



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:15 AM UTC

PDB ID : 5CJ2 / pdb_00005cj2
Title : Ran GDP Y39A mutant triclinic crystal form
Authors : Vetter, I.R.; Brucker, S.
Deposited on : 2015-07-13
Resolution : 1.75 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:

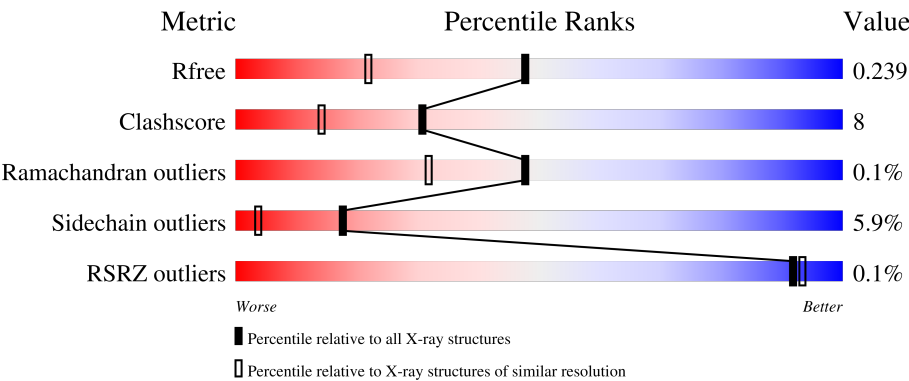
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	216	71% 15%5%9%
1	B	216	77% 12%•8%
1	C	216	70% 17%5%8%
1	D	216	75% 13%•8%
1	E	216	79% 11%•7%

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Mol	Chain	Length	Quality of chain
1	F	216	 75%15%•9%
1	G	216	 69%20%•9%
1	H	216	 75%12%•9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13388 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 GTP-binding nuclear protein Ran.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	1	0
			1583	1026	275	276	6			
1	B	199	Total	C	N	O	S	0	1	0
			1599	1036	278	279	6			
1	C	198	Total	C	N	O	S	0	1	0
			1590	1030	276	278	6			
1	D	198	Total	C	N	O	S	0	1	0
			1590	1031	276	277	6			
1	E	200	Total	C	N	O	S	0	1	0
			1606	1039	279	282	6			
1	F	197	Total	C	N	O	S	0	1	0
			1583	1026	275	276	6			
1	G	197	Total	C	N	O	S	0	1	0
			1583	1026	275	276	6			
1	H	197	Total	C	N	O	S	0	1	0
			1583	1026	275	276	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	ALA	TYR	engineered mutation	UNP P62826
B	39	ALA	TYR	engineered mutation	UNP P62826
C	39	ALA	TYR	engineered mutation	UNP P62826
D	39	ALA	TYR	engineered mutation	UNP P62826
E	39	ALA	TYR	engineered mutation	UNP P62826
F	39	ALA	TYR	engineered mutation	UNP P62826
G	39	ALA	TYR	engineered mutation	UNP P62826
H	39	ALA	TYR	engineered mutation	UNP P62826

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

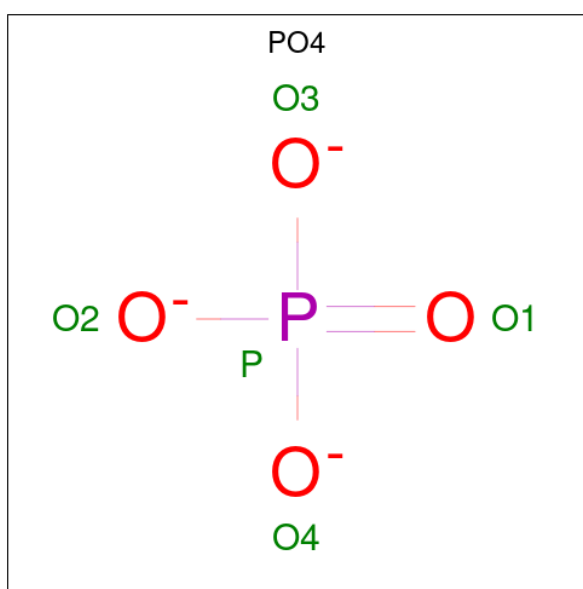
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	3	Total	Mg	0	0
			3	3		
3	C	3	Total	Mg	0	0
			3	3		
3	D	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		
3	G	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	36	Total	O	0	0
			36	36		
5	B	84	Total	O	0	0
			84	84		
5	C	52	Total	O	0	0
			52	52		

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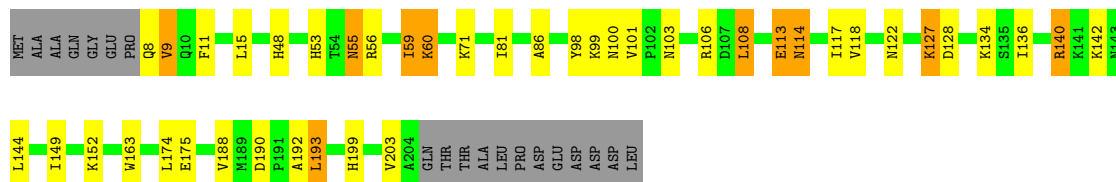
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	80	Total 80	O 80	0	0
5	E	49	Total 49	O 49	0	0
5	F	47	Total 47	O 47	0	0
5	G	42	Total 42	O 42	0	0
5	H	35	Total 35	O 35	0	0

3 Residue-property plots

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.

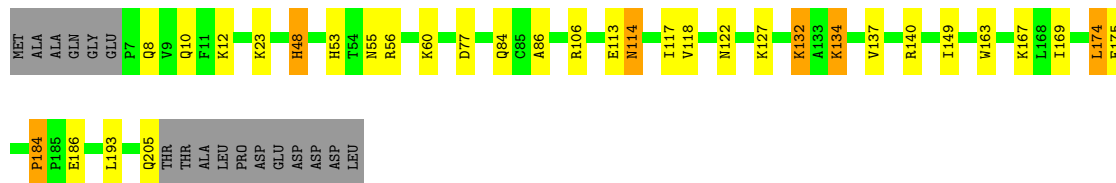
- Molecule 1: GTP-binding nuclear protein Ran

Chain A: 



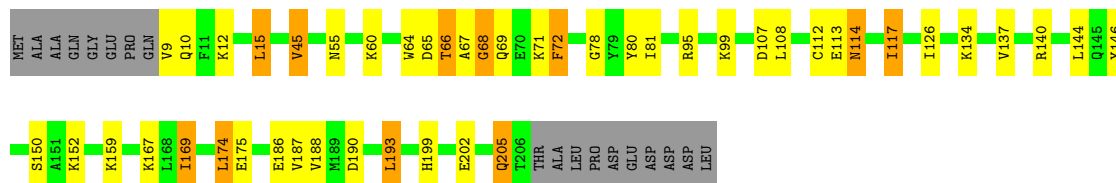
- Molecule 1: GTP-binding nuclear protein Ran

Chain B: 



- Molecule 1: GTP-binding nuclear protein Ran

Chain C: 



- Molecule 1: GTP-binding nuclear protein Ran

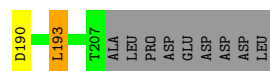
Chain D: 





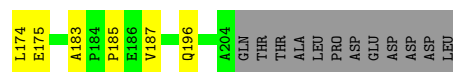
- Molecule 1: GTP-binding nuclear protein Ran

Chain E: 79% 11% 7%



- Molecule 1: GTP-binding nuclear protein Ran

Chain F: 75% 15% 9%



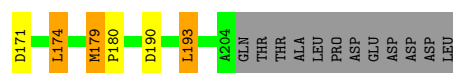
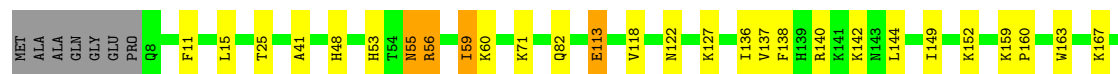
- Molecule 1: GTP-binding nuclear protein Ran

Chain G: 69% 20% 9%



- Molecule 1: GTP-binding nuclear protein Ran

Chain H: 75% 12% 9%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.19Å 80.73Å 91.65Å 97.66° 90.00° 90.01°	Depositor
Resolution (Å)	47.58 – 1.75 47.58 – 1.75	Depositor EDS
% Data completeness (in resolution range)	92.2 (47.58-1.75) 92.2 (47.58-1.75)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.197 , 0.239 0.197 , 0.239	Depositor DCC
R_{free} test set	7824 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	22.7	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 22.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.459 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13388	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.26 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.4087e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: MG, GDP, PO4

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	1.12	0/1625	1.22	5/2200 (0.2%)
1	B	1.28	3/1642 (0.2%)	1.29	3/2223 (0.1%)
1	C	1.27	4/1632 (0.2%)	1.29	10/2210 (0.5%)
1	D	1.32	6/1633 (0.4%)	1.29	2/2211 (0.1%)
1	E	1.22	2/1648 (0.1%)	1.23	2/2232 (0.1%)
1	F	1.16	2/1625 (0.1%)	1.21	4/2200 (0.2%)
1	G	1.18	1/1625 (0.1%)	1.19	2/2200 (0.1%)
1	H	1.13	1/1625 (0.1%)	1.18	0/2200
All	All	1.21	19/13055 (0.1%)	1.24	28/17676 (0.2%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	184	PRO	CA-C	6.71	1.55	1.51
1	C	146	TYR	N-CA	6.68	1.54	1.46
1	C	117	ILE	C-O	6.39	1.30	1.24
1	C	150	SER	C-O	-6.25	1.17	1.24
1	D	184	PRO	CA-C	6.15	1.57	1.52
1	G	101	VAL	CA-CB	6.05	1.57	1.54
1	B	184	PRO	CA-C	5.98	1.57	1.52
1	D	87	ILE	C-O	5.80	1.30	1.24
1	B	23	LYS	N-CA	5.54	1.52	1.46
1	D	128	ASP	C-O	5.54	1.30	1.24
1	C	159	LYS	CA-C	5.37	1.59	1.52
1	D	37	LYS	C-O	5.33	1.30	1.23
1	B	48	HIS	CA-C	5.26	1.58	1.52
1	H	174	LEU	N-CA	5.22	1.52	1.46
1	E	163	TRP	C-O	5.21	1.30	1.24
1	F	37	LYS	N-CA	5.17	1.52	1.46
1	D	23	LYS	N-CA	5.09	1.52	1.46
1	F	137	VAL	N-CA	5.05	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	101	VAL	CA-C	5.03	1.58	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	VAL	CA-C-N	-7.62	111.79	119.56
1	A	101	VAL	C-N-CA	-7.62	111.79	119.56
1	C	174	LEU	CA-CB-CG	6.67	139.63	116.30
1	G	31	LEU	N-CA-C	6.62	118.50	111.28
1	D	140	ARG	N-CA-C	-6.46	103.74	111.69
1	E	142	LYS	N-CA-C	6.23	120.92	112.88
1	C	114	ASN	N-CA-C	6.17	123.95	110.80
1	C	108	LEU	N-CA-C	5.91	117.52	111.14
1	B	114	ASN	N-CA-C	5.71	122.17	113.61
1	C	68	GLY	N-CA-C	5.71	123.52	115.30
1	C	187	VAL	CA-C-N	-5.69	115.76	122.93
1	C	187	VAL	C-N-CA	-5.69	115.76	122.93
1	A	100	ASN	CA-C-N	5.52	123.72	120.24
1	A	100	ASN	C-N-CA	5.52	123.72	120.24
1	C	169	ILE	N-CA-C	-5.49	104.97	113.16
1	C	80	TYR	N-CA-C	5.44	118.38	111.69
1	D	67	ALA	N-CA-C	-5.42	105.11	112.26
1	F	31	LEU	N-CA-C	5.42	117.18	111.28
1	B	186	GLU	CA-CB-CG	-5.41	103.28	114.10
1	G	111	VAL	N-CA-C	5.38	116.87	111.00
1	C	15	LEU	CB-CG-CD2	5.32	126.67	110.70
1	F	8	GLN	CA-C-N	-5.30	113.80	122.33
1	F	8	GLN	C-N-CA	-5.30	113.80	122.33
1	C	66	THR	N-CA-C	-5.28	103.56	110.53
1	B	77	ASP	N-CA-C	-5.24	105.74	111.82
1	F	103	ASN	N-CA-C	5.12	117.59	111.71
1	E	100	ASN	N-CA-C	5.10	119.38	113.20
1	A	98	TYR	N-CA-C	-5.02	105.89	111.36

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	1583	0	1609	37	0
1	B	1599	0	1625	27	0
1	C	1590	0	1616	27	0
1	D	1590	0	1617	28	0
1	E	1606	0	1631	16	0
1	F	1583	0	1609	19	0
1	G	1583	0	1609	39	0
1	H	1583	0	1609	30	0
2	A	28	0	12	2	0
2	B	28	0	12	0	0
2	C	28	0	12	0	0
2	D	28	0	12	2	0
2	E	28	0	12	0	0
2	F	28	0	12	1	0
2	G	28	0	12	4	0
2	H	28	0	12	2	0
3	A	1	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
5	A	36	0	0	3	0
5	B	84	0	0	6	0
5	C	52	0	0	2	0
5	D	80	0	0	4	0
5	E	49	0	0	1	0
5	F	47	0	0	2	0
5	G	42	0	0	3	0
5	H	35	0	0	5	0
All	All	13388	0	13021	216	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 8.

All (216) 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:C:68:GLY:O	1:C:71:LYS:HG2	1.35	1.19
1:E:137:VAL:HG12	1:E:140:ARG:NH1	1.76	1.00
1:E:55:ASN:ND2	1:E:174:LEU:HD12	1.77	0.99
1:E:55:ASN:HD21	1:E:174:LEU:HD12	1.27	0.98
1:B:137:VAL:HG12	1:B:140:ARG:HH11	1.26	0.97
1:E:137:VAL:HG12	1:E:140:ARG:HH11	1.31	0.95
1:B:8:GLN:NE2	1:B:10:GLN:HE21	1.66	0.93
1:B:8:GLN:HE21	1:B:10:GLN:NE2	1.69	0.90
1:D:96:VAL:HG23	5:D:459:HOH:O	1.72	0.89
1:G:55:ASN:ND2	1:G:175:GLU:H	1.72	0.87
1:D:106:ARG:HH21	1:D:106:ARG:HG2	1.39	0.87
1:G:137:VAL:HG12	1:G:140:ARG:NH1	1.92	0.84
1:B:8:GLN:HE21	1:B:10:GLN:HE21	0.85	0.84
1:E:142:LYS:O	1:E:143:ASN:HB3	1.74	0.84
1:A:127:LYS:HD2	1:A:127:LYS:C	2.04	0.82
1:B:56:ARG:NH2	5:B:401:HOH:O	2.12	0.81
1:F:55:ASN:ND2	1:F:175:GLU:H	1.79	0.81
1:A:113:GLU:O	1:A:113:GLU:HG2	1.78	0.79
1:G:78:GLY:O	1:G:81:ILE:HG22	1.87	0.74
1:F:78:GLY:O	1:F:81:ILE:HG22	1.90	0.72
1:A:56:ARG:HG3	1:A:56:ARG:O	1.90	0.71
1:B:106:ARG:HG2	1:B:106:ARG:HH21	1.54	0.71
1:B:137:VAL:HG12	1:B:140:ARG:NH1	2.04	0.70
1:C:10:GLN:HE21	1:C:60:LYS:HE3	1.57	0.70
1:C:152[A]:LYS:HD3	1:C:186:GLU:HB2	1.75	0.69
1:G:139:HIS:HA	1:G:144:LEU:HB2	1.73	0.68
1:G:53:HIS:HD2	5:G:439:HOH:O	1.75	0.68
1:G:199:HIS:HD2	5:H:427:HOH:O	1.78	0.67
1:E:169:ILE:HD12	1:E:174:LEU:HD21	1.77	0.67
1:G:96:VAL:HA	1:G:99:LYS:HD2	1.76	0.67
1:B:55:ASN:HD21	1:B:174:LEU:HB2	1.59	0.66
1:D:109:VAL:HG13	1:D:113:GLU:HA	1.78	0.65
1:A:152[A]:LYS:HG2	2:A:301:GDP:C6	2.30	0.65
1:C:55:ASN:H	1:C:55:ASN:HD22	1.44	0.65
1:H:152[B]:LYS:HE3	2:H:301:GDP:C4	2.33	0.64
1:F:118:VAL:HG23	1:F:164:LEU:HD21	1.80	0.64
1:G:55:ASN:HD21	1:G:174:LEU:HA	1.63	0.62
1:A:55:ASN:ND2	1:A:174:LEU:HD12	2.14	0.62
1:F:127:LYS:HE3	5:F:442:HOH:O	2.00	0.62
1:A:136:ILE:O	1:A:140:ARG:NH2	2.33	0.61
1:C:202:GLU:CG	5:C:450:HOH:O	2.48	0.61
1:G:55:ASN:HD22	1:G:175:GLU:H	1.43	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:GLN:HE22	1:A:60:LYS:NZ	1.99	0.60
1:C:137:VAL:O	1:C:140:ARG:HB2	2.00	0.60
1:G:23:LYS:NZ	2:G:301:GDP:O1B	2.34	0.60
1:B:12:LYS:H	1:B:84:GLN:HE21	1.50	0.60
1:G:127:LYS:HD3	1:G:193:LEU:HD21	1.84	0.60
1:A:53:HIS:HD2	5:A:434:HOH:O	1.85	0.58
1:C:67:ALA:N	1:C:69:GLN:OE1	2.34	0.58
1:E:137:VAL:O	1:E:140:ARG:HB2	2.03	0.58
1:A:59:ILE:HG12	1:A:60:LYS:N	2.19	0.58
1:G:48:HIS:HE1	5:G:421:HOH:O	1.86	0.58
1:B:12:LYS:H	1:B:84:GLN:NE2	2.01	0.58
1:D:53:HIS:HD2	5:D:473:HOH:O	1.88	0.57
1:A:103:ASN:ND2	1:A:106:ARG:NH1	2.53	0.57
1:B:55:ASN:ND2	1:B:175:GLU:H	2.03	0.57
1:G:95:ARG:O	1:G:99:LYS:HG3	2.05	0.57
1:G:137:VAL:HG12	1:G:140:ARG:HH11	1.68	0.56
1:F:55:ASN:HD21	1:F:174:LEU:HA	1.69	0.56
1:G:202:GLU:OE1	1:H:41:ALA:HB3	2.06	0.56
1:G:43:LEU:O	1:G:45:VAL:HG23	2.06	0.56
1:C:45:VAL:HG22	1:C:65:ASP:O	2.06	0.56
1:H:56:ARG:HH11	1:H:171:ASP:HB2	1.71	0.56
1:H:137:VAL:HG12	1:H:140:ARG:NH1	2.20	0.55
1:H:59:ILE:HG12	1:H:60:LYS:N	2.22	0.55
1:G:152[B]:LYS:HD2	2:G:301:GDP:C2	2.41	0.55
1:C:169:ILE:HD12	1:C:174:LEU:HD21	1.87	0.55
1:D:55:ASN:HD22	1:D:55:ASN:H	1.54	0.55
1:C:72:PHE:CD1	1:C:72:PHE:N	2.75	0.55
1:B:48:HIS:HE1	5:B:426:HOH:O	1.90	0.54
1:G:43:LEU:HA	1:G:76:ARG:HH22	1.72	0.54
1:F:163:TRP:CZ2	1:F:167:LYS:HE3	2.43	0.54
1:D:32:THR:OG1	1:G:53:HIS:HE1	1.91	0.54
1:G:139:HIS:CA	1:G:144:LEU:HB2	2.37	0.54
1:G:192:ALA:HB2	1:H:82:GLN:HG3	1.90	0.54
1:C:66:THR:HG23	5:C:401:HOH:O	2.07	0.53
1:H:163:TRP:CZ2	1:H:167:LYS:HE2	2.43	0.53
1:A:127:LYS:HD2	1:A:128:ASP:N	2.23	0.53
1:D:53:HIS:HE1	1:G:32:THR:OG1	1.91	0.53
1:G:142:LYS:HB2	1:G:144:LEU:HG	1.90	0.53
1:H:11:PHE:CD2	1:H:59:ILE:HD11	2.43	0.53
1:B:132:LYS:HE2	1:B:134:LYS:HE3	1.91	0.53
1:D:48:HIS:HE1	5:D:429:HOH:O	1.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:ASN:HD22	1:E:55:ASN:H	1.57	0.53
1:A:55:ASN:HD22	1:A:55:ASN:N	2.08	0.52
1:F:72:PHE:CD1	1:F:72:PHE:O	2.63	0.52
1:F:48:HIS:HE1	5:F:432:HOH:O	1.91	0.51
1:H:53:HIS:HD2	5:H:433:HOH:O	1.93	0.51
1:F:40:VAL:HG11	1:F:43:LEU:HD12	1.93	0.51
1:H:55:ASN:HD22	1:H:55:ASN:N	2.08	0.51
1:E:190:ASP:HB3	1:E:193:LEU:HB2	1.93	0.51
1:A:55:ASN:ND2	1:A:175:GLU:H	2.09	0.51
1:A:55:ASN:HD21	1:A:174:LEU:HD12	1.75	0.51
1:G:118:VAL:HG23	1:G:164:LEU:HD21	1.93	0.50
1:H:190:ASP:HB3	1:H:193:LEU:HB2	1.93	0.50
1:C:113:GLU:HB2	1:C:114:ASN:ND2	2.26	0.50
1:G:72:PHE:CD1	1:G:72:PHE:O	2.65	0.49
1:B:55:ASN:H	1:B:55:ASN:HD22	1.59	0.49
1:H:163:TRP:CE2	1:H:167:LYS:HE2	2.47	0.49
1:A:11:PHE:HD2	1:A:59:ILE:HD11	1.77	0.49
1:D:12:LYS:H	1:D:84:GLN:NE2	2.09	0.49
1:F:55:ASN:H	1:F:55:ASN:HD22	1.59	0.49
1:A:48:HIS:HD2	5:A:415:HOH:O	1.94	0.49
1:G:152[B]:LYS:HG3	2:G:301:GDP:C6	2.48	0.49
1:B:48:HIS:HD2	5:B:414:HOH:O	1.96	0.48
1:C:10:GLN:NE2	1:C:60:LYS:HE3	2.27	0.48
1:C:55:ASN:H	1:C:55:ASN:ND2	2.10	0.48
1:D:106:ARG:HH21	1:D:106:ARG:CG	2.20	0.48
1:H:48:HIS:HE1	5:H:408:HOH:O	1.97	0.48
1:C:12:LYS:HE3	1:C:64:TRP:CE2	2.49	0.48
1:A:56:ARG:O	1:A:56:ARG:CG	2.61	0.48
1:A:114:ASN:HD22	1:A:114:ASN:HA	1.50	0.48
1:C:117:ILE:HB	1:C:144:LEU:HD22	1.96	0.48
1:D:56:ARG:NH2	1:D:171:ASP:OD2	2.46	0.48
1:H:11:PHE:HD2	1:H:59:ILE:HD11	1.77	0.48
1:A:190:ASP:OD2	1:A:192:ALA:HB3	2.14	0.47
1:D:55:ASN:ND2	1:D:175:GLU:H	2.12	0.47
1:F:153:SER:HA	1:F:185:PRO:HB3	1.96	0.47
1:H:159:LYS:N	1:H:160:PRO:HD2	2.30	0.47
1:A:11:PHE:CD2	1:A:59:ILE:HD11	2.49	0.46
1:A:8:GLN:HE22	1:A:60:LYS:HZ2	1.64	0.46
1:A:103:ASN:ND2	1:A:106:ARG:HH12	2.12	0.46
1:C:12:LYS:HE3	1:C:64:TRP:CD2	2.50	0.46
1:D:106:ARG:HG2	1:D:106:ARG:NH2	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:GLN:HE22	1:B:60:LYS:NZ	2.14	0.46
1:G:24:THR:CG2	1:G:28:LYS:HE3	2.46	0.46
1:F:152[B]:LYS:NZ	2:F:301:GDP:O2'	2.49	0.46
1:G:192:ALA:CB	1:H:82:GLN:HG3	2.46	0.46
1:D:150:SER:HB3	1:D:155:TYR:HB3	1.98	0.46
1:B:53:HIS:HD2	5:B:475:HOH:O	1.99	0.46
1:B:106:ARG:HG2	1:B:106:ARG:NH2	2.27	0.46
1:D:137:VAL:HG12	1:D:140:ARG:NH1	2.31	0.46
1:G:139:HIS:CB	1:G:144:LEU:HB2	2.46	0.45
1:F:152[B]:LYS:HD3	1:F:187:VAL:HG13	1.98	0.45
1:H:55:ASN:N	1:H:55:ASN:ND2	2.64	0.45
1:A:55:ASN:HD21	1:A:174:LEU:HA	1.80	0.45
1:A:86:ALA:CB	1:A:108:LEU:HD21	2.46	0.45
1:C:137:VAL:HG12	1:C:140:ARG:HH11	1.81	0.45
1:A:113:GLU:O	1:A:113:GLU:CG	2.58	0.45
1:D:199:HIS:CE1	1:E:42:THR:O	2.69	0.45
1:F:31:LEU:HD21	1:F:183:ALA:HB2	1.98	0.45
1:D:152[B]:LYS:HG3	2:D:301:GDP:C5	2.52	0.45
1:B:86:ALA:HB3	1:B:117:ILE:HG12	1.99	0.44
1:C:137:VAL:HG12	1:C:140:ARG:NH1	2.33	0.44
1:H:55:ASN:HD21	1:H:174:LEU:HA	1.81	0.44
5:B:417:HOH:O	1:C:199:HIS:HD2	2.00	0.44
1:C:55:ASN:HD21	1:C:174:LEU:HA	1.83	0.44
1:D:12:LYS:H	1:D:84:GLN:HE21	1.66	0.44
1:D:12:LYS:HE3	1:D:64:TRP:CD2	2.53	0.44
1:F:142:LYS:HB2	1:F:144:LEU:HG	2.00	0.44
1:A:81:ILE:HD12	1:A:81:ILE:HA	1.88	0.43
1:C:78:GLY:O	1:C:81:ILE:HG22	2.18	0.43
1:C:99:LYS:HE2	1:C:99:LYS:HB3	1.59	0.43
1:D:103:ASN:HD22	1:D:106:ARG:NH1	2.16	0.43
1:F:55:ASN:HD22	1:F:175:GLU:H	1.58	0.43
1:G:136:ILE:HG22	1:G:139:HIS:CE1	2.52	0.43
1:H:179:MET:SD	1:H:180:PRO:HD2	2.57	0.43
1:C:190:ASP:HB3	1:C:193:LEU:HB2	2.01	0.43
1:G:79:TYR:CD1	1:G:79:TYR:C	2.96	0.43
1:D:103:ASN:ND2	1:D:106:ARG:NH1	2.67	0.43
1:G:123:LYS:HB3	1:G:126:ILE:HD12	2.01	0.43
1:G:95:ARG:HG3	1:G:131:VAL:HG22	2.01	0.43
1:H:136:ILE:O	1:H:140:ARG:NH2	2.52	0.43
1:A:48:HIS:HE1	5:A:410:HOH:O	2.02	0.43
1:E:66:THR:HG23	5:E:401:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:13:LEU:C	1:F:13:LEU:HD23	2.44	0.43
1:H:48:HIS:HD2	5:H:413:HOH:O	2.00	0.43
1:E:83:ALA:HB3	1:E:112:CYS:SG	2.59	0.42
1:G:152[B]:LYS:HG3	2:G:301:GDP:C5	2.55	0.42
1:H:142:LYS:HB2	1:H:144:LEU:HG	2.01	0.42
1:A:152[A]:LYS:HG2	2:A:301:GDP:C5	2.54	0.42
1:B:167:LYS:HA	1:B:167:LYS:HD2	1.84	0.42
1:D:140:ARG:HE	1:D:140:ARG:HB2	1.36	0.42
1:A:199:HIS:CE1	1:F:76:ARG:HH11	2.37	0.42
1:D:190:ASP:HB3	1:D:193:LEU:HB2	2.02	0.42
1:G:13:LEU:HD23	1:G:13:LEU:C	2.45	0.42
1:A:9:VAL:O	1:A:9:VAL:CG2	2.67	0.42
1:G:48:HIS:HD2	5:G:402:HOH:O	2.03	0.42
1:H:122:ASN:HA	1:H:149:ILE:HG13	2.01	0.42
1:D:152[B]:LYS:HG3	2:D:301:GDP:C6	2.54	0.42
1:A:203:VAL:HG12	1:A:203:VAL:O	2.19	0.41
1:E:55:ASN:HD21	1:E:174:LEU:HA	1.84	0.41
1:H:55:ASN:ND2	1:H:55:ASN:H	2.18	0.41
1:A:55:ASN:ND2	1:A:55:ASN:N	2.67	0.41
1:C:55:ASN:ND2	1:C:175:GLU:H	2.18	0.41
1:A:122:ASN:HA	1:A:149:ILE:HG13	2.02	0.41
1:A:142:LYS:HB2	1:A:144:LEU:HG	2.02	0.41
1:D:103:ASN:ND2	1:D:106:ARG:HH11	2.19	0.41
1:H:138:PHE:CZ	1:H:142:LYS:HG3	2.55	0.41
1:G:137:VAL:HG12	1:G:140:ARG:HH12	1.80	0.41
1:G:153:SER:HA	1:G:185:PRO:HB3	2.02	0.41
1:H:25:THR:HG21	1:H:152[A]:LYS:HE2	2.02	0.41
1:H:152[A]:LYS:HG2	2:H:301:GDP:C6	2.56	0.41
1:A:118:VAL:HG22	1:A:163:TRP:CE3	2.56	0.41
1:B:106:ARG:NH2	1:B:106:ARG:CG	2.84	0.41
1:B:174:LEU:C	1:B:174:LEU:HD23	2.46	0.41
1:C:205:GLN:O	1:C:205:GLN:HG3	2.19	0.41
1:H:113:GLU:HG2	5:H:435:HOH:O	2.21	0.41
1:A:190:ASP:HB3	1:A:193:LEU:HB2	2.03	0.41
1:B:163:TRP:CD1	5:B:433:HOH:O	2.74	0.41
1:D:55:ASN:HD21	1:D:174:LEU:HA	1.86	0.41
1:G:70:GLU:C	1:G:72:PHE:H	2.29	0.41
1:D:53:HIS:CD2	5:D:473:HOH:O	2.70	0.41
1:E:79:TYR:CD1	1:E:79:TYR:C	2.98	0.41
1:H:118:VAL:HG22	1:H:163:TRP:CE3	2.56	0.41
1:B:122:ASN:HA	1:B:149:ILE:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:ILE:HD12	1:B:174:LEU:HD11	2.03	0.40
1:B:8:GLN:NE2	1:B:10:GLN:NE2	2.45	0.40
1:B:118:VAL:HG22	1:B:163:TRP:CE3	2.57	0.40
1:F:171:ASP:HA	1:F:172:PRO:HD3	1.96	0.40
1:C:126:ILE:HD12	1:C:126:ILE:HG23	1.87	0.40
1:E:12:LYS:HE3	1:E:64:TRP:CD2	2.56	0.40
1:H:56:ARG:NH1	1:H:171:ASP:HB2	2.35	0.40
1:A:86:ALA:HB3	1:A:117:ILE:HG12	2.03	0.40
1:D:114:ASN:HD22	1:D:114:ASN:HA	1.55	0.40
1:E:127:LYS:HE3	1:E:127:LYS:HB3	1.88	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	196/216 (91%)	190 (97%)	6 (3%)	0	100	100
1	B	198/216 (92%)	193 (98%)	5 (2%)	0	100	100
1	C	197/216 (91%)	188 (95%)	9 (5%)	0	100	100
1	D	197/216 (91%)	190 (96%)	6 (3%)	1 (0%)	24	11
1	E	199/216 (92%)	188 (94%)	11 (6%)	0	100	100
1	F	196/216 (91%)	193 (98%)	3 (2%)	0	100	100
1	G	196/216 (91%)	192 (98%)	4 (2%)	0	100	100
1	H	196/216 (91%)	191 (97%)	4 (2%)	1 (0%)	24	11
All	All	1575/1728 (91%)	1525 (97%)	48 (3%)	2 (0%)	48	32

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	113	GLU
1	D	143	ASN

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	170/184 (92%)	155 (91%)	15 (9%)	9	1
1	B	172/184 (94%)	163 (95%)	9 (5%)	21	5
1	C	171/184 (93%)	159 (93%)	12 (7%)	14	2
1	D	171/184 (93%)	160 (94%)	11 (6%)	16	3
1	E	173/184 (94%)	160 (92%)	13 (8%)	12	2
1	F	170/184 (92%)	164 (96%)	6 (4%)	32	12
1	G	170/184 (92%)	163 (96%)	7 (4%)	27	8
1	H	170/184 (92%)	162 (95%)	8 (5%)	23	6
All	All	1367/1472 (93%)	1286 (94%)	81 (6%)	18	4

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	15	LEU
1	A	55	ASN
1	A	59	ILE
1	A	60	LYS
1	A	71	LYS
1	A	99	LYS
1	A	108	LEU
1	A	113	GLU
1	A	114	ASN
1	A	127	LYS
1	A	134	LYS
1	A	140	ARG
1	A	188	VAL

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Mol	Chain	Res	Type
1	A	193	LEU
1	B	113	GLU
1	B	114	ASN
1	B	127	LYS
1	B	132	LYS
1	B	134	LYS
1	B	174	LEU
1	B	184	PRO
1	B	193	LEU
1	B	205	GLN
1	C	9	VAL
1	C	15	LEU
1	C	45	VAL
1	C	72	PHE
1	C	95	ARG
1	C	107	ASP
1	C	112	CYS
1	C	134	LYS
1	C	167	LYS
1	C	188	VAL
1	C	193	LEU
1	C	205	GLN
1	D	50	LEU
1	D	106	ARG
1	D	113	GLU
1	D	114	ASN
1	D	134	LYS
1	D	140	ARG
1	D	152[A]	LYS
1	D	152[B]	LYS
1	D	174	LEU
1	D	186	GLU
1	D	193	LEU
1	E	9	VAL
1	E	15	LEU
1	E	45	VAL
1	E	95	ARG
1	E	99	LYS
1	E	106	ARG
1	E	127	LYS
1	E	134	LYS
1	E	140	ARG

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Mol	Chain	Res	Type
1	E	143	ASN
1	E	144	LEU
1	E	179	MET
1	E	193	LEU
1	F	9	VAL
1	F	56	ARG
1	F	108	LEU
1	F	127	LYS
1	F	134	LYS
1	F	196	GLN
1	G	15	LEU
1	G	95	ARG
1	G	108	LEU
1	G	114	ASN
1	G	127	LYS
1	G	140	ARG
1	G	141	LYS
1	H	15	LEU
1	H	55	ASN
1	H	56	ARG
1	H	59	ILE
1	H	71	LYS
1	H	127	LYS
1	H	179	MET
1	H	193	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	10	GLN
1	A	48	HIS
1	A	53	HIS
1	A	55	ASN
1	A	62	ASN
1	A	103	ASN
1	A	105	HIS
1	A	114	ASN
1	B	8	GLN
1	B	48	HIS
1	B	53	HIS
1	B	55	ASN

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Mol	Chain	Res	Type
1	B	62	ASN
1	B	84	GLN
1	B	103	ASN
1	B	114	ASN
1	B	145	GLN
1	C	10	GLN
1	C	48	HIS
1	C	53	HIS
1	C	55	ASN
1	C	62	ASN
1	C	103	ASN
1	C	105	HIS
1	C	114	ASN
1	C	139	HIS
1	C	145	GLN
1	C	199	HIS
1	D	48	HIS
1	D	53	HIS
1	D	55	ASN
1	D	84	GLN
1	D	103	ASN
1	D	114	ASN
1	D	139	HIS
1	D	145	GLN
1	D	199	HIS
1	E	10	GLN
1	E	48	HIS
1	E	55	ASN
1	E	103	ASN
1	E	143	ASN
1	E	145	GLN
1	E	196	GLN
1	E	199	HIS
1	F	10	GLN
1	F	48	HIS
1	F	55	ASN
1	F	103	ASN
1	F	105	HIS
1	F	139	HIS
1	F	145	GLN
1	G	10	GLN
1	G	48	HIS

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Mol	Chain	Res	Type
1	G	53	HIS
1	G	55	ASN
1	G	62	ASN
1	G	105	HIS
1	G	139	HIS
1	G	145	GLN
1	G	199	HIS
1	H	48	HIS
1	H	53	HIS
1	H	55	ASN
1	H	62	ASN
1	H	103	ASN
1	H	105	HIS
1	H	196	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 12 are monoatomic - leaving 10 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	A	301	3	29,30,30	1.13	2 (6%)	45,47,47	1.59	11 (24%)
4	PO4	B	304	3	4,4,4	0.82	0	6,6,6	0.94	0
2	GDP	F	301	3	29,30,30	1.26	4 (13%)	45,47,47	1.55	5 (11%)
2	GDP	C	301	3	29,30,30	1.50	5 (17%)	45,47,47	1.62	7 (15%)
2	GDP	H	301	3	29,30,30	1.20	3 (10%)	45,47,47	1.54	8 (17%)
4	PO4	C	304	3	4,4,4	0.52	0	6,6,6	0.84	0
2	GDP	E	301	3	29,30,30	1.22	2 (6%)	45,47,47	1.53	6 (13%)
2	GDP	D	301	3	29,30,30	1.37	6 (20%)	45,47,47	1.44	8 (17%)
2	GDP	G	301	3	29,30,30	1.08	2 (6%)	45,47,47	1.74	8 (17%)
2	GDP	B	301	3	29,30,30	1.25	5 (17%)	45,47,47	1.65	9 (20%)

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	A	301	3	-	0/16/32/32	0/3/3/3
2	GDP	F	301	3	-	0/16/32/32	0/3/3/3
2	GDP	C	301	3	-	1/16/32/32	0/3/3/3
2	GDP	H	301	3	-	2/16/32/32	0/3/3/3
2	GDP	E	301	3	-	2/16/32/32	0/3/3/3
2	GDP	D	301	3	-	2/16/32/32	0/3/3/3
2	GDP	G	301	3	-	0/16/32/32	0/3/3/3
2	GDP	B	301	3	-	0/16/32/32	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	GDP	C5-C4	3.61	1.48	1.38
2	G	301	GDP	C5-C4	3.44	1.48	1.38
2	E	301	GDP	C5-C4	3.42	1.48	1.38
2	D	301	GDP	C5-C4	3.40	1.48	1.38
2	C	301	GDP	PA-O3A	3.28	1.63	1.59
2	C	301	GDP	O6-C6	3.22	1.29	1.23
2	A	301	GDP	C5-C4	3.16	1.47	1.38
2	A	301	GDP	C4-N9	-3.15	1.30	1.38
2	C	301	GDP	C5-C4	3.14	1.47	1.38
2	H	301	GDP	C4-N9	-2.93	1.30	1.38
2	H	301	GDP	C5-C4	2.89	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	GDP	C5-C4	2.85	1.46	1.38
2	C	301	GDP	C4-N9	-2.80	1.30	1.38
2	E	301	GDP	C2-N3	2.75	1.39	1.33
2	F	301	GDP	C4-N9	-2.69	1.31	1.38
2	D	301	GDP	O6-C6	2.63	1.28	1.23
2	B	301	GDP	C4-N3	2.49	1.39	1.34
2	C	301	GDP	C2-N3	2.49	1.39	1.33
2	F	301	GDP	PA-O3A	-2.44	1.56	1.59
2	B	301	GDP	O4'-C1'	2.40	1.47	1.42
2	B	301	GDP	O6-C6	2.39	1.28	1.23
2	F	301	GDP	C6-N1	-2.25	1.34	1.38
2	D	301	GDP	PA-O2A	-2.21	1.45	1.55
2	B	301	GDP	C4-N9	-2.18	1.32	1.38
2	G	301	GDP	C4-N9	-2.14	1.32	1.38
2	H	301	GDP	C5'-C4'	2.08	1.57	1.51
2	D	301	GDP	C4-N9	-2.08	1.32	1.38
2	D	301	GDP	C2-N3	2.04	1.38	1.33
2	D	301	GDP	O4'-C1'	2.02	1.46	1.42

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	GDP	C5-C4-N3	-5.18	120.15	128.39
2	F	301	GDP	C5-C4-N3	-5.12	120.24	128.39
2	B	301	GDP	C5-C4-N3	-4.93	120.54	128.39
2	G	301	GDP	C2-N3-C4	4.57	120.17	112.30
2	G	301	GDP	C6-C5-N7	4.52	138.51	130.29
2	G	301	GDP	C5-C4-N3	-4.49	121.25	128.39
2	C	301	GDP	N9-C4-N3	4.19	134.34	125.95
2	E	301	GDP	C5-C4-N3	-4.17	121.75	128.39
2	E	301	GDP	C2-N3-C4	4.08	119.32	112.30
2	F	301	GDP	C2-N3-C4	4.04	119.26	112.30
2	A	301	GDP	C5-C4-N3	-4.03	121.98	128.39
2	H	301	GDP	C5-C4-N3	-3.73	122.45	128.39
2	C	301	GDP	C2-N3-C4	3.73	118.72	112.30
2	F	301	GDP	C6-C5-N7	3.72	137.07	130.29
2	B	301	GDP	C2-N3-C4	3.67	118.61	112.30
2	H	301	GDP	N9-C4-N3	3.58	133.11	125.95
2	A	301	GDP	N9-C4-N3	3.49	132.94	125.95
2	F	301	GDP	N9-C4-N3	3.49	132.93	125.95
2	E	301	GDP	N9-C4-N3	3.47	132.90	125.95
2	B	301	GDP	C6-C5-N7	3.47	136.60	130.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	GDP	C5-C4-N3	-3.44	122.91	128.39
2	G	301	GDP	N9-C4-N3	3.40	132.76	125.95
2	H	301	GDP	C2-N3-C4	3.19	117.79	112.30
2	B	301	GDP	N9-C4-N3	3.17	132.30	125.95
2	D	301	GDP	C6-C5-N7	2.96	135.68	130.29
2	E	301	GDP	C6-C5-N7	2.93	135.63	130.29
2	A	301	GDP	C2-N3-C4	2.88	117.27	112.30
2	H	301	GDP	O6-C6-C5	-2.76	119.25	126.53
2	D	301	GDP	O2B-PB-O3A	2.74	113.81	104.64
2	A	301	GDP	O6-C6-C5	-2.72	119.34	126.53
2	F	301	GDP	C4-C5-N7	-2.72	106.36	110.67
2	G	301	GDP	C4-C5-N7	-2.65	106.46	110.67
2	A	301	GDP	O2A-PA-O1A	2.64	124.70	112.44
2	D	301	GDP	C4-C5-N7	-2.62	106.52	110.67
2	G	301	GDP	C6-C5-C4	-2.60	114.92	118.83
2	G	301	GDP	O4'-C1'-N9	-2.58	102.50	108.36
2	C	301	GDP	O6-C6-C5	-2.56	119.78	126.53
2	H	301	GDP	C6-C5-N7	2.53	134.89	130.29
2	E	301	GDP	C2'-C1'-N9	-2.50	106.29	113.25
2	B	301	GDP	C5-C6-N1	2.48	119.56	113.25
2	B	301	GDP	C4-C5-N7	-2.42	106.84	110.67
2	A	301	GDP	C2-N1-C6	-2.41	120.75	125.11
2	D	301	GDP	N9-C4-N3	2.39	130.74	125.95
2	B	301	GDP	O3'-C3'-C2'	-2.35	104.30	111.82
2	B	301	GDP	C2-N1-C6	-2.34	120.86	125.11
2	H	301	GDP	C8-N9-C4	2.33	110.39	106.03
2	C	301	GDP	O2B-PB-O3A	-2.32	96.86	104.64
2	A	301	GDP	O3B-PB-O2B	2.31	116.47	107.80
2	A	301	GDP	C6-C5-N7	2.28	134.44	130.29
2	B	301	GDP	C2'-C3'-C4'	2.27	107.00	102.61
2	C	301	GDP	O3'-C3'-C2'	-2.23	104.66	111.82
2	A	301	GDP	O3A-PA-O1A	-2.23	104.00	110.70
2	G	301	GDP	O4'-C1'-C2'	-2.20	101.90	106.62
2	D	301	GDP	O4'-C4'-C5'	2.17	116.29	109.33
2	D	301	GDP	O3'-C3'-C2'	-2.15	104.91	111.82
2	H	301	GDP	C5-C6-N1	2.11	118.63	113.25
2	A	301	GDP	C5-C6-N1	2.07	118.52	113.25
2	E	301	GDP	O3B-PB-O2B	2.07	115.55	107.80
2	C	301	GDP	O5'-PA-O1A	2.06	117.09	108.94
2	A	301	GDP	O3'-C3'-C4'	-2.05	105.20	111.08
2	D	301	GDP	C8-N7-C5	2.04	107.90	104.26
2	H	301	GDP	C5'-C4'-C3'	-2.02	107.95	115.21

There are no chirality outliers.

All (7) torsion outliers are listed below:

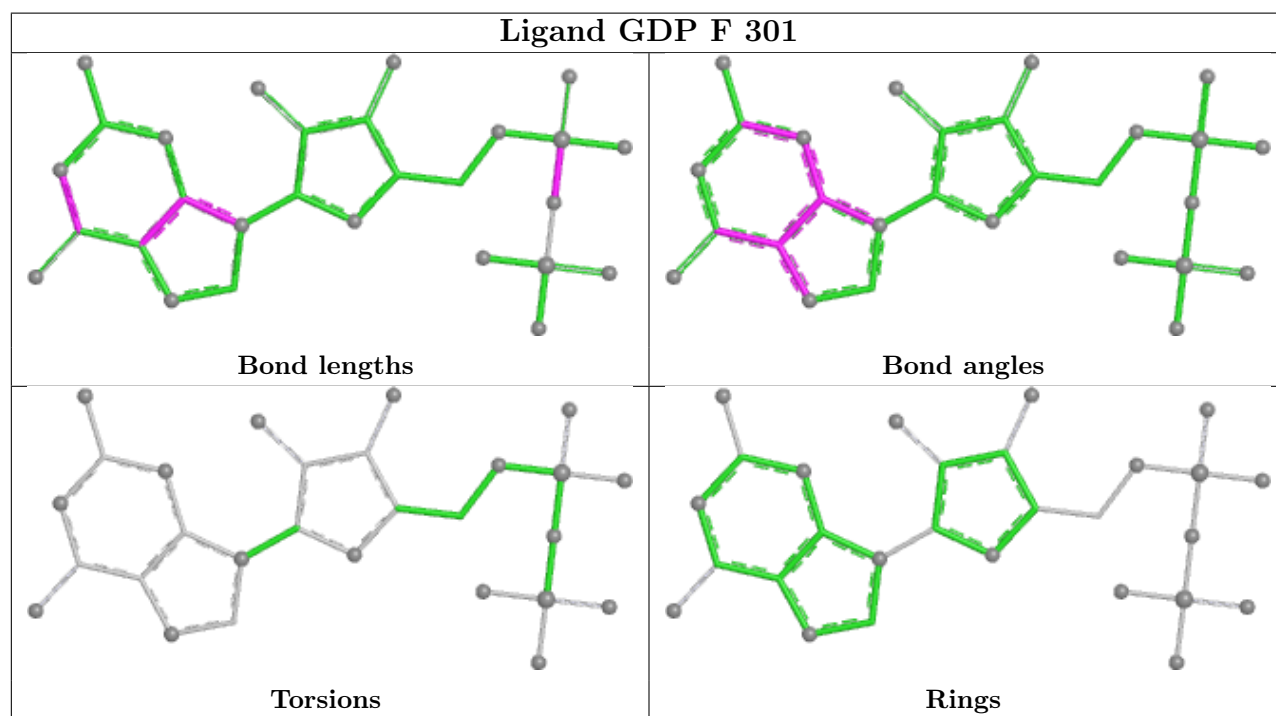
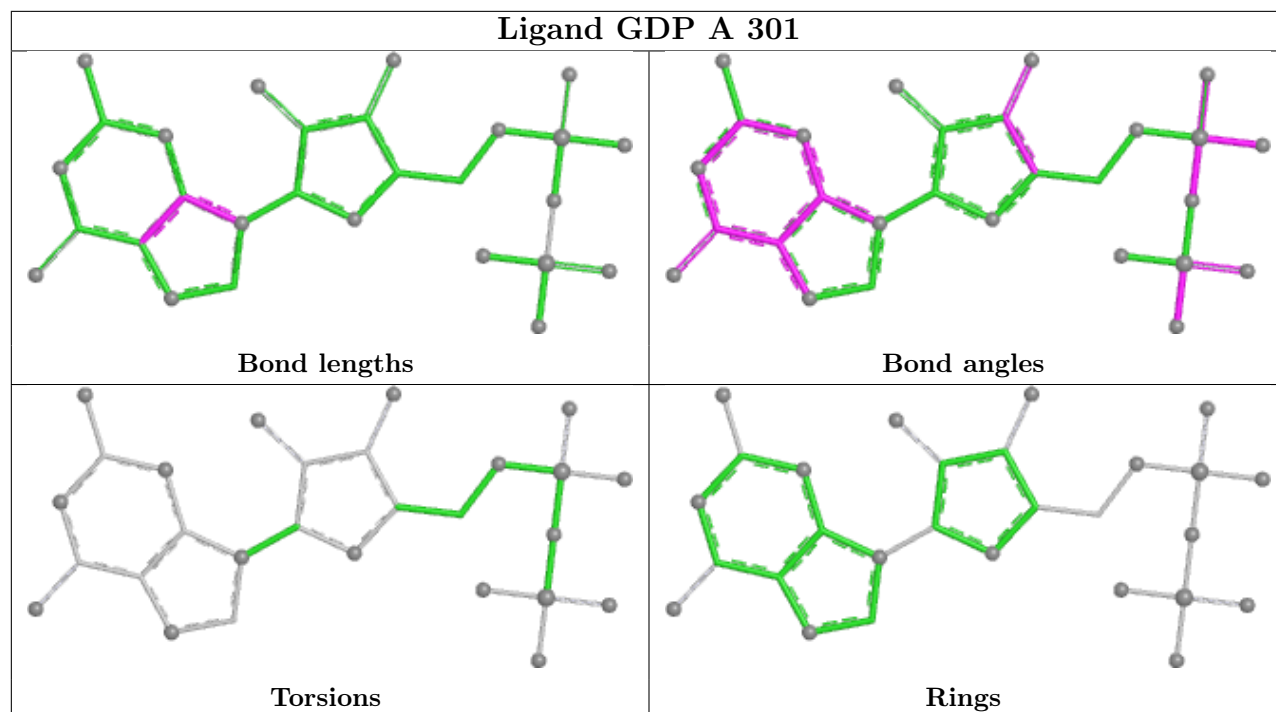
Mol	Chain	Res	Type	Atoms
2	H	301	GDP	PA-O3A-PB-O2B
2	E	301	GDP	PA-O3A-PB-O1B
2	H	301	GDP	PA-O3A-PB-O1B
2	E	301	GDP	PA-O3A-PB-O2B
2	C	301	GDP	C5'-O5'-PA-O1A
2	D	301	GDP	PA-O3A-PB-O1B
2	D	301	GDP	PA-O3A-PB-O2B

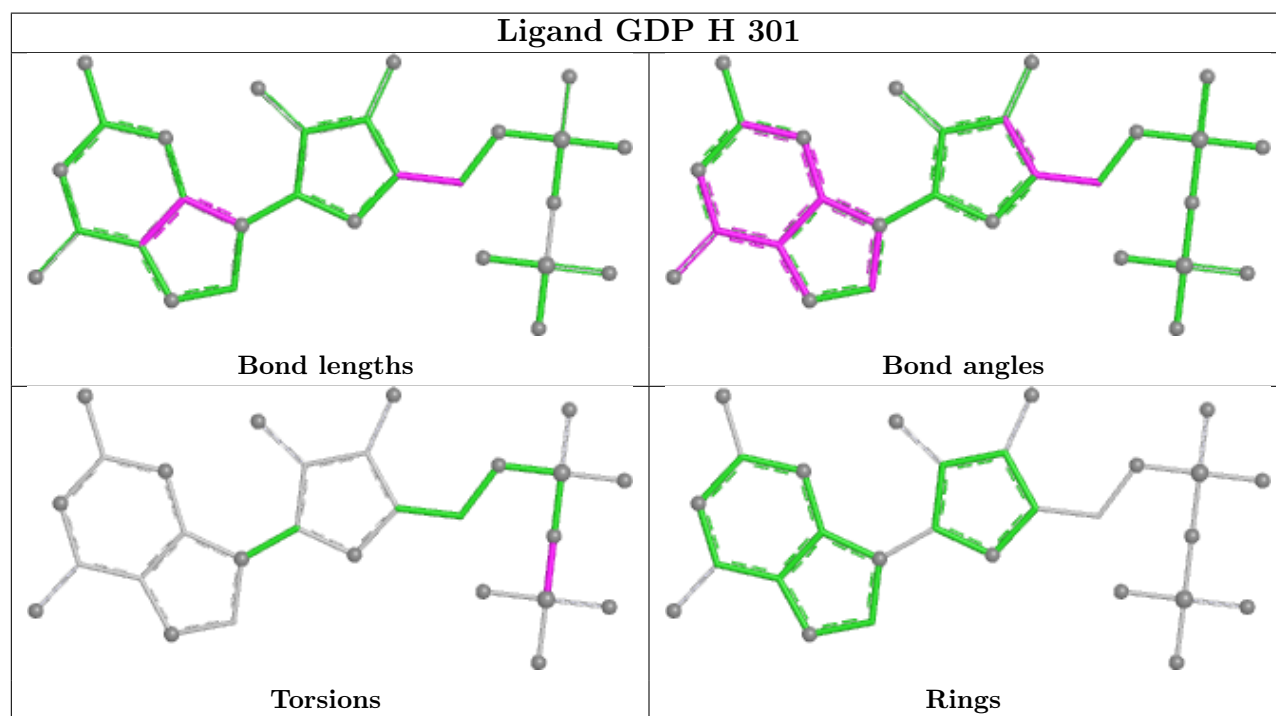
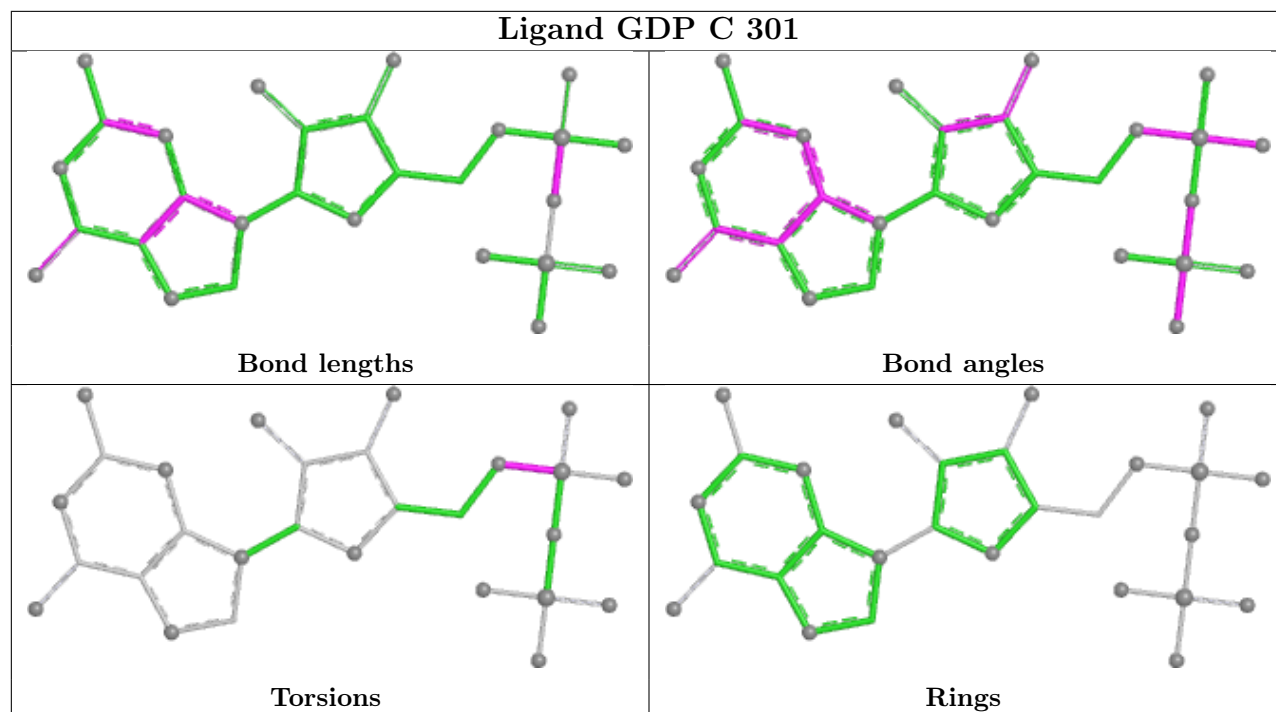
There are no ring outliers.

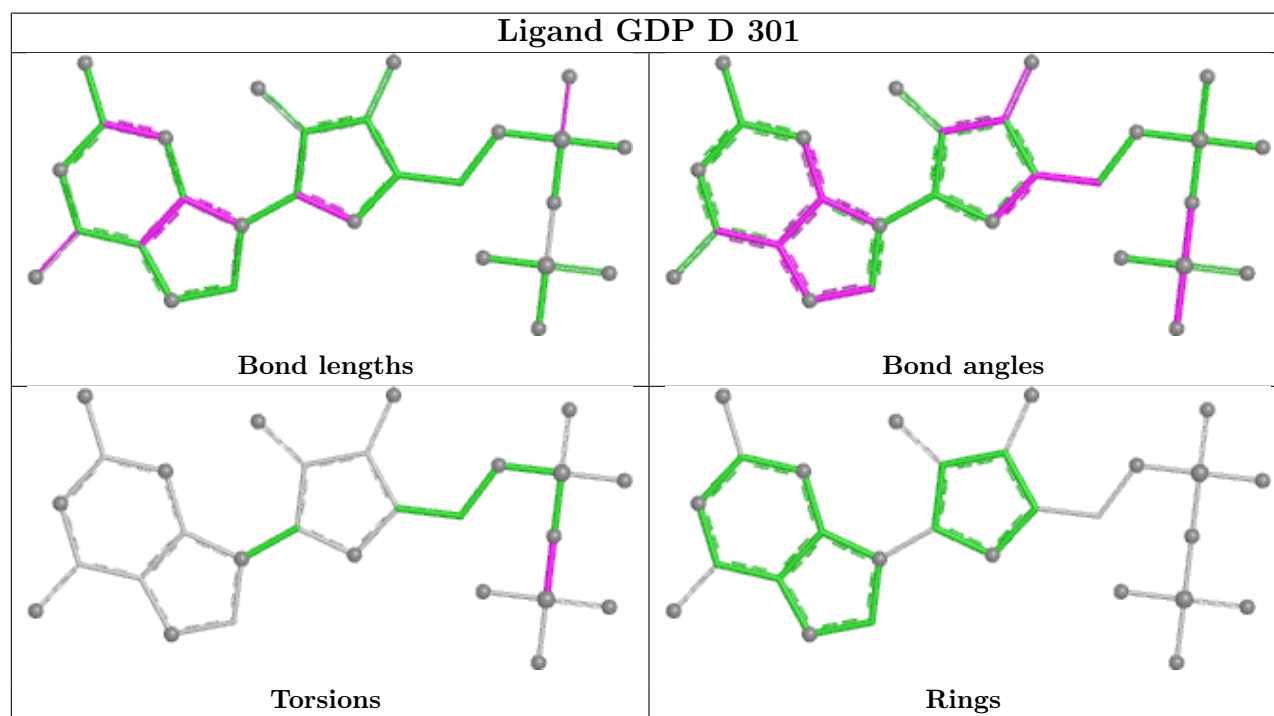
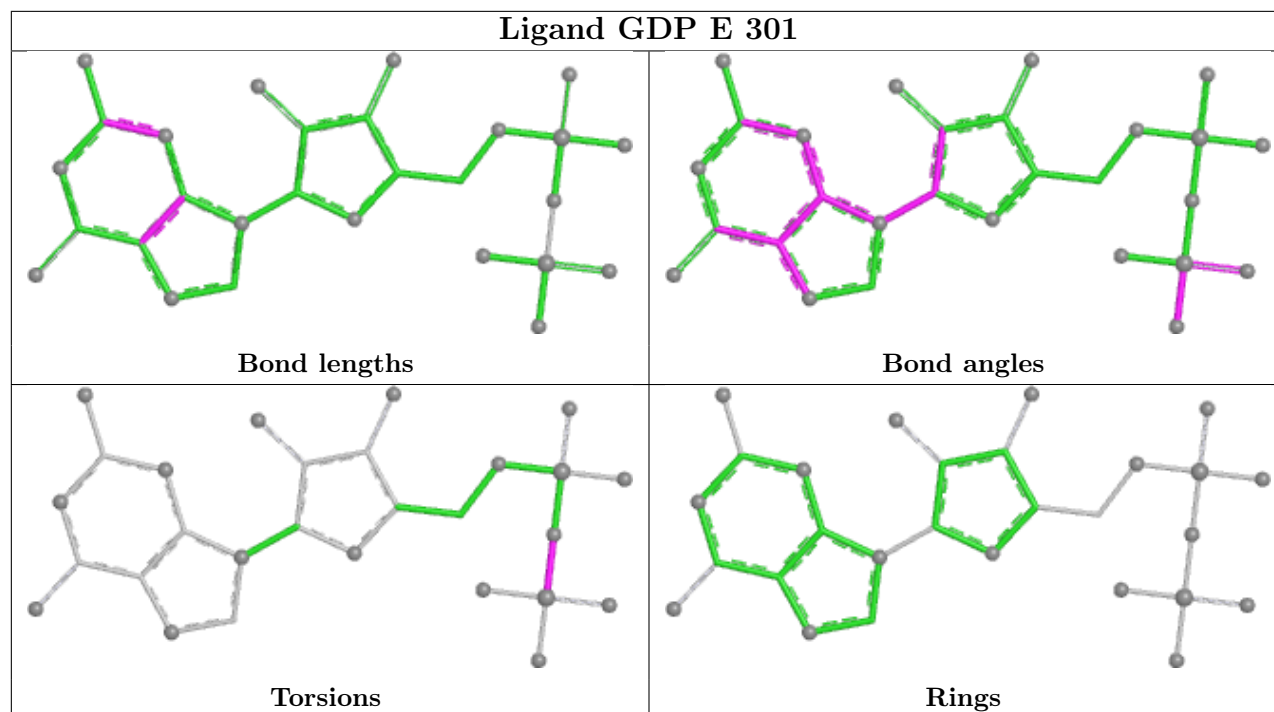
5 monomers are involved in 11 short contacts:

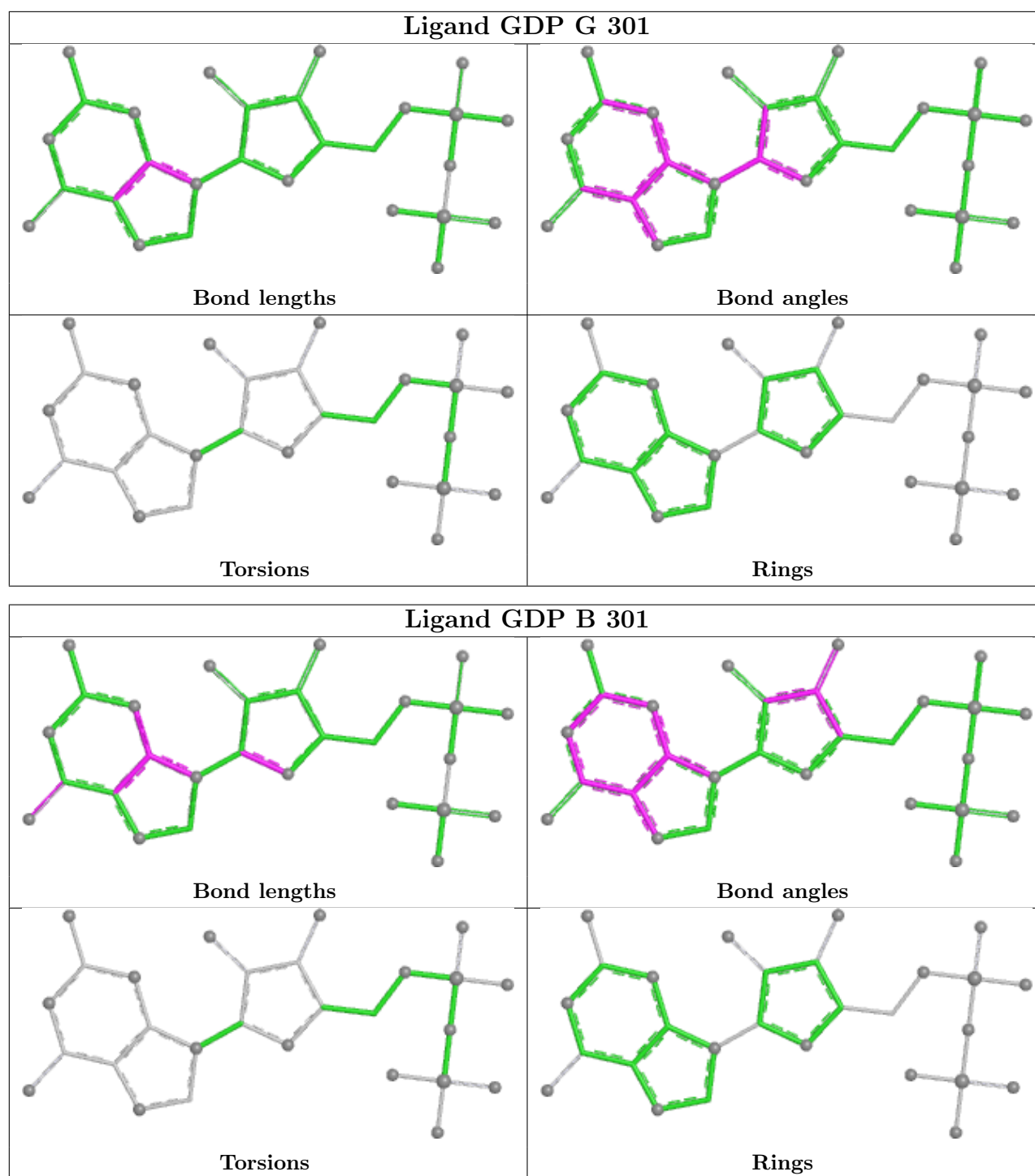
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	GDP	2	0
2	F	301	GDP	1	0
2	H	301	GDP	2	0
2	D	301	GDP	2	0
2	G	301	GDP	4	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	197/216 (91%)	-0.65	0	100	100	15, 28, 54, 77	1 (0%)
1	B	199/216 (92%)	-0.83	0	100	100	12, 20, 44, 63	1 (0%)
1	C	198/216 (91%)	-0.61	0	100	100	12, 26, 55, 69	1 (0%)
1	D	198/216 (91%)	-0.81	0	100	100	11, 20, 42, 58	1 (0%)
1	E	200/216 (92%)	-0.68	1 (0%)	87	90	13, 26, 55, 67	1 (0%)
1	F	197/216 (91%)	-0.64	0	100	100	14, 29, 51, 75	1 (0%)
1	G	197/216 (91%)	-0.62	1 (0%)	87	90	14, 30, 51, 81	1 (0%)
1	H	197/216 (91%)	-0.53	0	100	100	15, 28, 52, 69	1 (0%)
All	All	1583/1728 (91%)	-0.67	2 (0%)	92	93	11, 26, 52, 81	8 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	170	GLY	2.6
1	E	41	ALA	2.1

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 oligosaccharides in this entry.

6.4 Ligands ⓘ

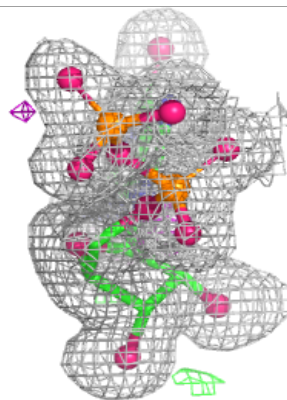
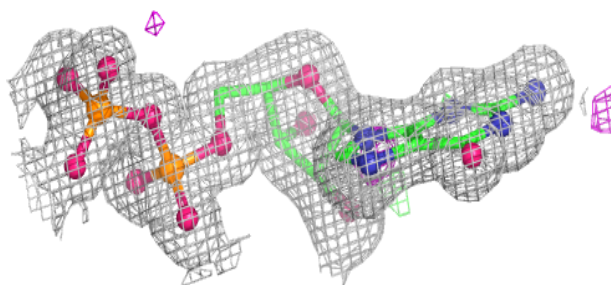
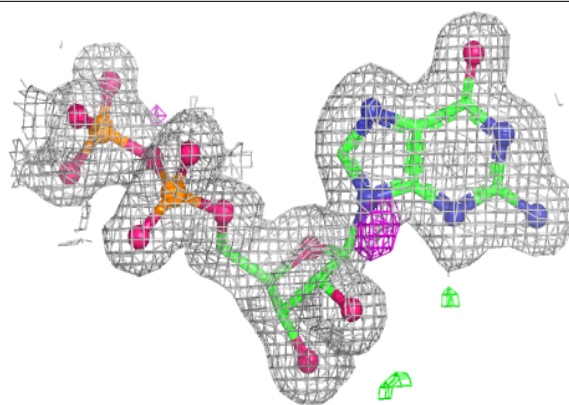
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	MG	B	303	1/1	0.98	0.07	26,26,26,26	0
2	GDP	B	301	28/28	0.99	0.03	13,16,20,23	0
2	GDP	C	301	28/28	0.99	0.03	16,20,25,33	0
2	GDP	D	301	28/28	0.99	0.03	12,16,20,24	0
2	GDP	E	301	28/28	0.99	0.04	17,19,25,31	0
2	GDP	F	301	28/28	0.99	0.03	19,24,30,34	0
2	GDP	G	301	28/28	0.99	0.04	20,24,28,33	0
2	GDP	H	301	28/28	0.99	0.04	19,23,26,27	0
3	MG	A	302	1/1	0.99	0.02	23,23,23,23	0
2	GDP	A	301	28/28	0.99	0.03	19,25,27,28	0
3	MG	B	305	1/1	0.99	0.07	25,25,25,25	0
3	MG	C	302	1/1	0.99	0.04	19,19,19,19	0
3	MG	C	303	1/1	0.99	0.08	26,26,26,26	0
3	MG	C	305	1/1	0.99	0.06	25,25,25,25	0
3	MG	D	302	1/1	0.99	0.04	14,14,14,14	0
3	MG	E	302	1/1	0.99	0.06	20,20,20,20	0
3	MG	F	302	1/1	0.99	0.04	23,23,23,23	0
3	MG	G	302	1/1	0.99	0.02	23,23,23,23	0
3	MG	H	302	1/1	0.99	0.02	24,24,24,24	0
4	PO4	B	304	5/5	0.99	0.08	24,25,28,28	0
4	PO4	C	304	5/5	0.99	0.08	23,25,26,26	0
3	MG	B	302	1/1	1.00	0.01	15,15,15,15	0

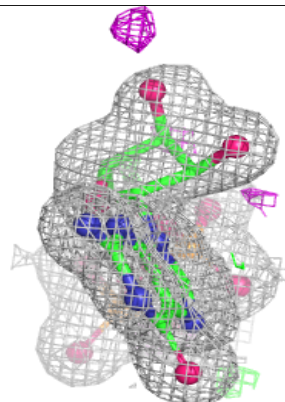
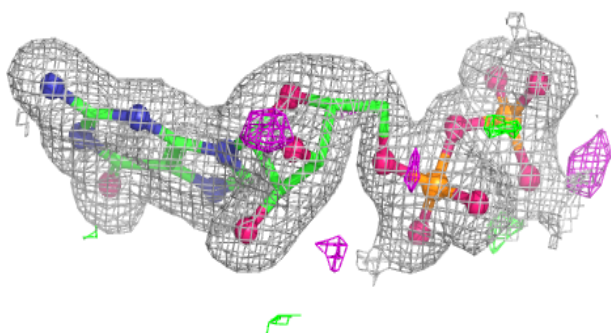
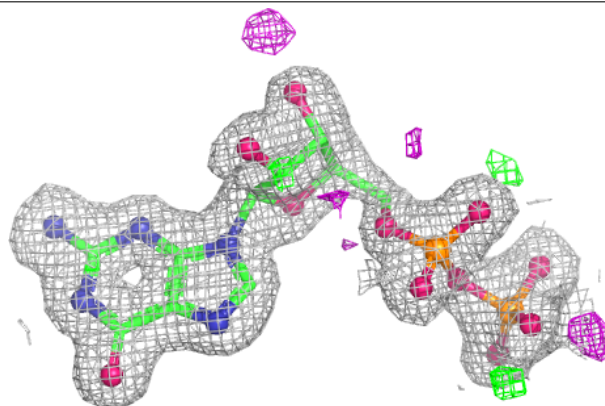
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP B 301:

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

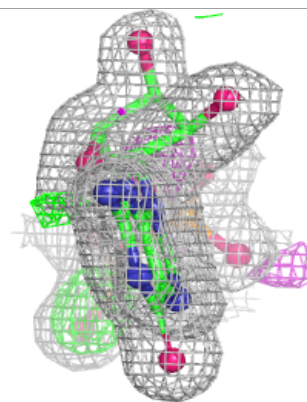
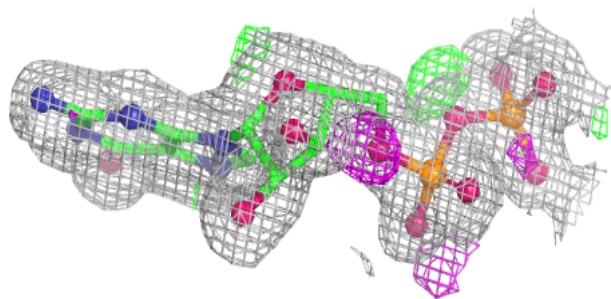
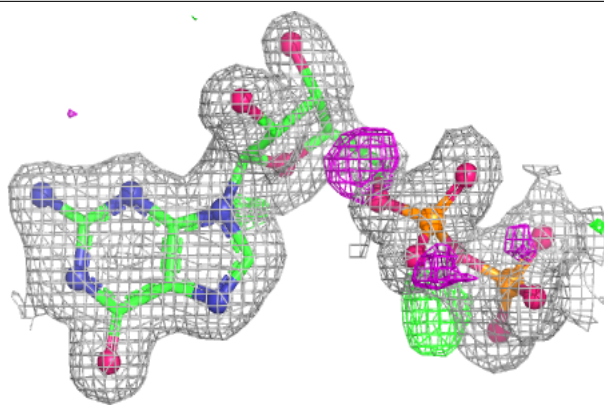
**Electron density around GDP C 301:**

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

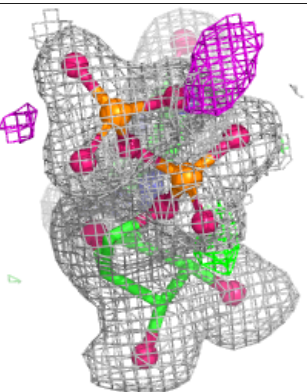
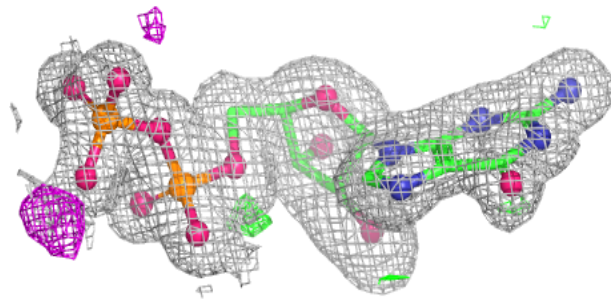
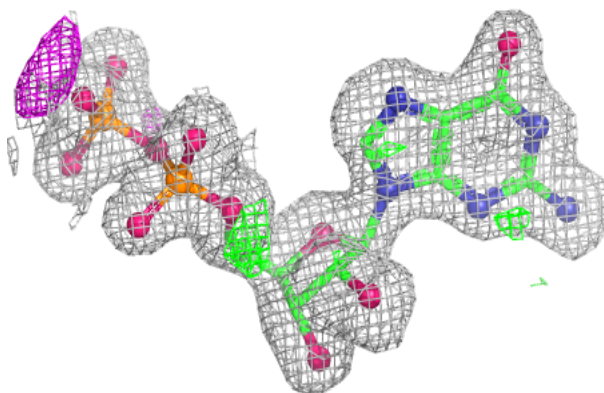


Electron density around GDP D 301:

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

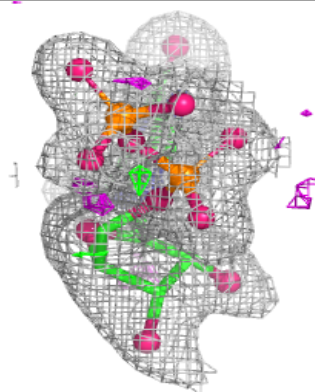
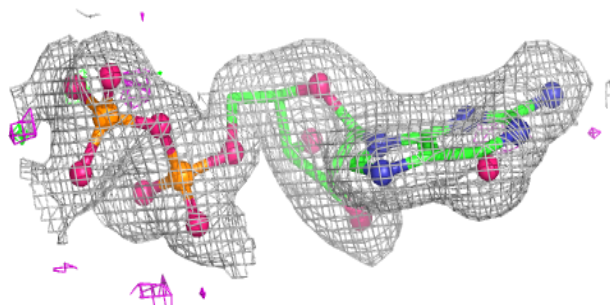
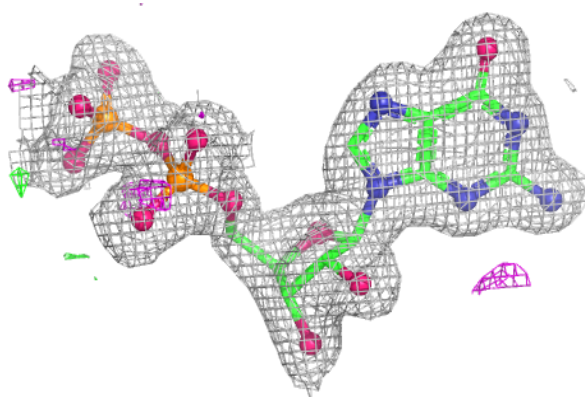
**Electron density around GDP E 301:**

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

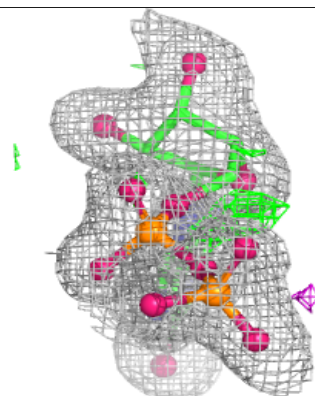
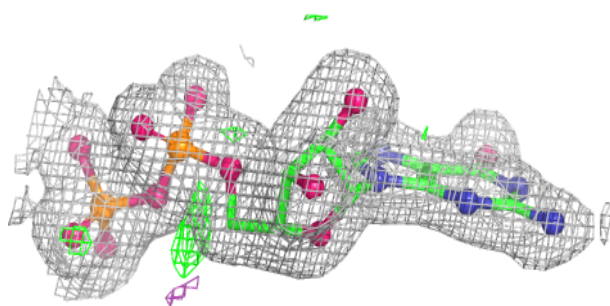
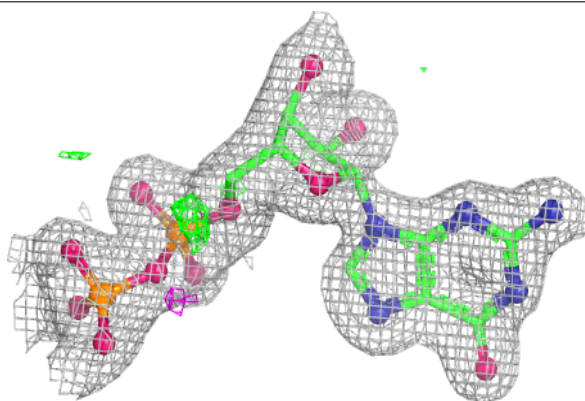


Electron density around GDP F 301:

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

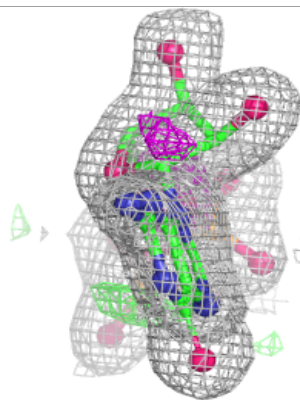
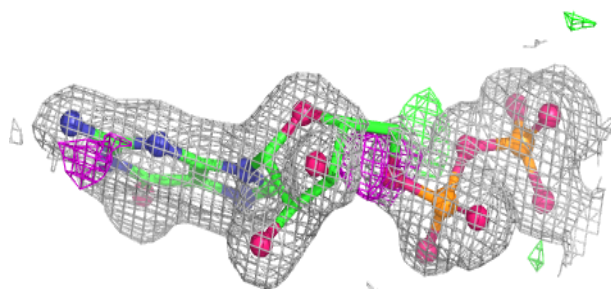
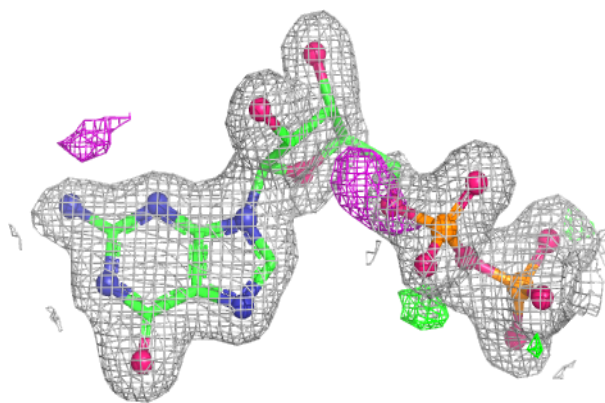
**Electron density around GDP G 301:**

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

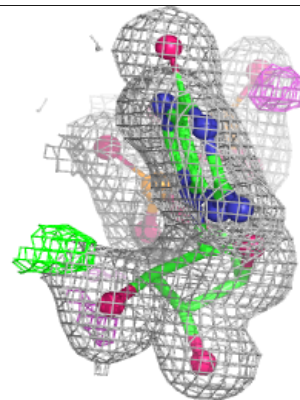
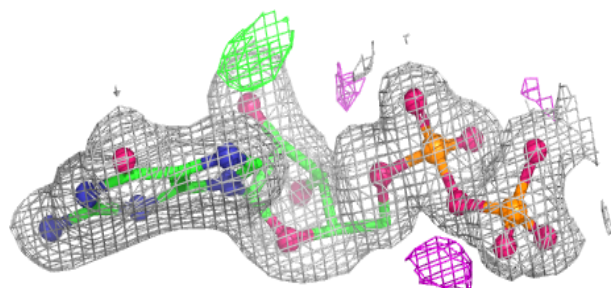
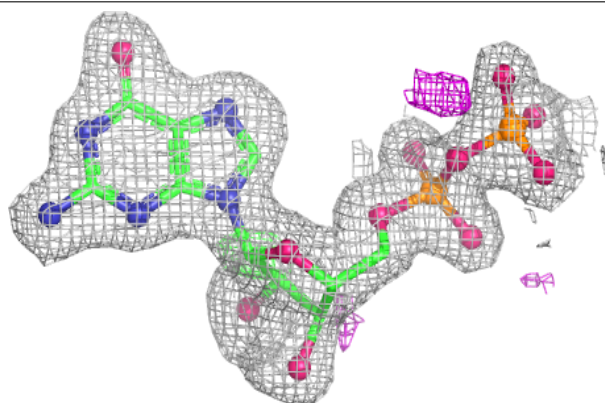


Electron density around GDP H 301:

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

**Electron density around GDP A 301:**

$2mF_o-DF_c$ (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.