C2-N3-C4	4.86	120.91	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	401	GDP	C2-N3-C4	4.83	120.87	115.36
3	D	401	GDP	C2-N3-C4	4.69	120.71	115.36
3	B	401	GDP	C2-N3-C4	4.65	120.67	115.36
3	B	401	GDP	C5-C6-N1	-4.03	117.91	123.43
3	C	401	GDP	C5-C6-N1	-4.00	117.96	123.43
3	B	401	GDP	C6-N1-C2	3.97	122.24	115.93
3	A	401	GDP	C6-N1-C2	3.96	122.22	115.93
3	D	401	GDP	C5-C6-N1	-3.94	118.05	123.43
3	A	401	GDP	C6-C5-C4	-3.94	117.04	120.80
3	A	401	GDP	C5-C6-N1	-3.90	118.09	123.43
3	D	401	GDP	C6-N1-C2	3.88	122.09	115.93
3	C	401	GDP	C6-N1-C2	3.80	121.97	115.93
3	D	401	GDP	C6-C5-C4	-3.66	117.31	120.80
3	B	401	GDP	C6-C5-C4	-3.60	117.36	120.80
3	D	401	GDP	PA-O3A-PB	-3.56	120.62	132.83
3	A	401	GDP	PA-O3A-PB	-3.53	120.71	132.83
3	C	401	GDP	PA-O3A-PB	-3.53	120.72	132.83
3	A	401	GDP	N3-C2-N1	-3.35	122.76	127.22
3	B	401	GDP	PA-O3A-PB	-3.28	121.59	132.83
5	B	403	CIT	C3-C4-C5	-3.26	109.76	114.98
5	B	402	CIT	C3-C4-C5	-3.16	109.93	114.98
3	B	401	GDP	N3-C2-N1	-3.15	123.02	127.22
3	C	401	GDP	C3'-C2'-C1'	3.15	105.72	100.98
3	D	401	GDP	N3-C2-N1	-3.14	123.03	127.22
3	C	401	GDP	C6-C5-C4	-3.13	117.81	120.80
5	B	402	CIT	C3-C2-C1	-3.07	110.07	114.98
5	C	402	CIT	C3-C4-C5	-3.00	110.18	114.98
3	C	401	GDP	N3-C2-N1	-2.99	123.24	127.22
3	A	401	GDP	C4-C5-N7	-2.93	106.35	109.40
3	B	401	GDP	C4-C5-N7	-2.88	106.40	109.40
3	D	401	GDP	C4-C5-N7	-2.77	106.51	109.40
3	C	401	GDP	C4-C5-N7	-2.66	106.63	109.40
5	B	403	CIT	C3-C2-C1	-2.58	110.85	114.98
5	C	402	CIT	C3-C2-C1	-2.51	110.96	114.98
3	D	401	GDP	C3'-C2'-C1'	2.48	104.71	100.98
5	C	403	CIT	C3-C4-C5	-2.47	111.03	114.98
3	B	401	GDP	C3'-C2'-C1'	2.46	104.69	100.98

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	GDP	C5'-O5'-PA-O1A
3	C	401	GDP	C5'-O5'-PA-O1A
3	D	401	GDP	C5'-O5'-PA-O1A
3	D	401	GDP	C5'-O5'-PA-O2A
3	B	401	GDP	C5'-O5'-PA-O1A
3	A	401	GDP	O4'-C4'-C5'-O5'
5	B	402	CIT	C2-C3-C4-C5
5	C	403	CIT	C1-C2-C3-O7
5	C	403	CIT	C1-C2-C3-C4
3	A	401	GDP	C5'-O5'-PA-O3A
3	C	401	GDP	C5'-O5'-PA-O3A
3	B	401	GDP	C5'-O5'-PA-O3A
3	A	401	GDP	C5'-O5'-PA-O2A
3	C	401	GDP	C5'-O5'-PA-O2A
3	B	401	GDP	C5'-O5'-PA-O2A
5	C	403	CIT	C1-C2-C3-C6
3	A	401	GDP	C3'-C4'-C5'-O5'
3	D	401	GDP	C5'-O5'-PA-O3A

There are no ring outliers.

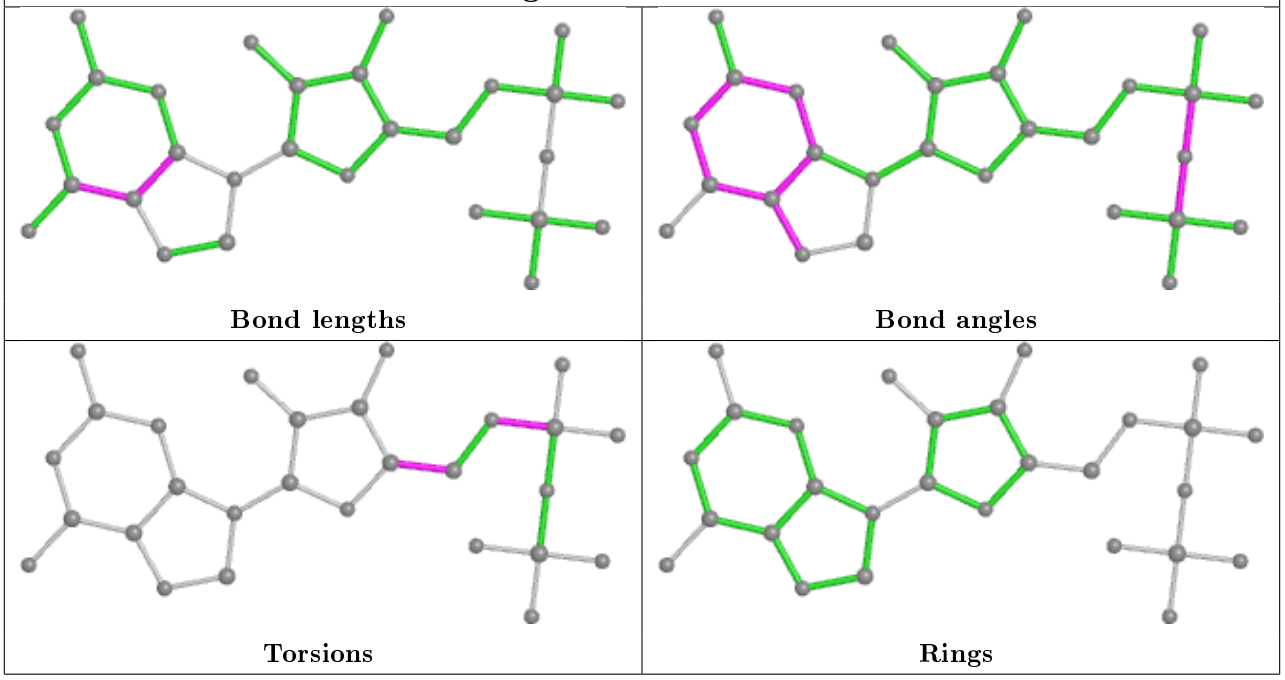
8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	403	CIT	1	0
5	B	402	CIT	3	0
3	A	401	GDP	2	0
3	C	401	GDP	3	0
3	D	401	GDP	1	0
5	C	402	CIT	1	0
3	B	401	GDP	4	0
5	C	403	CIT	1	0

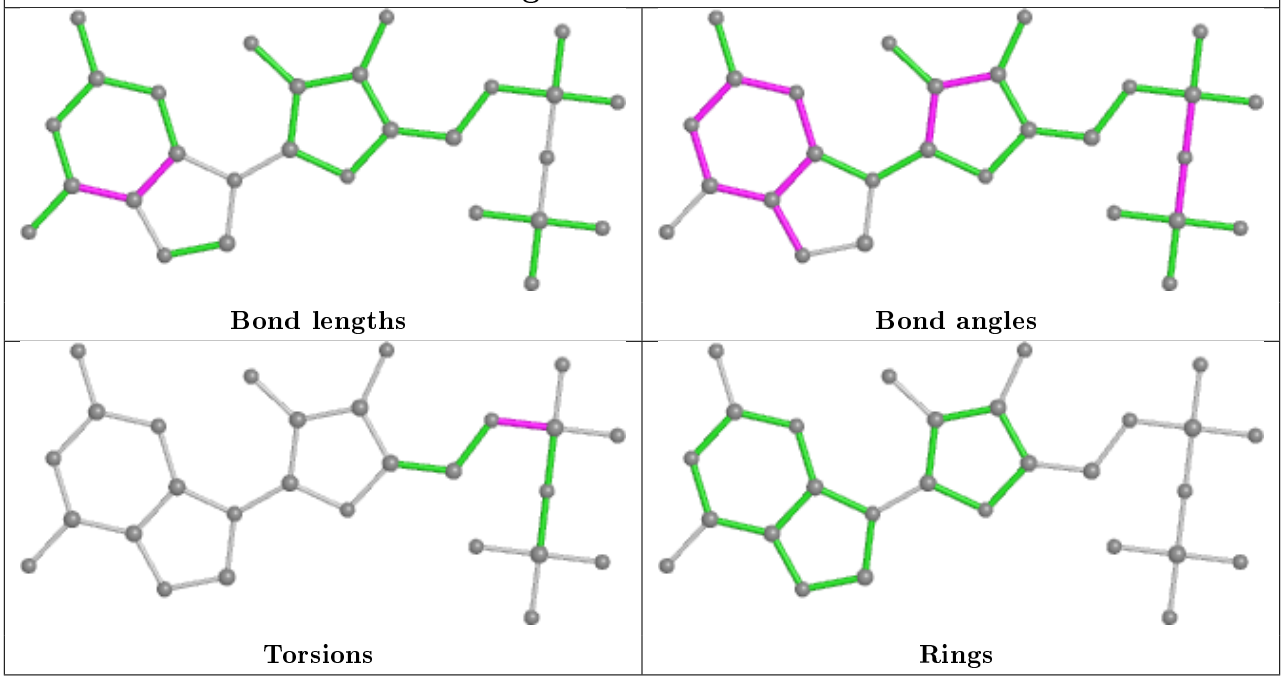
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

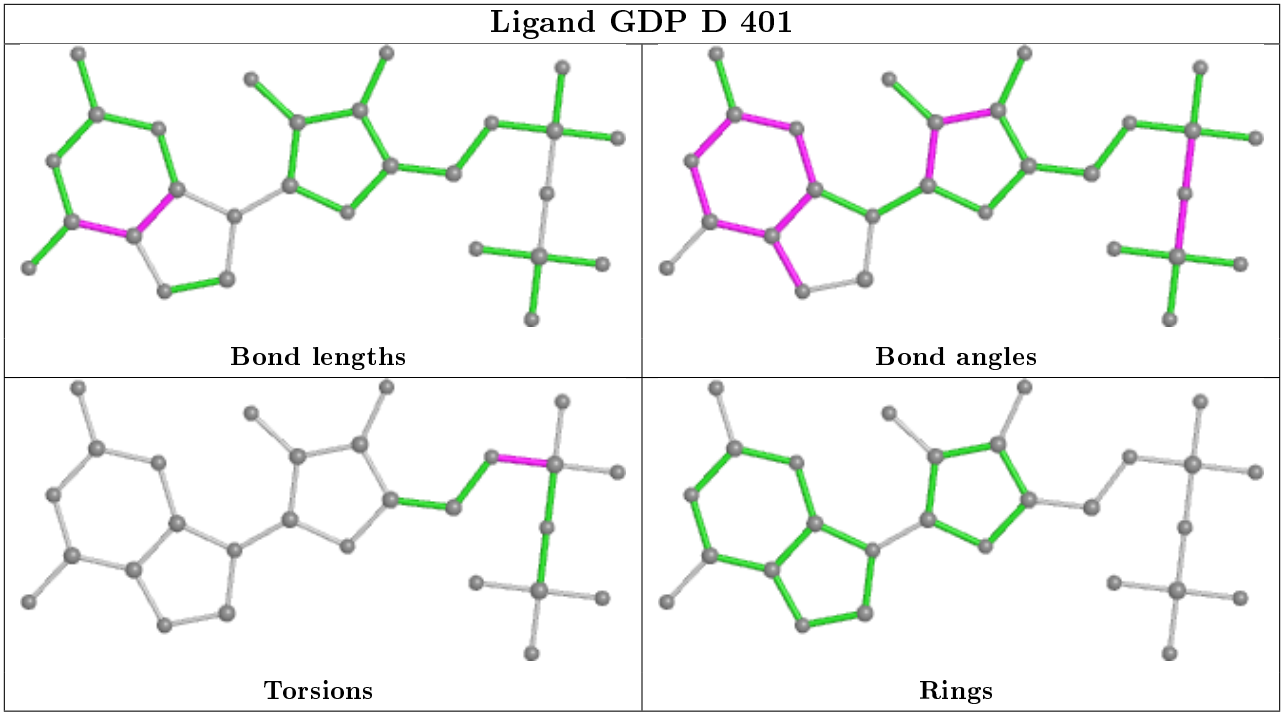
equivalents in the CSD to analyse the geometry.

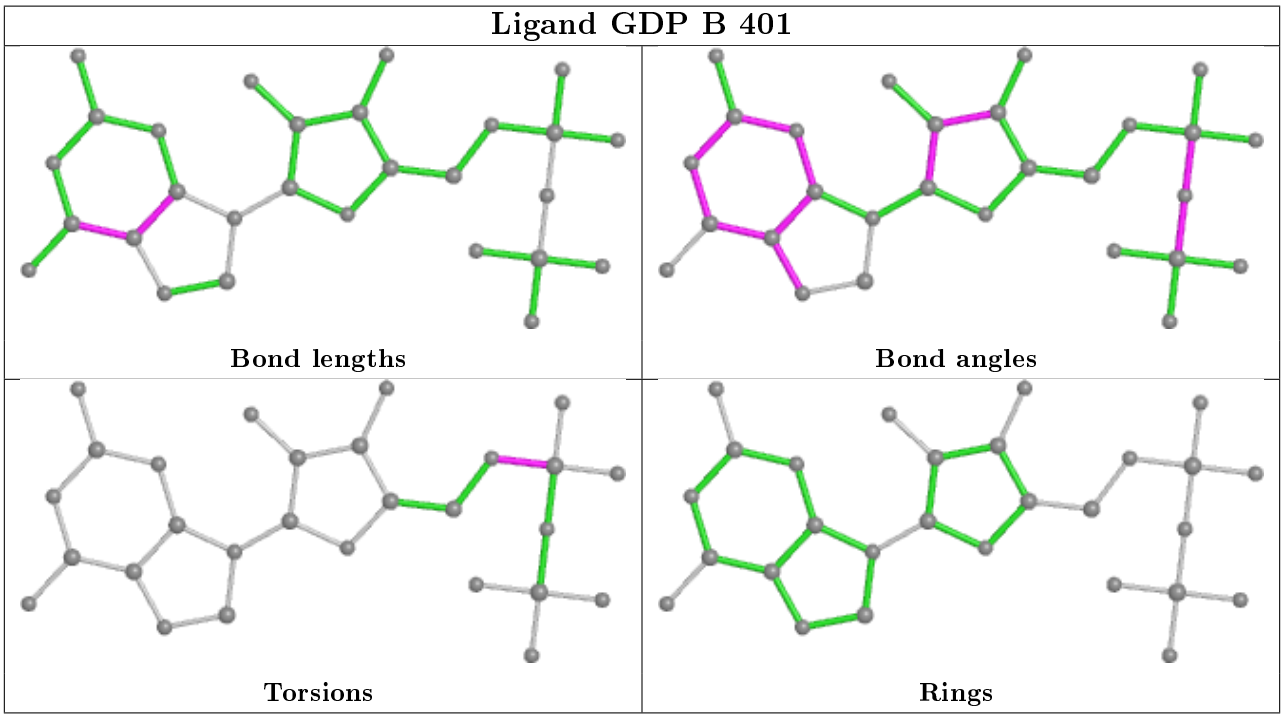
Ligand GDP A 401



Ligand GDP C 401







5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	319/330 (96%)	0.05	5 (1%) 72 68	60, 97, 142, 167	0
1	B	313/330 (94%)	0.18	15 (4%) 30 29	55, 99, 157, 178	0
1	C	317/330 (96%)	0.16	10 (3%) 47 45	50, 100, 169, 191	0
1	D	317/330 (96%)	0.18	14 (4%) 34 32	57, 99, 151, 166	0
2	E	21/25 (84%)	0.12	0 100 100	82, 102, 137, 144	0
2	F	22/25 (88%)	0.08	0 100 100	80, 96, 122, 144	0
2	G	22/25 (88%)	0.16	0 100 100	81, 100, 136, 152	0
2	Z	21/25 (84%)	0.52	2 (9%) 8 10	97, 125, 153, 163	0
All	All	1352/1420 (95%)	0.15	46 (3%) 45 42	50, 100, 154, 191	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	162	ILE	3.9
1	A	165	SER	3.5
1	B	155	TYR	3.5
1	B	95	PHE	3.4
1	C	116	GLU	3.3
1	B	164	GLN	3.3
1	D	98	ALA	3.2
1	D	179	VAL	3.0
1	D	97	GLU	3.0
1	D	180	LYS	2.9
1	B	167	TYR	2.8
1	D	314	LYS	2.7
1	B	163	SER	2.7
1	D	126	VAL	2.7
1	D	95	PHE	2.7
1	C	102	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	175	LEU	2.6
1	C	97	GLU	2.5
1	B	127	ILE	2.5
1	A	167	TYR	2.5
1	B	168	ILE	2.5
1	C	95	PHE	2.5
1	D	96	GLY	2.4
1	C	168	ILE	2.4
1	C	113	SER	2.3
1	D	101	ALA	2.3
1	A	164	GLN	2.3
2	Z	623	ASP	2.3
1	A	168	ILE	2.3
1	C	98	ALA	2.3
1	D	118	VAL	2.2
1	B	93	ILE	2.2
2	Z	635	ARG	2.2
1	B	61	TYR	2.1
1	B	125	GLY	2.1
1	C	69	TYR	2.1
1	D	182	THR	2.1
1	B	96	GLY	2.1
1	B	98	ALA	2.1
1	C	118	VAL	2.1
1	B	69	TYR	2.1
1	D	43	GLU	2.1
1	A	195	TYR	2.1
1	D	195	TYR	2.1
1	D	215	PHE	2.0
1	C	96	GLY	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 carbohydrates in this entry.

6.4 Ligands

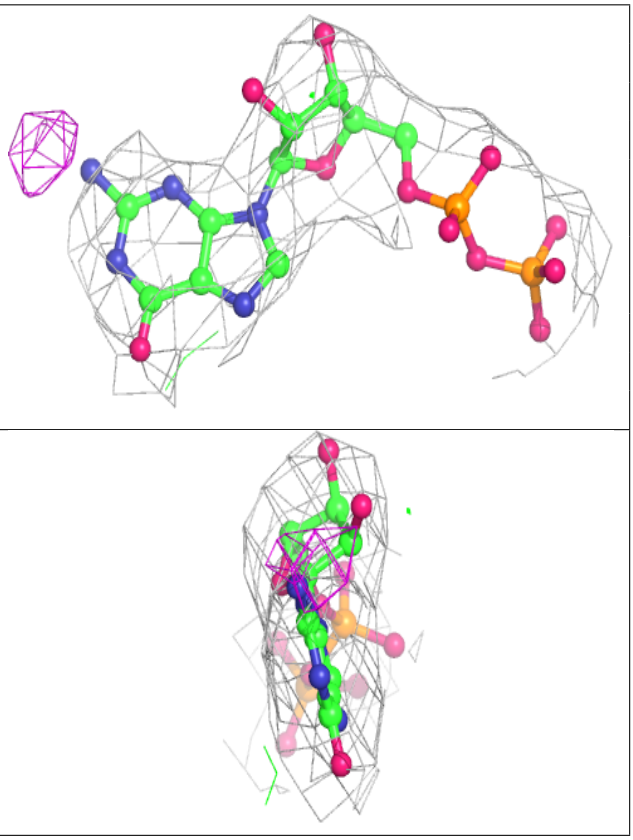
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	SO4	B	404	5/5	0.81	0.25	130,132,163,163	0
4	SO4	A	402	5/5	0.84	0.22	144,160,185,189	0
4	SO4	C	404	5/5	0.88	0.12	127,156,165,171	0
5	CIT	C	403	13/13	0.89	0.30	83,102,121,121	0
5	CIT	C	402	13/13	0.90	0.23	76,94,114,126	0
5	CIT	B	402	13/13	0.92	0.33	86,105,120,121	0
5	CIT	B	403	13/13	0.93	0.28	76,93,112,130	0
3	GDP	A	401	28/28	0.97	0.20	77,88,99,120	0
3	GDP	C	401	28/28	0.97	0.21	60,80,94,110	0
3	GDP	B	401	28/28	0.97	0.23	66,93,109,122	0
3	GDP	D	401	28/28	0.97	0.23	53,80,98,110	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.

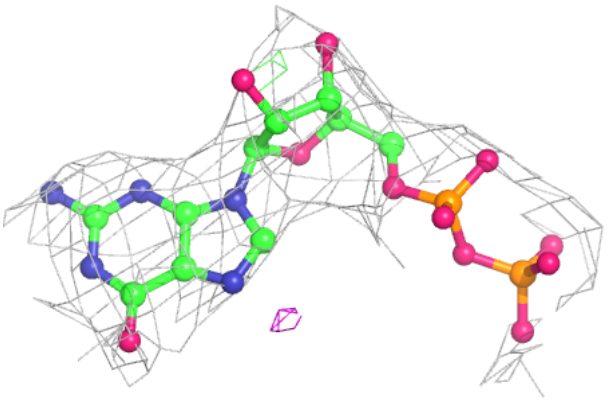
Electron density around GDP A 401:

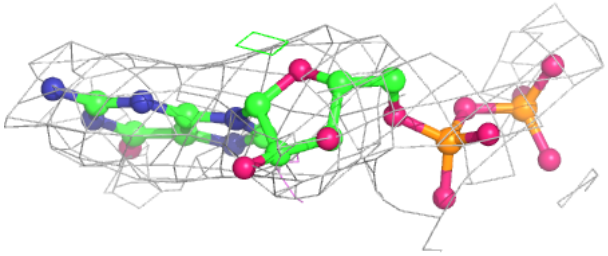
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

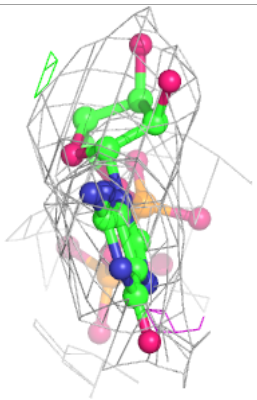


Electron density around GDP C 401:

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

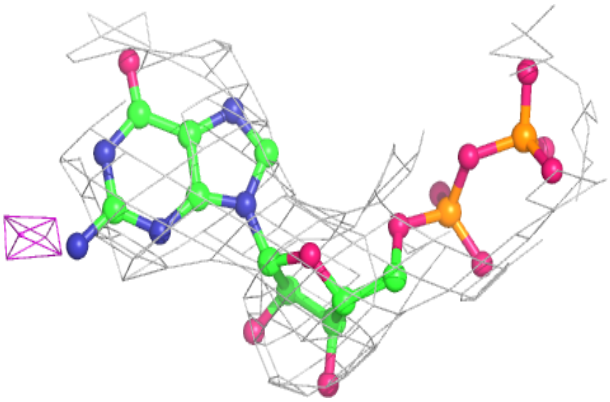


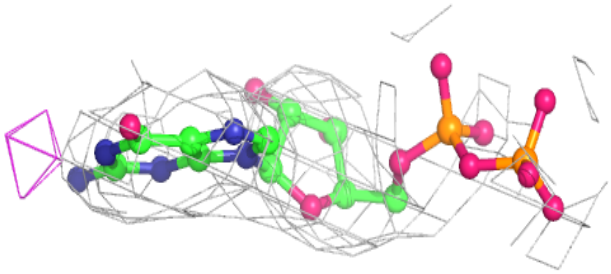


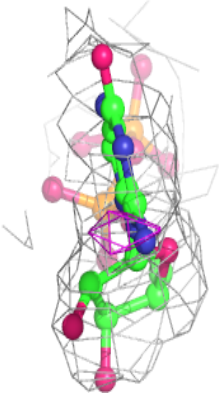


Electron density around GDP B 401:

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

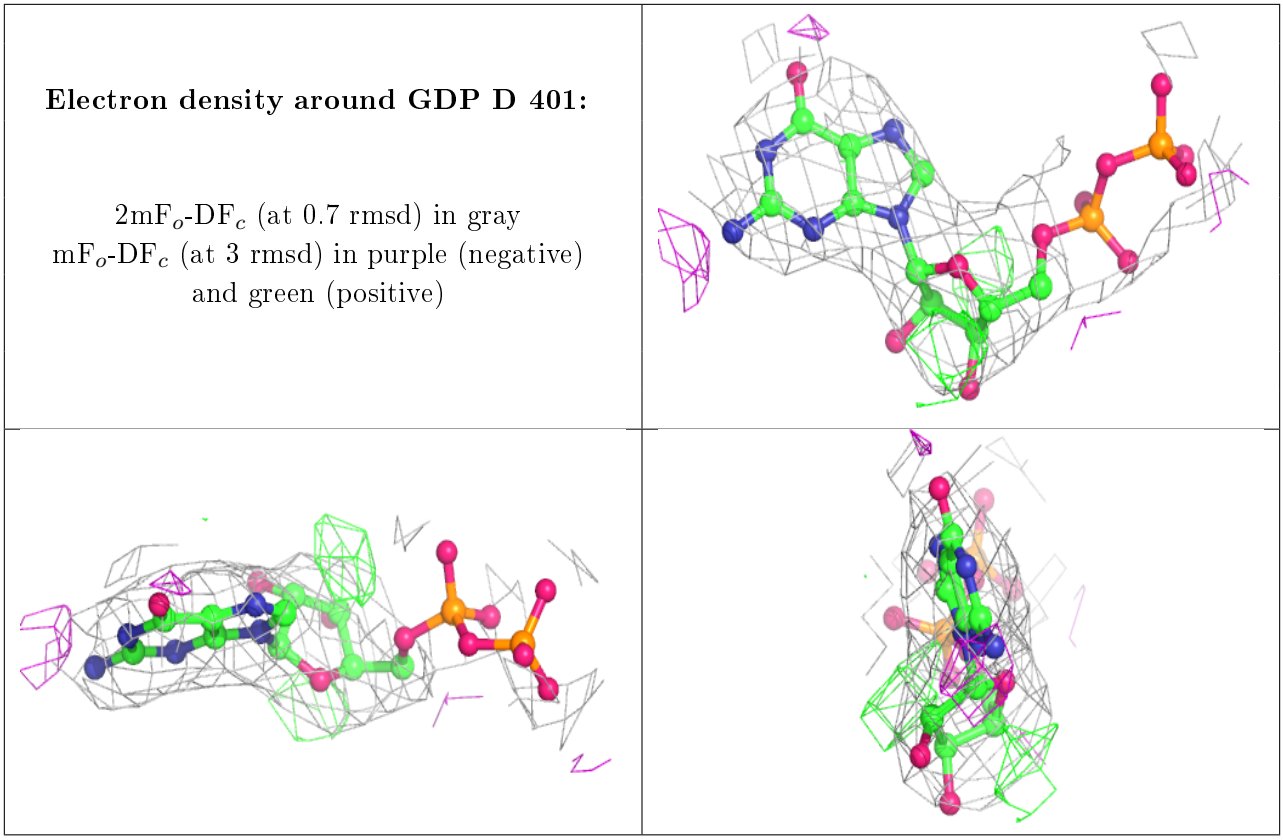






Electron density around GDP D 401:

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



6.5 Other polymers (i)

There are no such residues in this entry.