



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 04:09 pm BST

PDB ID : 6JSJ
Title : Structural analysis of a trimeric assembly of the mitochondrial dynamin-like GTPase Mgm1
Authors : Yan, L.; Li, L.
Deposited on : 2019-04-08
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

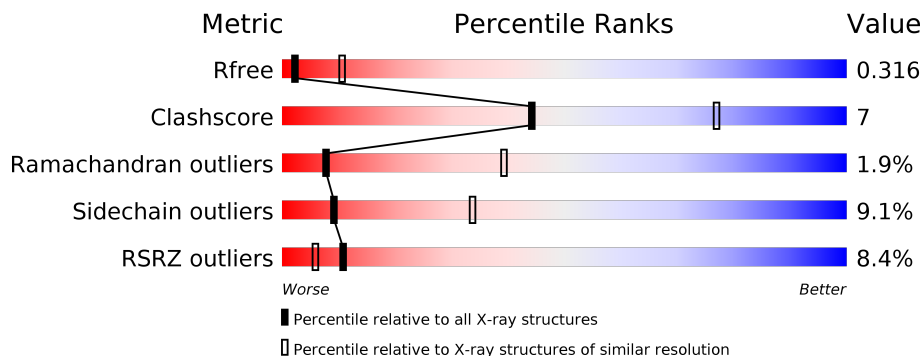
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	698	
1	B	698	
1	C	698	

2 Entry composition [i](#)

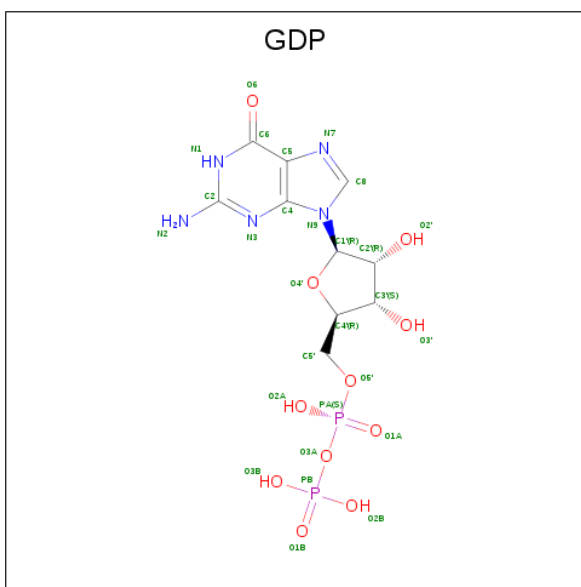
There are 3 unique types of molecules in this entry. The entry contains 15082 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dynamin-like GTPase MGM1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	625	Total 5014	C 3185	N 851	O 956	S 22	0	0	0
1	B	624	Total 5001	C 3178	N 848	O 953	S 22	0	0	0
1	C	619	Total 4958	C 3151	N 840	O 946	S 21	0	0	0

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by author).



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

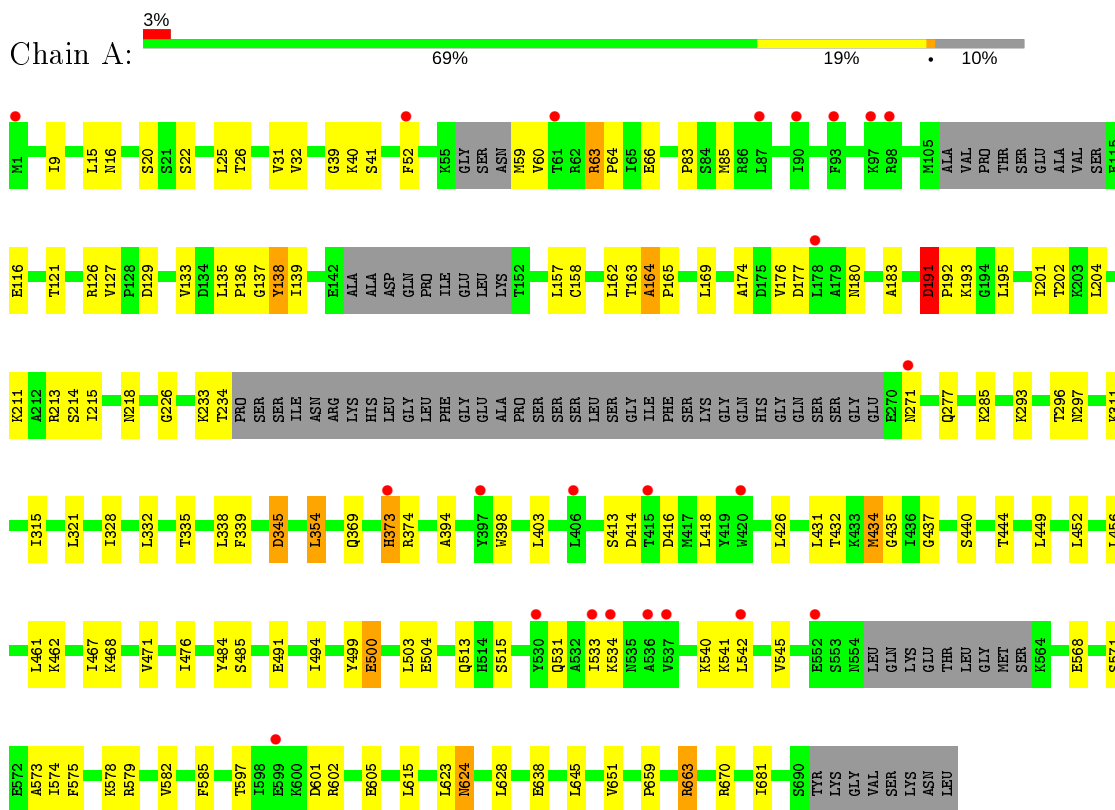
- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	10	Total I 10 10	0	0
3	A	9	Total I 9 9	0	0
3	C	6	Total I 6 6	0	0

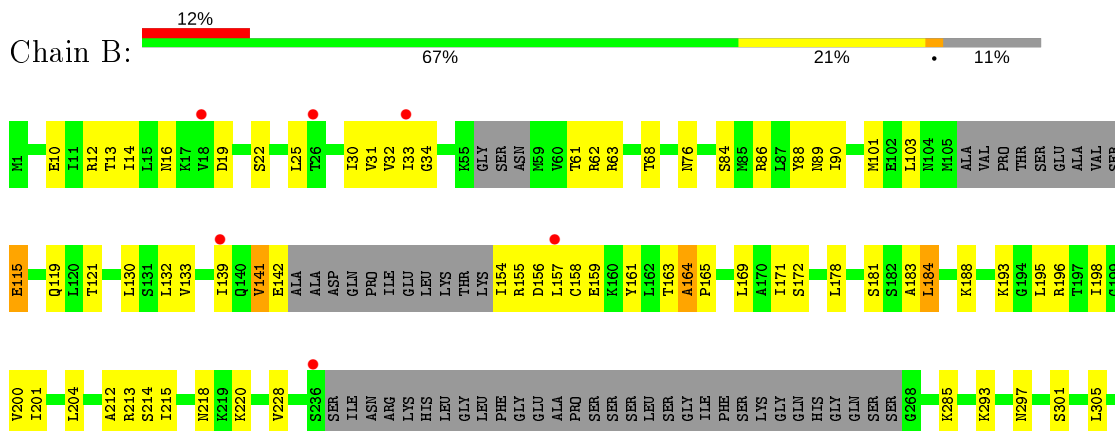
3 Residue-property plots [i](#)

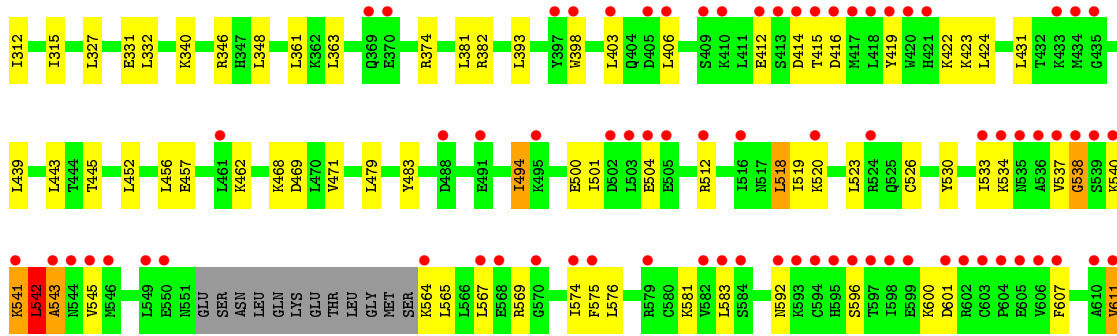
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Dynamin-like GTPase MGM1, mitochondrial

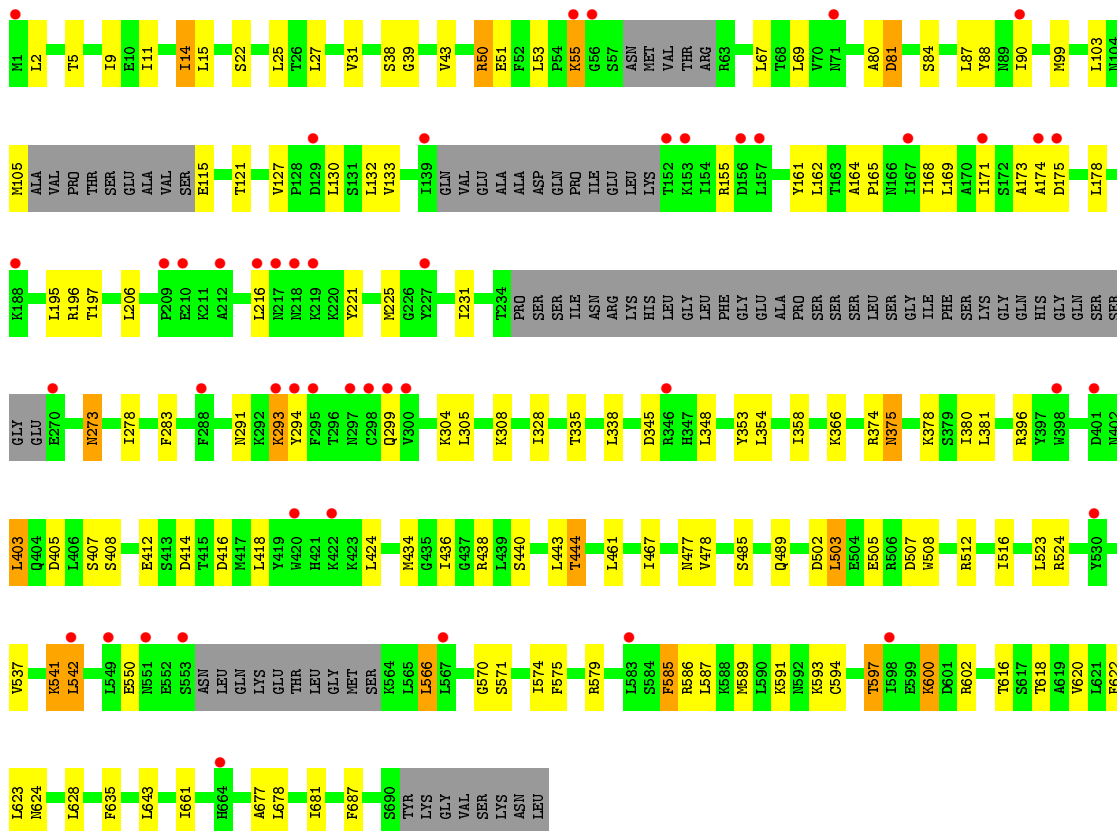


- Molecule 1: Dynamin-like GTPase MGM1, mitochondrial





• Molecule 1: Dynamamin-like GTPase MGM1, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	152.94Å 152.94Å 236.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.17 – 3.20 49.16 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.17-3.20) 100.0 (49.16-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 3.19Å)	Xtrriage
Refinement program	PHENIX v1.0	Depositor
R, R_{free}	0.243 , 0.306 0.267 , 0.316	Depositor DCC
R_{free} test set	2292 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	118.5	Xtrriage
Anisotropy	0.302	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 115.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15082	wwPDB-VP
Average B, all atoms (Å ²)	135.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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, IOD

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	0.45	0/5078	0.69	0/6830
1	B	0.46	0/5066	0.72	1/6815 (0.0%)
1	C	0.45	0/5022	0.67	0/6754
All	All	0.45	0/15166	0.69	1/20399 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	538	GLY	N-CA-C	16.31	153.88	113.10

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	5014	0	5214	55	0
1	B	5001	0	5198	89	0
1	C	4958	0	5155	65	0
2	A	28	0	12	0	0
2	B	28	0	12	0	0
2	C	28	0	12	0	0
3	A	9	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	10	0	0	3	0
3	C	6	0	0	3	0
All	All	15082	0	15603	203	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 7.

All (203) 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:541:LYS:HA	1:B:542:LEU:CB	1.69	1.22
1:B:541:LYS:HA	1:B:542:LEU:HB3	1.18	1.16
1:B:541:LYS:CA	1:B:542:LEU:CB	2.30	1.06
1:B:542:LEU:O	1:B:542:LEU:HD13	1.55	1.04
1:B:541:LYS:N	1:B:542:LEU:HB2	1.74	1.03
1:B:537:VAL:HG22	1:B:538:GLY:N	1.74	1.02
1:B:541:LYS:H	1:B:542:LEU:HB2	1.23	1.01
1:B:537:VAL:CG2	1:B:538:GLY:H	1.74	0.99
1:B:541:LYS:CA	1:B:542:LEU:HB2	1.94	0.98
1:B:540:LYS:O	1:B:541:LYS:HD3	1.68	0.94
1:B:541:LYS:HG2	1:B:541:LYS:O	1.65	0.93
1:B:537:VAL:CG2	1:B:538:GLY:N	2.30	0.92
1:A:191:ASP:HB3	1:A:192:PRO:HA	1.57	0.84
1:C:403:LEU:HB3	1:C:585:PHE:HZ	1.43	0.84
1:B:542:LEU:HD22	1:B:542:LEU:O	1.79	0.82
1:B:541:LYS:CG	1:B:541:LYS:O	2.30	0.80
1:B:542:LEU:CD1	1:B:542:LEU:O	2.30	0.80
1:B:540:LYS:O	1:B:541:LYS:CG	2.30	0.79
1:B:540:LYS:O	1:B:541:LYS:CD	2.30	0.79
1:B:542:LEU:O	1:B:543:ALA:CB	2.32	0.77
1:C:174:ALA:HA	1:C:178:LEU:HD21	1.68	0.75
1:B:541:LYS:HA	1:B:542:LEU:HB2	1.58	0.75
1:B:541:LYS:O	1:B:545:VAL:HG23	1.87	0.74
1:B:537:VAL:HG23	1:B:538:GLY:H	1.51	0.73
1:B:530:TYR:HA	1:C:293:LYS:HE2	1.72	0.70
1:B:613:ASP:HA	1:B:616:THR:HB	1.72	0.70
1:A:440:SER:O	1:A:444:THR:HG22	1.92	0.69
1:A:191:ASP:HB3	1:A:192:PRO:CA	2.22	0.69
1:C:407:SER:HB3	1:C:589:MET:SD	2.34	0.68
1:B:542:LEU:HD22	1:B:542:LEU:C	2.14	0.67
1:B:624:ASN:HA	1:B:628:LEU:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:TYR:H	1:B:76:ASN:HD21	1.44	0.65
1:A:164:ALA:HB1	1:A:165:PRO:HD2	1.77	0.65
1:B:84:SER:HB3	3:B:705:IOD:I	2.66	0.65
1:A:138:TYR:HD1	1:A:139:ILE:H	1.44	0.64
1:C:440:SER:O	1:C:444:THR:HG22	1.98	0.63
1:C:566:LEU:HD13	1:C:566:LEU:H	1.63	0.63
1:B:141:VAL:HA	1:B:155:ARG:HG3	1.80	0.63
1:B:541:LYS:CA	1:B:542:LEU:HB3	2.03	0.63
1:B:142:GLU:HB3	1:B:154:ILE:HG21	1.80	0.62
1:A:164:ALA:HB1	1:A:165:PRO:CD	2.29	0.62
1:A:271:ASN:HB3	1:C:477:ASN:OD1	1.99	0.62
1:A:461:LEU:HD22	1:A:467:ILE:HG21	1.82	0.62
1:A:452:LEU:HD21	1:A:471:VAL:HG12	1.82	0.61
1:B:542:LEU:O	1:B:542:LEU:CD2	2.47	0.61
1:B:540:LYS:O	1:B:541:LYS:HG2	2.00	0.61
1:C:678:LEU:HA	1:C:681:ILE:HG22	1.82	0.61
1:B:542:LEU:O	1:B:543:ALA:HB2	1.99	0.61
1:C:537:VAL:HG12	1:C:541:LYS:HD2	1.83	0.59
1:B:163:THR:HA	1:B:196:ARG:HH22	1.67	0.59
1:A:449:LEU:HD11	1:A:476:ILE:HD13	1.85	0.59
1:A:624:ASN:HA	1:A:628:LEU:HB2	1.83	0.58
1:C:461:LEU:HD22	1:C:467:ILE:HG21	1.85	0.58
1:B:155:ARG:HB3	1:B:158:CYS:HB2	1.87	0.56
1:B:22:SER:HA	1:B:25:LEU:HD13	1.87	0.56
1:A:311:LYS:O	1:A:315:ILE:HG12	2.05	0.56
1:B:607:PHE:O	1:B:611:VAL:HB	2.04	0.56
1:C:624:ASN:HA	1:C:628:LEU:HB2	1.86	0.56
1:B:457:GLU:HA	1:B:462:LYS:HB3	1.87	0.56
1:C:403:LEU:HB3	1:C:585:PHE:CZ	2.32	0.56
1:B:172:SER:O	1:B:201:ILE:HA	2.06	0.56
1:C:14:ILE:HD11	1:C:677:ALA:HB2	1.88	0.56
1:B:542:LEU:O	1:B:542:LEU:CG	2.52	0.55
1:C:81:ASP:HB2	1:C:121:THR:HB	1.87	0.55
1:B:452:LEU:HD21	1:B:471:VAL:HG12	1.88	0.55
1:B:439:LEU:O	1:B:443:LEU:HB2	2.08	0.54
1:B:534:LYS:HE3	1:B:540:LYS:NZ	2.22	0.54
1:A:31:VAL:HG12	1:A:133:VAL:HB	1.91	0.53
1:B:381:LEU:HD23	1:B:616:THR:HG23	1.90	0.53
1:B:31:VAL:HG12	1:B:133:VAL:HB	1.90	0.53
1:A:193:LYS:HD3	1:A:195:LEU:HD11	1.90	0.53
1:C:537:VAL:HG11	1:C:542:LEU:HD23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:THR:HG21	1:A:623:LEU:HD22	1.91	0.53
1:C:15:LEU:HD11	1:C:328:ILE:HD11	1.92	0.52
1:B:537:VAL:HG22	1:B:538:GLY:H	1.42	0.52
1:A:663:ARG:HG2	3:A:704:IOD:I	2.80	0.52
1:C:38:SER:HB2	1:C:173:ALA:HB2	1.91	0.52
1:A:138:TYR:OH	1:A:183:ALA:HA	2.10	0.52
1:B:596:SER:HB3	1:B:600:LYS:H	1.75	0.52
1:B:181:SER:OG	1:B:184:LEU:HB2	2.10	0.51
1:B:542:LEU:O	1:B:543:ALA:HB3	2.10	0.51
1:A:32:VAL:HG12	1:A:169:LEU:HB3	1.91	0.51
1:B:412:GLU:H	1:B:416:ASP:HB3	1.75	0.51
1:C:358:ILE:HG21	1:C:643:LEU:HD11	1.93	0.50
1:B:611:VAL:O	1:B:615:LEU:HG	2.11	0.50
1:C:31:VAL:HG12	1:C:133:VAL:HB	1.94	0.50
1:C:53:LEU:HB3	1:C:55:LYS:HD2	1.93	0.50
1:A:158:CYS:O	1:A:162:LEU:HB2	2.13	0.49
1:A:321:LEU:HD22	1:A:681:ILE:HG23	1.93	0.49
1:C:51:GLU:HB2	1:C:273:ASN:HD21	1.76	0.49
1:A:332:LEU:HA	1:A:335:THR:HG22	1.94	0.49
1:C:412:GLU:H	1:C:416:ASP:HB2	1.78	0.49
1:B:61:THR:HG23	3:B:710:IOD:I	2.83	0.49
1:C:434:MET:CE	1:C:436:ILE:HG13	2.42	0.49
1:C:505:GLU:HA	1:C:508:TRP:HB3	1.95	0.49
1:A:174:ALA:C	1:A:176:VAL:H	2.15	0.49
1:A:575:PHE:CZ	1:B:297:ASN:HB2	2.48	0.49
1:C:5:THR:O	1:C:9:ILE:HG12	2.13	0.49
1:A:515:SER:HB2	1:A:605:GLU:HB3	1.95	0.49
1:B:540:LYS:O	1:B:541:LYS:CB	2.61	0.49
1:A:373:HIS:HD1	1:A:628:LEU:HD23	1.78	0.48
1:C:69:LEU:HB3	1:C:127:VAL:HG13	1.96	0.48
1:A:211:LYS:HE3	1:A:215:ILE:HD11	1.96	0.48
1:B:382:ARG:HG3	1:B:616:THR:HG21	1.94	0.48
1:C:485:SER:O	1:C:489:GLN:HB2	2.13	0.48
1:C:348:LEU:HD21	1:C:661:ILE:HG23	1.94	0.48
1:A:339:PHE:CD2	1:A:345:ASP:HA	2.49	0.48
1:B:494:ILE:HD11	1:B:615:LEU:HB3	1.96	0.48
1:C:155:ARG:HD2	1:C:155:ARG:H	1.79	0.48
1:A:431:LEU:O	1:A:434:MET:HB3	2.13	0.47
1:A:574:ILE:HG22	1:A:578:LYS:HE2	1.97	0.47
1:C:381:LEU:HD23	1:C:616:THR:HG23	1.96	0.47
1:A:174:ALA:HB2	1:A:201:ILE:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:ALA:HB1	1:B:165:PRO:CD	2.45	0.47
1:A:22:SER:HA	1:A:25:LEU:HD23	1.97	0.47
1:B:30:ILE:HB	1:B:132:LEU:HD23	1.95	0.47
1:B:534:LYS:HE3	1:B:540:LYS:HZ1	1.79	0.47
1:C:162:LEU:HD22	1:C:168:ILE:HD12	1.97	0.47
1:B:228:VAL:HG11	1:B:305:LEU:HB2	1.97	0.47
1:C:571:SER:HA	1:C:574:ILE:HD12	1.97	0.47
1:A:32:VAL:HG23	1:A:40:LYS:HE2	1.97	0.47
1:C:622:PHE:N	1:C:622:PHE:HD1	2.13	0.47
1:A:394:ALA:HA	1:A:398:TRP:HB2	1.97	0.47
1:A:432:THR:HG22	1:A:615:LEU:HD11	1.96	0.47
1:A:571:SER:HA	1:A:574:ILE:HD12	1.97	0.46
1:B:642:ARG:HA	1:B:645:LEU:HD12	1.97	0.46
1:B:682:ASP:O	1:B:686:VAL:HG23	2.16	0.46
1:C:168:ILE:HG23	1:C:197:THR:HG23	1.97	0.46
1:C:622:PHE:CD1	1:C:622:PHE:N	2.82	0.46
1:A:582:VAL:HA	1:A:585:PHE:CE2	2.50	0.46
1:C:444:THR:HG21	1:C:623:LEU:HD22	1.98	0.46
1:B:34:GLY:HA2	1:B:183:ALA:HB2	1.96	0.46
1:B:541:LYS:N	1:B:542:LEU:CB	2.56	0.46
1:C:353:TYR:HA	3:C:706:IOD:I	2.86	0.46
1:B:68:THR:HB	1:B:121:THR:HG22	1.98	0.45
1:A:15:LEU:HD11	1:A:328:ILE:HD11	1.99	0.45
1:C:512:ARG:O	1:C:516:ILE:HG12	2.16	0.45
1:A:177:ASP:HB3	1:A:180:ASN:HD22	1.80	0.45
1:C:478:VAL:HG21	1:C:635:PHE:HA	1.98	0.45
1:A:293:LYS:HZ1	1:C:524:ARG:HH22	1.63	0.45
1:B:332:LEU:HD13	1:B:674:LEU:HB3	1.99	0.45
1:C:31:VAL:HG11	1:C:161:TYR:HB3	1.98	0.45
1:C:587:LEU:HG	1:C:591:LYS:HE2	1.97	0.45
1:B:212:ALA:HA	1:B:215:ILE:HD12	1.98	0.45
1:C:67:LEU:HD23	1:C:132:LEU:HD13	1.98	0.45
1:B:220:LYS:HG3	3:B:711:IOD:I	2.87	0.44
1:B:518:LEU:HD23	1:B:519:ILE:HG13	1.99	0.44
1:B:519:ILE:O	1:B:523:LEU:HB2	2.17	0.44
1:C:43:VAL:HG21	1:C:171:ILE:HG12	1.99	0.44
1:A:531:GLN:HA	1:A:534:LYS:HB2	1.99	0.44
1:C:542:LEU:HD11	1:C:570:GLY:HA2	1.99	0.44
1:A:456:LEU:HD22	1:A:468:LYS:HG2	2.00	0.44
1:C:403:LEU:HD22	1:C:586:ARG:HD3	1.99	0.44
1:A:354:LEU:HG	1:A:651:VAL:HG13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:LYS:HE3	1:B:195:LEU:HD21	1.99	0.44
1:A:437:GLY:HA3	1:A:491:GLU:HG2	2.00	0.44
1:C:22:SER:HA	1:C:25:LEU:HD12	2.00	0.44
1:C:50:ARG:HG3	1:C:273:ASN:HB3	1.99	0.44
1:A:541:LYS:O	1:A:545:VAL:HG23	2.18	0.44
1:B:171:ILE:HG13	1:B:200:VAL:HG13	2.00	0.44
1:A:158:CYS:HA	1:A:162:LEU:HD23	2.00	0.43
1:A:659:PRO:O	1:A:663:ARG:HB2	2.18	0.43
1:C:299:GLN:HE21	1:C:308:LYS:HD2	1.83	0.43
1:B:84:SER:HB2	1:B:119:GLN:HB2	1.99	0.43
1:B:10:GLU:O	1:B:14:ILE:HG12	2.17	0.43
1:B:156:ASP:HA	1:B:159:GLU:HG2	2.01	0.43
1:C:291:ASN:HB2	1:C:294:TYR:HB2	2.01	0.43
1:C:512:ARG:HD2	1:C:594:CYS:O	2.19	0.43
1:A:63:ARG:HH22	1:A:157:LEU:HD11	1.84	0.42
1:B:88:TYR:O	1:B:90:ILE:HG13	2.20	0.42
1:B:63:ARG:HH21	1:B:103:LEU:HD12	1.84	0.42
1:A:83:PRO:C	1:A:85:MET:H	2.22	0.42
1:C:2:LEU:HD13	1:C:687:PHE:HZ	1.85	0.42
1:C:11:ILE:HG21	1:C:681:ILE:HD12	2.01	0.42
1:A:213:ARG:HH21	1:A:296:THR:HG23	1.85	0.42
1:B:198:ILE:HD11	1:B:312:ILE:HG21	2.01	0.42
1:B:31:VAL:HG11	1:B:161:TYR:HB3	2.02	0.41
1:A:215:ILE:O	1:A:218:ASN:HB2	2.20	0.41
1:C:396:ARG:HD3	3:C:702:IOD:I	2.90	0.41
1:B:346:ARG:HH12	1:B:348:LEU:HD12	1.84	0.41
1:C:594:CYS:HA	1:C:600:LYS:HG2	2.02	0.41
1:B:431:LEU:HD21	1:B:612:SER:HB3	2.02	0.41
1:B:63:ARG:HB3	1:B:115:GLU:HG3	2.02	0.41
1:C:378:LYS:HA	1:C:620:VAL:HG11	2.02	0.41
1:A:39:GLY:HA3	1:A:202:THR:HG21	2.03	0.41
1:B:445:THR:HG23	1:B:479:LEU:HD13	2.02	0.41
1:B:456:LEU:HD22	1:B:468:LYS:HG2	2.03	0.41
1:B:419:TYR:HA	1:B:422:LYS:HE2	2.03	0.41
1:C:164:ALA:HB1	1:C:165:PRO:HD2	2.03	0.41
1:C:374:ARG:HG3	1:C:375:ASN:H	1.85	0.41
1:A:494:ILE:HB	1:A:615:LEU:HD23	2.03	0.41
1:C:537:VAL:HB	1:C:542:LEU:HB2	2.03	0.41
1:A:297:ASN:HB2	1:C:575:PHE:CE2	2.56	0.41
1:C:537:VAL:HG13	3:C:707:IOD:I	2.91	0.41
1:B:564:LYS:HD2	1:B:565:LEU:HG	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:THR:H	1:C:225:MET:HG3	1.85	0.41
1:A:533:ILE:HG21	1:A:573:ALA:HB2	2.03	0.40
1:C:566:LEU:CD1	1:C:566:LEU:H	2.30	0.40
1:B:530:TYR:CE1	1:B:576:LEU:HD13	2.57	0.40
1:C:99:MET:O	1:C:103:LEU:HB2	2.22	0.40
1:B:540:LYS:HB3	1:B:541:LYS:H	1.59	0.40
1:B:32:VAL:HG12	1:B:169:LEU:HB3	2.03	0.40
1:C:80:ALA:HB3	1:C:90:ILE:HB	2.03	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	613/698 (88%)	561 (92%)	37 (6%)	15 (2%)	6	34
1	B	612/698 (88%)	554 (90%)	46 (8%)	12 (2%)	7	38
1	C	607/698 (87%)	556 (92%)	44 (7%)	7 (1%)	13	49
All	All	1832/2094 (88%)	1671 (91%)	127 (7%)	34 (2%)	8	39

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	PRO
1	A	191	ASP
1	A	226	GLY
1	A	374	ARG
1	A	597	THR
1	B	89	ASN
1	B	141	VAL
1	B	374	ARG
1	B	542	LEU

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Mol	Chain	Res	Type
1	C	196	ARG
1	C	597	THR
1	A	137	GLY
1	A	164	ALA
1	A	373	HIS
1	A	500	GLU
1	B	19	ASP
1	B	301	SER
1	B	543	ALA
1	C	408	SER
1	A	413	SER
1	A	601	ASP
1	B	164	ALA
1	B	500	GLU
1	A	52	PHE
1	B	483	TYR
1	B	520	LYS
1	C	195	LEU
1	C	503	LEU
1	A	20	SER
1	C	88	TYR
1	A	63	ARG
1	B	218	ASN
1	C	39	GLY
1	A	435	GLY

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	579/638 (91%)	529 (91%)	50 (9%)	10	38
1	B	577/638 (90%)	521 (90%)	56 (10%)	8	31
1	C	572/638 (90%)	520 (91%)	52 (9%)	9	34
All	All	1728/1914 (90%)	1570 (91%)	158 (9%)	9	34

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ILE
1	A	16	ASN
1	A	26	THR
1	A	41	SER
1	A	59	MET
1	A	60	VAL
1	A	64	PRO
1	A	66	GLU
1	A	116	GLU
1	A	121	THR
1	A	126	ARG
1	A	127	VAL
1	A	129	ASP
1	A	135	LEU
1	A	138	TYR
1	A	163	THR
1	A	191	ASP
1	A	204	LEU
1	A	214	SER
1	A	233	LYS
1	A	234	THR
1	A	277	GLN
1	A	285	LYS
1	A	338	LEU
1	A	345	ASP
1	A	354	LEU
1	A	369	GLN
1	A	403	LEU
1	A	414	ASP
1	A	416	ASP
1	A	418	LEU
1	A	426	LEU
1	A	434	MET
1	A	462	LYS
1	A	485	SER
1	A	499	TYR
1	A	500	GLU
1	A	503	LEU
1	A	504	GLU
1	A	513	GLN
1	A	540	LYS
1	A	542	LEU

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Mol	Chain	Res	Type
1	A	568	GLU
1	A	579	ARG
1	A	602	ARG
1	A	624	ASN
1	A	638	GLU
1	A	645	LEU
1	A	663	ARG
1	A	670	ARG
1	B	12	ARG
1	B	13	THR
1	B	16	ASN
1	B	33	ILE
1	B	62	ARG
1	B	86	ARG
1	B	101	MET
1	B	115	GLU
1	B	130	LEU
1	B	139	ILE
1	B	157	LEU
1	B	178	LEU
1	B	184	LEU
1	B	188	LYS
1	B	204	LEU
1	B	213	ARG
1	B	214	SER
1	B	285	LYS
1	B	293	LYS
1	B	315	ILE
1	B	327	LEU
1	B	331	GLU
1	B	340	LYS
1	B	361	LEU
1	B	363	LEU
1	B	393	LEU
1	B	398	TRP
1	B	403	LEU
1	B	406	LEU
1	B	414	ASP
1	B	415	THR
1	B	423	LYS
1	B	424	LEU
1	B	469	ASP

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Mol	Chain	Res	Type
1	B	494	ILE
1	B	501	ILE
1	B	504	GLU
1	B	512	ARG
1	B	518	LEU
1	B	526	CYS
1	B	533	ILE
1	B	541	LYS
1	B	542	LEU
1	B	567	LEU
1	B	569	ARG
1	B	574	ILE
1	B	575	PHE
1	B	581	LYS
1	B	583	LEU
1	B	592	ASN
1	B	601	ASP
1	B	611	VAL
1	B	623	LEU
1	B	649	GLU
1	B	652	GLU
1	B	674	LEU
1	C	14	ILE
1	C	27	LEU
1	C	50	ARG
1	C	55	LYS
1	C	81	ASP
1	C	84	SER
1	C	87	LEU
1	C	105	MET
1	C	115	GLU
1	C	130	LEU
1	C	169	LEU
1	C	175	ASP
1	C	206	LEU
1	C	216	LEU
1	C	221	TYR
1	C	231	ILE
1	C	273	ASN
1	C	278	ILE
1	C	283	PHE
1	C	293	LYS

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Mol	Chain	Res	Type
1	C	304	LYS
1	C	305	LEU
1	C	335	THR
1	C	338	LEU
1	C	345	ASP
1	C	354	LEU
1	C	366	LYS
1	C	375	ASN
1	C	380	ILE
1	C	403	LEU
1	C	405	ASP
1	C	414	ASP
1	C	418	LEU
1	C	424	LEU
1	C	438	ARG
1	C	443	LEU
1	C	444	THR
1	C	502	ASP
1	C	503	LEU
1	C	507	ASP
1	C	523	LEU
1	C	541	LYS
1	C	542	LEU
1	C	550	GLU
1	C	566	LEU
1	C	579	ARG
1	C	585	PHE
1	C	593	LYS
1	C	597	THR
1	C	600	LYS
1	C	602	ARG
1	C	618	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	ASN
1	A	277	GLN
1	A	330	GLN
1	A	369	GLN
1	B	76	ASN
1	B	282	GLN

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Mol	Chain	Res	Type
1	C	24	HIS
1	C	36	GLN
1	C	299	GLN
1	C	460	GLN
1	C	525	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 25 are monoatomic - leaving 3 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	$\# Z > 2$
2	GDP	B	701	-	24,30,30	1.68	4 (16%)	31,47,47	1.84	5 (16%)
2	GDP	C	701	-	24,30,30	1.69	4 (16%)	31,47,47	1.77	5 (16%)
2	GDP	A	701	-	24,30,30	1.64	4 (16%)	31,47,47	1.82	4 (12%)

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	GDP	B	701	-	-	5/12/32/32	0/3/3/3
2	GDP	C	701	-	-	7/12/32/32	0/3/3/3
2	GDP	A	701	-	-	7/12/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	GDP	O6-C6	4.79	1.36	1.24
2	A	701	GDP	O6-C6	4.71	1.36	1.24
2	B	701	GDP	O6-C6	4.71	1.36	1.24
2	A	701	GDP	C6-C5	-4.17	1.34	1.41
2	C	701	GDP	C6-C5	-4.10	1.34	1.41
2	B	701	GDP	C6-C5	-4.09	1.34	1.41
2	C	701	GDP	O4'-C1'	2.66	1.44	1.41
2	C	701	GDP	C5-C4	-2.44	1.34	1.40
2	B	701	GDP	C5-C4	-2.43	1.34	1.40
2	B	701	GDP	O4'-C1'	2.38	1.44	1.41
2	A	701	GDP	C5-C4	-2.32	1.34	1.40
2	A	701	GDP	O4'-C1'	2.16	1.44	1.41

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	GDP	N3-C2-N1	-6.15	119.02	127.22
2	A	701	GDP	N3-C2-N1	-6.04	119.17	127.22
2	C	701	GDP	N3-C2-N1	-5.71	119.60	127.22
2	C	701	GDP	C2-N3-C4	4.44	120.43	115.36
2	B	701	GDP	C2-N3-C4	4.28	120.24	115.36
2	A	701	GDP	C2-N3-C4	4.25	120.21	115.36
2	B	701	GDP	C6-N1-C2	2.69	120.21	115.93
2	A	701	GDP	C6-N1-C2	2.68	120.19	115.93
2	C	701	GDP	O4'-C1'-C2'	-2.64	103.07	106.93
2	B	701	GDP	PA-O3A-PB	-2.47	124.35	132.83
2	A	701	GDP	O4'-C1'-C2'	-2.29	103.59	106.93
2	C	701	GDP	C6-N1-C2	2.15	119.34	115.93
2	B	701	GDP	O3B-PB-O2B	2.04	115.45	107.64
2	C	701	GDP	O3B-PB-O2B	2.02	115.35	107.64

There are no chirality outliers.

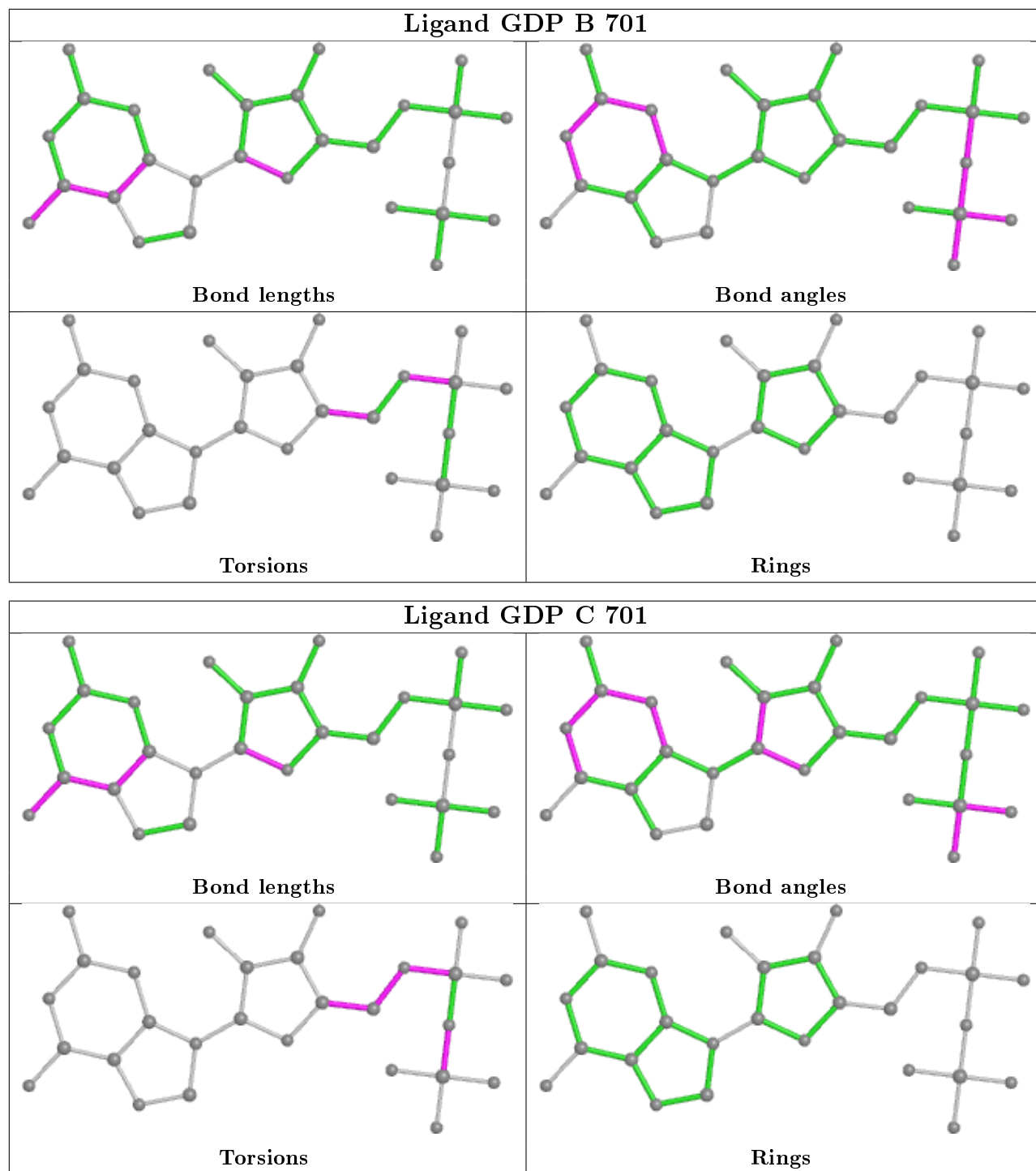
All (19) torsion outliers are listed below:

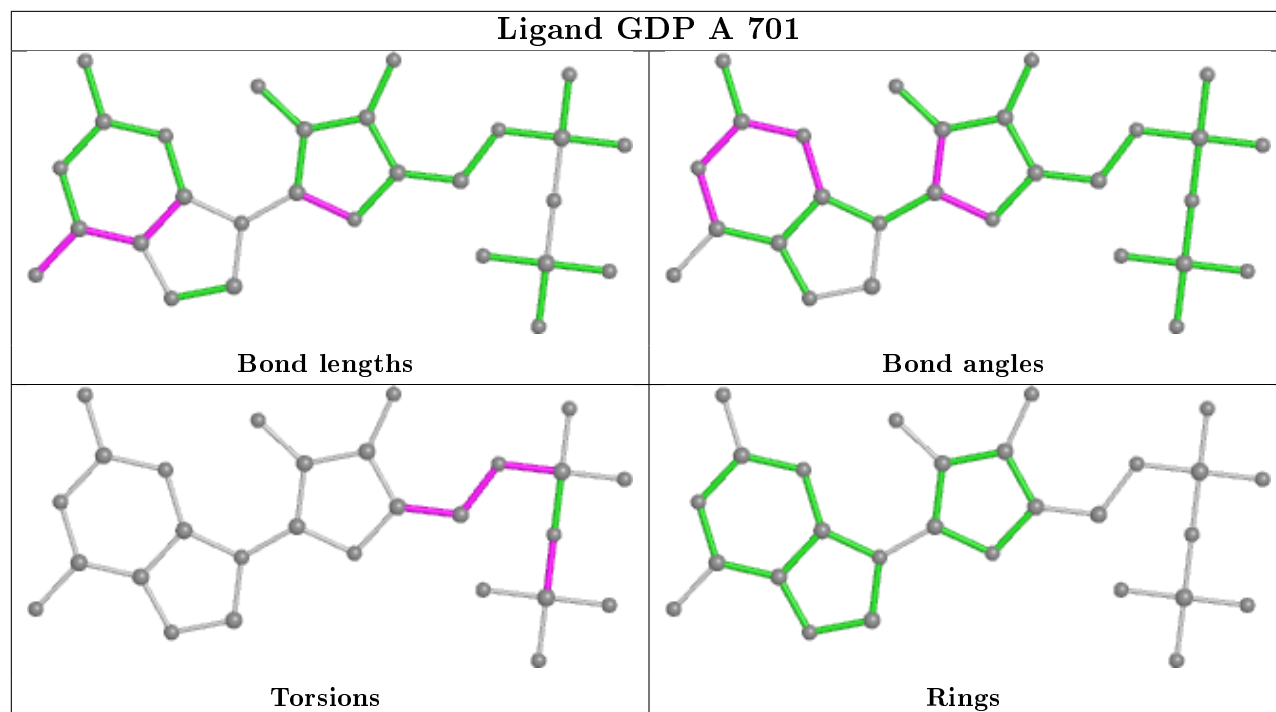
Mol	Chain	Res	Type	Atoms
2	C	701	GDP	PA-O3A-PB-O3B
2	C	701	GDP	C5'-O5'-PA-O3A
2	C	701	GDP	C5'-O5'-PA-O2A
2	C	701	GDP	O4'-C4'-C5'-O5'
2	A	701	GDP	PA-O3A-PB-O2B
2	A	701	GDP	C5'-O5'-PA-O3A
2	B	701	GDP	C5'-O5'-PA-O1A
2	C	701	GDP	C3'-C4'-C5'-O5'
2	A	701	GDP	O4'-C4'-C5'-O5'
2	A	701	GDP	C3'-C4'-C5'-O5'
2	B	701	GDP	O4'-C4'-C5'-O5'
2	B	701	GDP	C3'-C4'-C5'-O5'
2	A	701	GDP	C4'-C5'-O5'-PA
2	A	701	GDP	C5'-O5'-PA-O1A
2	B	701	GDP	C5'-O5'-PA-O2A
2	C	701	GDP	PA-O3A-PB-O1B
2	C	701	GDP	C4'-C5'-O5'-PA
2	A	701	GDP	PA-O3A-PB-O3B
2	B	701	GDP	C5'-O5'-PA-O3A

There are no ring outliers.

No monomer is involved in short contacts.

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	625/698 (89%)	0.33	23 (3%) 41 26	79, 118, 163, 200	0
1	B	624/698 (89%)	0.79	86 (13%) 2 2	24, 130, 196, 224	0
1	C	619/698 (88%)	0.44	47 (7%) 13 7	85, 144, 188, 217	0
All	All	1868/2094 (89%)	0.52	156 (8%) 11 6	24, 130, 188, 224	0

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	606	VAL	11.9
1	B	605	GLU	9.4
1	B	604	PRO	9.3
1	B	544	ASN	8.2
1	B	535	ASN	8.2
1	B	597	THR	8.2
1	B	397	TYR	7.2
1	C	139	ILE	7.0
1	B	418	LEU	6.9
1	B	603	CYS	6.7
1	B	598	ILE	6.3
1	C	216	LEU	6.2
1	B	610	ALA	6.1
1	B	602	ARG	6.0
1	B	538	GLY	5.9
1	B	502	ASP	5.7
1	C	152	THR	5.6
1	C	293	LYS	5.4
1	C	219	LYS	5.4
1	B	592	ASN	5.2
1	B	398	TRP	5.2
1	B	611	VAL	5.0
1	B	413	SER	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	607	PHE	4.8
1	B	567	LEU	4.7
1	B	495	LYS	4.7
1	B	595	HIS	4.6
1	A	536	ALA	4.6
1	B	549	LEU	4.6
1	B	409	SER	4.5
1	A	420	TRP	4.3
1	B	435	GLY	4.2
1	B	414	ASP	4.2
1	B	545	VAL	4.2
1	B	546	MET	4.1
1	B	503	LEU	4.1
1	C	549	LEU	4.1
1	B	543	ALA	4.0
1	B	403	LEU	4.0
1	C	295	PHE	4.0
1	B	504	GLU	3.9
1	B	612	SER	3.8
1	B	582	VAL	3.8
1	C	553	SER	3.7
1	B	416	ASP	3.7
1	B	539	SER	3.7
1	B	157	LEU	3.7
1	B	568	GLU	3.7
1	B	433	LYS	3.6
1	B	417	MET	3.6
1	B	593	LYS	3.6
1	B	421	HIS	3.6
1	A	542	LEU	3.6
1	A	537	VAL	3.6
1	C	398	TRP	3.5
1	C	210	GLU	3.5
1	C	300	VAL	3.5
1	B	516	ILE	3.5
1	B	415	THR	3.5
1	A	599	GLU	3.4
1	B	419	TYR	3.4
1	C	1	MET	3.4
1	B	534	LYS	3.4
1	B	405	ASP	3.3
1	C	129	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	26	THR	3.3
1	A	271	ASN	3.3
1	C	174	ALA	3.2
1	B	583	LEU	3.2
1	B	541	LYS	3.2
1	C	153	LYS	3.2
1	B	594	CYS	3.2
1	A	397	TYR	3.2
1	A	178	LEU	3.1
1	A	373	HIS	3.1
1	B	574	ILE	3.1
1	C	542	LEU	3.1
1	B	599	GLU	3.1
1	A	61	THR	3.1
1	C	227	TYR	3.1
1	B	540	LYS	3.0
1	A	533	ILE	3.0
1	B	370	GLU	3.0
1	B	488	ASP	3.0
1	C	175	ASP	3.0
1	A	90	ILE	3.0
1	B	614	LYS	3.0
1	C	298	CYS	3.0
1	C	401	ASP	3.0
1	C	664	HIS	2.9
1	C	90	ILE	2.9
1	B	410	LYS	2.9
1	A	415	THR	2.8
1	C	422	LYS	2.8
1	C	299	GLN	2.8
1	B	412	GLU	2.8
1	B	564	LYS	2.8
1	B	575	PHE	2.8
1	B	420	TRP	2.7
1	A	97	LYS	2.7
1	B	369	GLN	2.7
1	B	533	ILE	2.7
1	C	420	TRP	2.6
1	B	491	GLU	2.6
1	B	139	ILE	2.6
1	B	550	GLU	2.6
1	A	93	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	406	LEU	2.6
1	C	530	TYR	2.6
1	C	294	TYR	2.5
1	A	52	PHE	2.5
1	C	156	ASP	2.5
1	A	530	TYR	2.5
1	B	536	ALA	2.5
1	C	297	ASN	2.4
1	C	212	ALA	2.4
1	B	524	ARG	2.4
1	C	71	ASN	2.4
1	C	209	PRO	2.4
1	C	346	ARG	2.4
1	A	87	LEU	2.4
1	A	1	MET	2.4
1	C	56	GLY	2.4
1	B	674	LEU	2.3
1	C	551	ASN	2.3
1	B	236	SER	2.3
1	B	596	SER	2.3
1	B	579	ARG	2.3
1	C	188	LYS	2.3
1	B	584	SER	2.3
1	C	218	ASN	2.2
1	C	583	LEU	2.2
1	A	534	LYS	2.2
1	C	288	PHE	2.2
1	C	270	GLU	2.2
1	B	520	LYS	2.2
1	B	601	ASP	2.2
1	A	552	GLU	2.2
1	B	33	ILE	2.2
1	B	505	GLU	2.2
1	C	598	ILE	2.2
1	B	406	LEU	2.1
1	B	667	LEU	2.1
1	C	171	ILE	2.1
1	B	570	GLY	2.1
1	C	567	LEU	2.1
1	B	537	VAL	2.1
1	C	157	LEU	2.1
1	B	18	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	98	ARG	2.0
1	C	217	ASN	2.0
1	C	167	ILE	2.0
1	B	512	ARG	2.0
1	C	55	LYS	2.0
1	B	461	LEU	2.0
1	B	434	MET	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 [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.

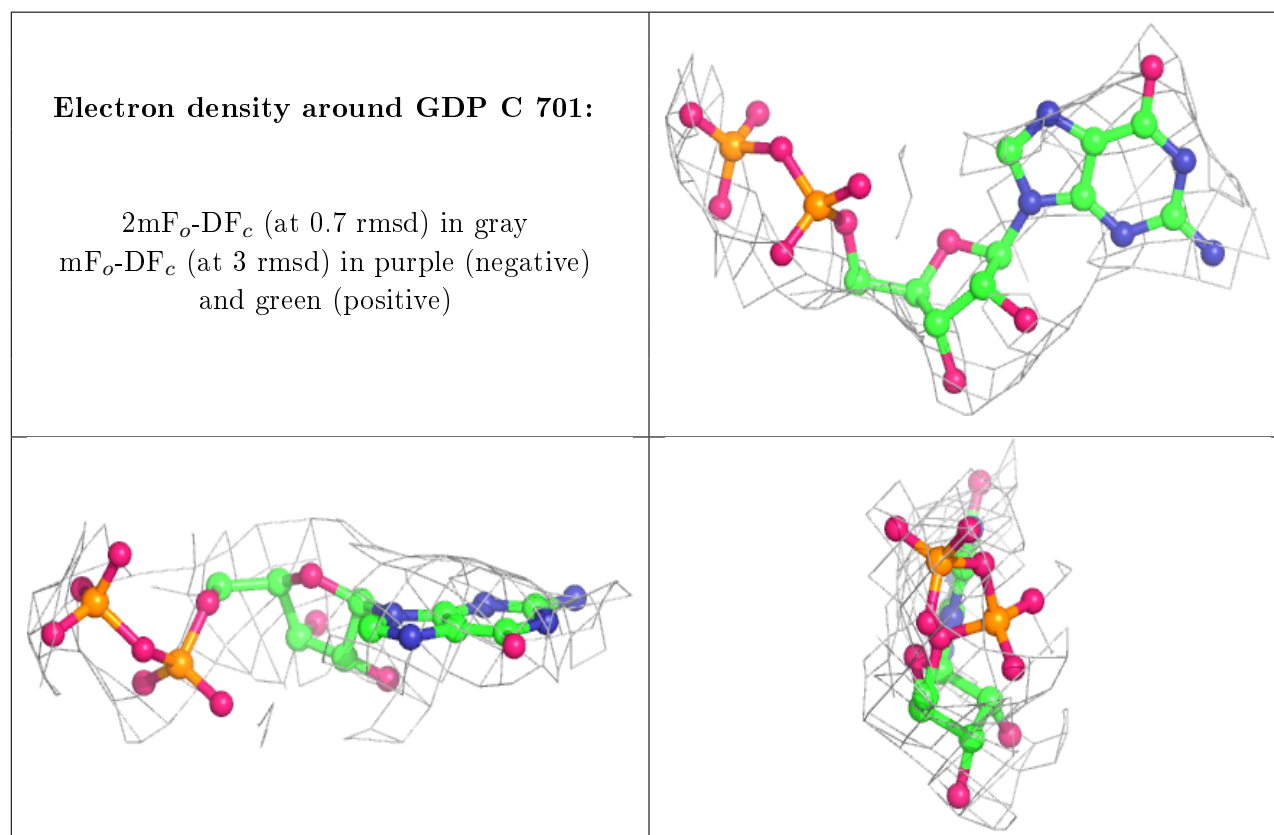
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	IOD	B	706	1/1	-0.44	0.26	300,300,300,300	0
3	IOD	A	707	1/1	0.27	0.25	262,262,262,262	0
3	IOD	B	707	1/1	0.34	0.19	285,285,285,285	0
3	IOD	B	709	1/1	0.37	0.24	300,300,300,300	0
3	IOD	B	711	1/1	0.37	0.18	294,294,294,294	0
3	IOD	A	704	1/1	0.45	0.22	255,255,255,255	0
3	IOD	B	708	1/1	0.51	0.20	275,275,275,275	0
3	IOD	A	708	1/1	0.52	0.20	231,231,231,231	0
3	IOD	C	706	1/1	0.58	0.12	240,240,240,240	0
3	IOD	B	702	1/1	0.62	0.30	222,222,222,222	0
3	IOD	C	707	1/1	0.65	0.12	229,229,229,229	0
3	IOD	B	710	1/1	0.65	0.24	291,291,291,291	0
3	IOD	B	703	1/1	0.66	0.38	241,241,241,241	0
3	IOD	A	703	1/1	0.67	0.27	216,216,216,216	0
3	IOD	C	704	1/1	0.71	0.23	242,242,242,242	0
3	IOD	A	706	1/1	0.72	0.16	216,216,216,216	0

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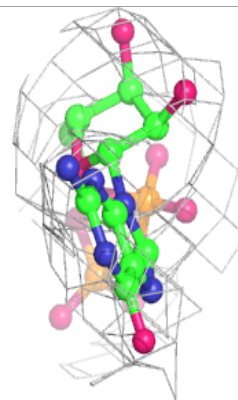
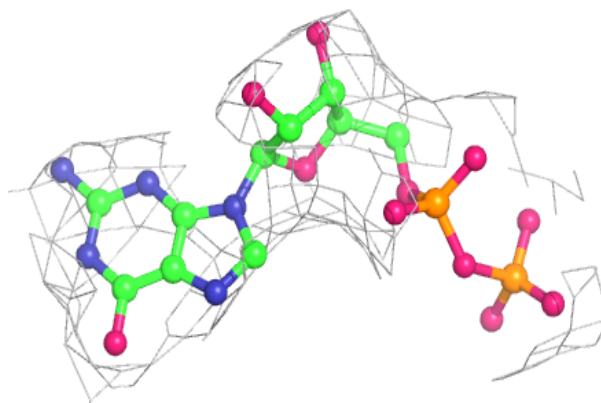
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GDP	C	701	28/28	0.80	0.21	223,226,228,229	0
3	IOD	C	703	1/1	0.83	0.21	219,219,219,219	0
3	IOD	C	705	1/1	0.85	0.17	215,215,215,215	0
3	IOD	A	709	1/1	0.87	0.12	189,189,189,189	0
3	IOD	B	704	1/1	0.88	0.35	250,250,250,250	0
3	IOD	A	705	1/1	0.90	0.07	173,173,173,173	0
3	IOD	A	710	1/1	0.91	0.15	194,194,194,194	0
3	IOD	A	702	1/1	0.91	0.17	135,135,135,135	0
3	IOD	B	705	1/1	0.91	0.11	165,165,165,165	0
2	GDP	A	701	28/28	0.91	0.14	122,133,148,149	0
2	GDP	B	701	28/28	0.92	0.20	125,131,140,141	0
3	IOD	C	702	1/1	0.98	0.21	139,139,139,139	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.

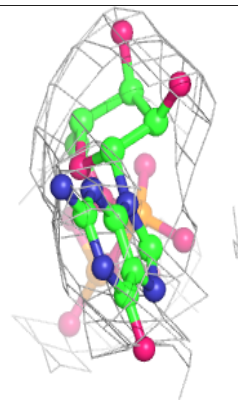
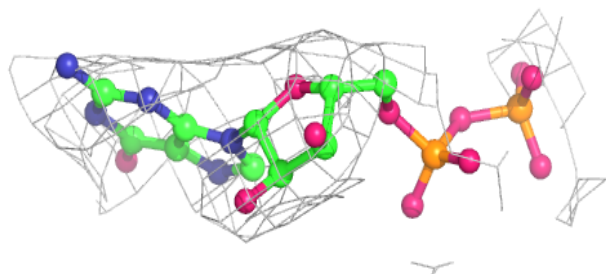
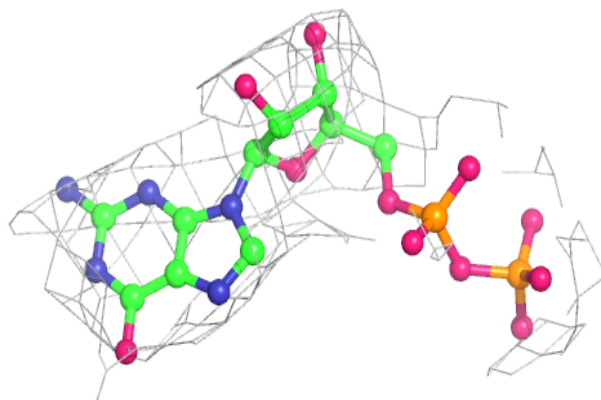


Electron density around GDP A 701:

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

**Electron density around GDP B 701:**

$2mF_o-DF_c$ (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.