



Full wwPDB X-ray Structure Validation Report

May 17, 2020 – 11:31 am BST

PDB ID : 5CJ2
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 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

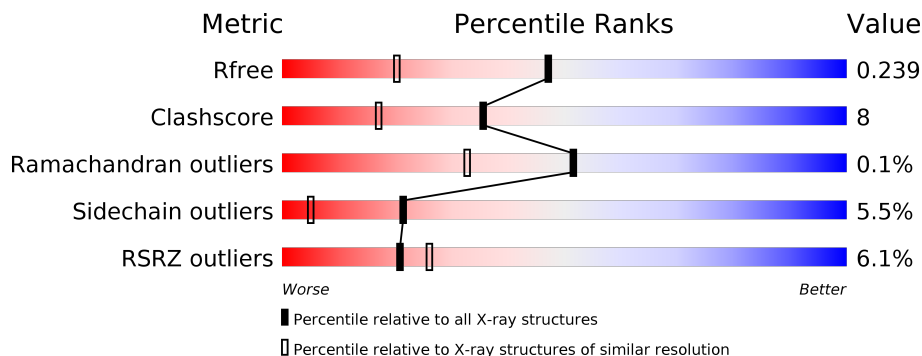
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



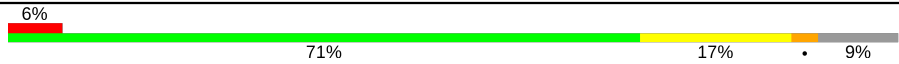

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 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	216	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 72%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center; margin-top: 5px;">6% 72% 15% • 9%</p>
1	B	216	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 76%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center; margin-top: 5px;">2% 76% 14% • 8%</p>
1	C	216	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 71%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center; margin-top: 5px;">9% 71% 18% • 8%</p>
1	D	216	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 77%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center; margin-top: 5px;">2% 77% 11% • 8%</p>
1	E	216	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 79%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center; margin-top: 5px;">5% 79% 12% • 7%</p>
1	F	216	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 75%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center; margin-top: 5px;">7% 75% 14% • 9%</p>

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Mol	Chain	Length	Quality of chain
1	G	216	
1	H	216	

2 Entry composition i

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.

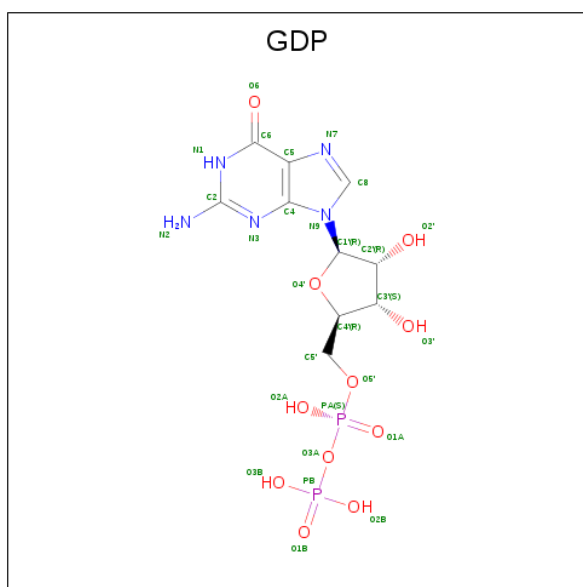
- Molecule 1 is a protein called GTP-binding nuclear protein Ran.

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

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 (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

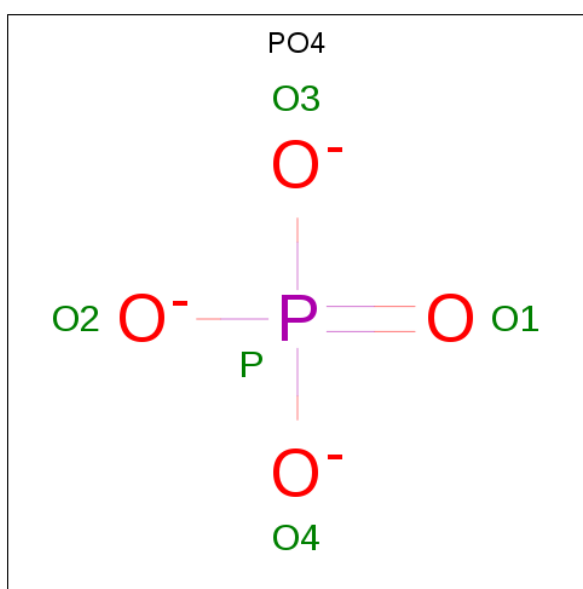
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	G	1	1	1	0	0
3	D	1	1	1	0	0
3	E	1	1	1	0	0
3	H	1	1	1	0	0

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

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 5 is water.

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

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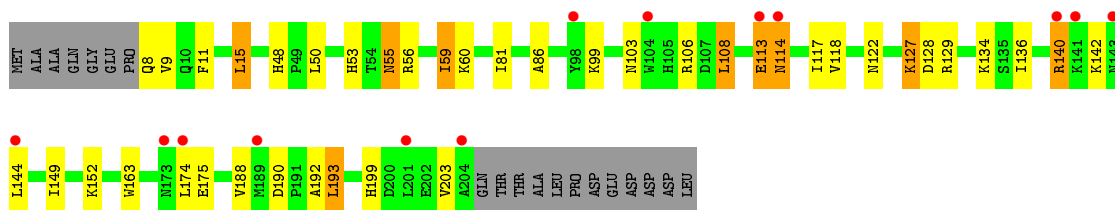
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	80	Total 80	O 80	0	0
5	E	49	Total 49	O 49	0	0
5	F	47	Total 47	O 47	0	0
5	G	42	Total 42	O 42	0	0
5	H	35	Total 35	O 35	0	0

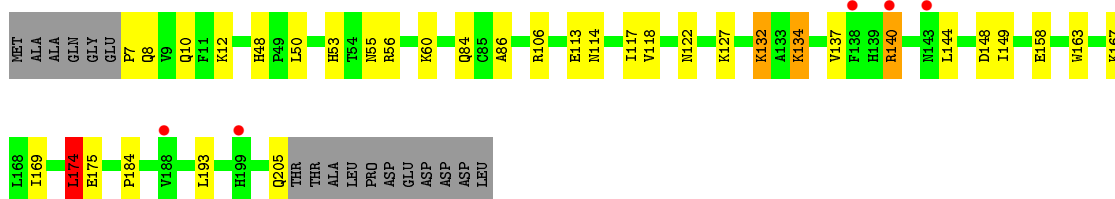
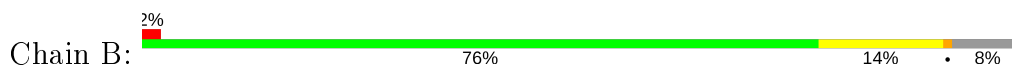
3 Residue-property plots [i](#)

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.

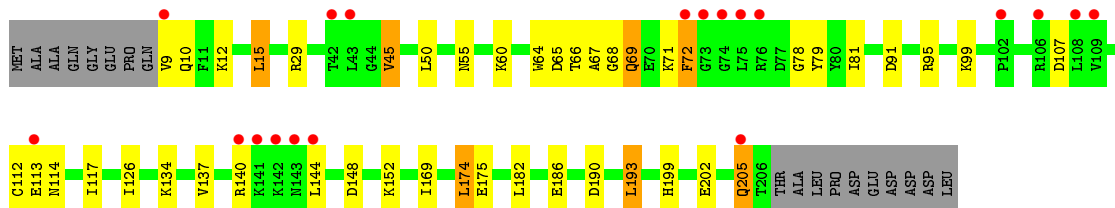
- Molecule 1: GTP-binding nuclear protein Ran



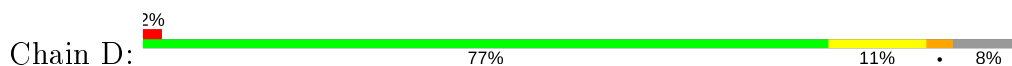
- Molecule 1: GTP-binding nuclear protein Ran

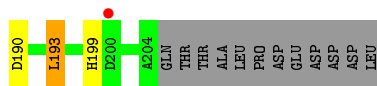


- Molecule 1: GTP-binding nuclear protein Ran

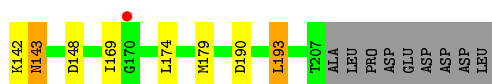
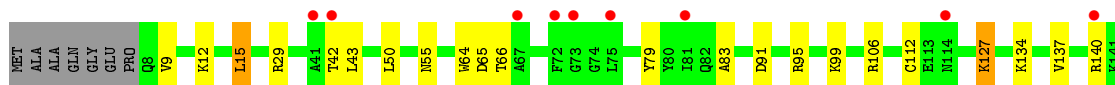
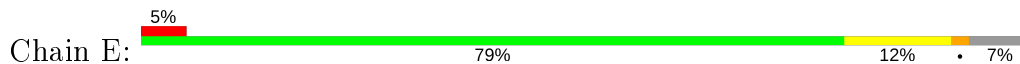


- Molecule 1: GTP-binding nuclear protein Ran

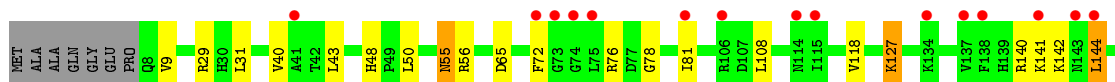
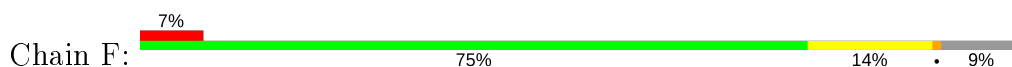




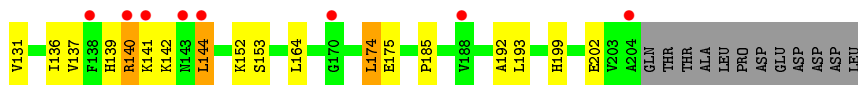
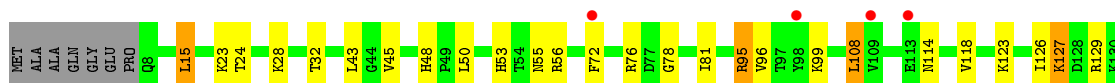
- Molecule 1: GTP-binding nuclear protein Ran



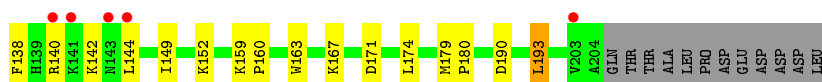
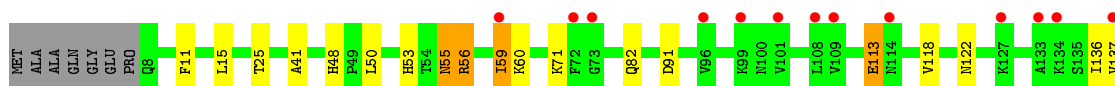
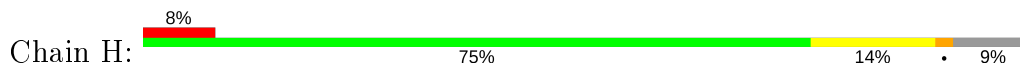
- Molecule 1: GTP-binding nuclear protein Ran



- Molecule 1: GTP-binding nuclear protein Ran



- Molecule 1: GTP-binding nuclear protein Ran



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)	Xtrriage
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	Xtrriage
Anisotropy	0.037	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 23.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.459 for h,-k,-l	Xtrriage
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

Xtrriage'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: GDP, PO4, MG

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	0.85	0/1625	0.98	5/2200 (0.2%)
1	B	1.00	1/1642 (0.1%)	1.09	5/2223 (0.2%)
1	C	0.95	0/1632	1.10	9/2210 (0.4%)
1	D	0.98	0/1633	1.06	4/2211 (0.2%)
1	E	0.90	0/1648	1.04	11/2232 (0.5%)
1	F	0.88	0/1625	0.98	4/2200 (0.2%)
1	G	0.90	0/1625	0.99	6/2200 (0.3%)
1	H	0.85	0/1625	0.99	4/2200 (0.2%)
All	All	0.92	1/13055 (0.0%)	1.03	48/17676 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	158	GLU	CD-OE1	5.05	1.31	1.25

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	174	LEU	CA-CB-CG	10.58	139.63	115.30
1	C	15	LEU	CB-CG-CD2	9.22	126.67	111.00
1	C	148	ASP	CB-CG-OD1	7.97	125.47	118.30
1	G	15	LEU	CB-CG-CD2	7.72	124.13	111.00
1	A	50	LEU	CB-CG-CD2	7.59	123.91	111.00
1	C	29	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	C	148	ASP	CB-CG-OD2	-7.04	111.97	118.30
1	D	50	LEU	CB-CG-CD1	6.82	122.59	111.00
1	E	148	ASP	CB-CG-OD1	6.73	124.36	118.30
1	E	148	ASP	CB-CG-OD2	-6.69	112.28	118.30
1	E	91	ASP	CB-CG-OD2	-6.67	112.29	118.30
1	E	65	ASP	CB-CG-OD1	6.61	124.25	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	50	LEU	CB-CG-CD2	6.54	122.12	111.00
1	D	174	LEU	CA-CB-CG	6.30	129.78	115.30
1	H	50	LEU	CB-CG-CD2	6.29	121.70	111.00
1	F	144	LEU	CA-CB-CG	6.25	129.66	115.30
1	B	148	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	D	50	LEU	CB-CG-CD2	6.21	121.55	111.00
1	E	91	ASP	CB-CG-OD1	6.20	123.88	118.30
1	E	50	LEU	CB-CG-CD2	6.13	121.42	111.00
1	G	50	LEU	CB-CG-CD2	6.13	121.42	111.00
1	G	129	ARG	NE-CZ-NH1	-6.06	117.27	120.30
1	A	129	ARG	NE-CZ-NH1	-6.04	117.28	120.30
1	F	50	LEU	CB-CG-CD2	5.97	121.15	111.00
1	E	29	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	C	91	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	H	56	ARG	NE-CZ-NH1	-5.90	117.35	120.30
1	A	129	ARG	NE-CZ-NH2	5.87	123.24	120.30
1	G	144	LEU	CA-CB-CG	5.84	128.73	115.30
1	F	29	ARG	NE-CZ-NH1	-5.83	117.38	120.30
1	E	15	LEU	CB-CG-CD2	5.60	120.51	111.00
1	C	50	LEU	CB-CG-CD2	5.50	120.34	111.00
1	G	174	LEU	CB-CG-CD1	-5.46	101.72	111.00
1	E	79	TYR	CB-CG-CD1	-5.45	117.73	121.00
1	C	79	TYR	CB-CG-CD2	-5.37	117.78	121.00
1	C	182	LEU	CB-CG-CD1	-5.37	101.87	111.00
1	F	65	ASP	CB-CG-OD1	5.35	123.12	118.30
1	H	91	ASP	CB-CG-OD1	5.35	123.12	118.30
1	B	144	LEU	CA-CB-CG	5.32	127.53	115.30
1	B	174	LEU	CA-CB-CG	5.30	127.49	115.30
1	E	50	LEU	CB-CG-CD1	5.29	119.99	111.00
1	A	15	LEU	CB-CG-CD2	5.28	119.98	111.00
1	E	43	LEU	CA-CB-CG	-5.27	103.17	115.30
1	B	50	LEU	CB-CG-CD1	5.25	119.93	111.00
1	H	50	LEU	CB-CG-CD1	5.21	119.85	111.00
1	D	108	LEU	CB-CG-CD1	-5.18	102.20	111.00
1	G	108	LEU	CA-CB-CG	5.04	126.89	115.30
1	A	50	LEU	CB-CG-CD1	5.02	119.53	111.00

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	1583	0	1609	37	0
1	B	1599	0	1625	25	0
1	C	1590	0	1616	27	0
1	D	1590	0	1617	29	0
1	E	1606	0	1631	15	0
1	F	1583	0	1609	18	0
1	G	1583	0	1609	36	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	5	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	210	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 (210) 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:HG2	1:D:106:ARG:HH21	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: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:A:127:LYS:HD2	1:A:127:LYS:C	2.04	0.78
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:HH21	1:B:106:ARG:HG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:G:142:LYS:HB2	1:G:144:LEU:HG	1.90	0.53
1:D:53:HIS:HE1	1:G:32:THR:OG1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:55:ASN:H	1:E:55:ASN:HD22	1.57	0.53
1:A:55:ASN:N	1:A:55:ASN:HD22	2.08	0.52
1:F:72:PHE:O	1:F:72:PHE:CD1	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:G:23:LYS:NZ	2:G:301:GDP:O1B	2.34	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:HD22	1:B:55:ASN:H	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:HD22	1:F:55:ASN:H	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:55:ASN:ND2	1:C:55:ASN:H	2.10	0.48
1:C:10:GLN:NE2	1:C:60:LYS:HE3	2.27	0.48
1:D:106:ARG:CG	1:D:106:ARG:HH21	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:CG	1:A:56:ARG:O	2.61	0.48
1:A:114:ASN:HA	1:A:114:ASN:HD22	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:D:150:SER:CB	1:D:153:SER:HG	2.28	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:NH2	1:D:106:ARG:HG2	2.18	0.46
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:106:ARG:NH2	1:B:106:ARG:HG2	2.27	0.46
1:B:53:HIS:HD2	5:B:475:HOH:O	1.99	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:ND2	1:H:55:ASN:N	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:CG	1:A:113:GLU:O	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:HB3	1:C:99:LYS:HE2	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HD2	1:B:167:LYS:HA	1.84	0.42
1:D:140:ARG:HB2	1:D:140:ARG:HE	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:A:9:VAL:CG2	1:A:9:VAL:O	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:C:205:GLN:O	1:C:205:GLN:HG3	2.19	0.41
1:E:55:ASN:HD21	1:E:174:LEU:HA	1.84	0.41
1:H:55:ASN:H	1:H:55:ASN:ND2	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:CG	1:B:106:ARG:NH2	2.84	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:D:55:ASN:HD21	1:D:174:LEU:HA	1.86	0.41
1:D:53:HIS:CD2	5:D:473:HOH:O	2.70	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
1:B:169:ILE:HD12	1:B:174:LEU:HD11	2.03	0.40
1:B:118:VAL:HG22	1:B:163:TRP:CE3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:GLN:NE2	1:B:10:GLN:NE2	2.45	0.40
1:F:171:ASP:HA	1:F:172:PRO:HD3	1.96	0.40
1:C:126:ILE:HG23	1:C:126:ILE:HD12	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:HA	1:D:114:ASN:HD22	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 [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	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%)	29	12
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%)	29	12
All	All	1575/1728 (91%)	1525 (97%)	48 (3%)	2 (0%)	51	33

All (2) Ramachandran outliers are listed below:

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

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	170/184 (92%)	158 (93%)	12 (7%)	14	2
1	B	172/184 (94%)	161 (94%)	11 (6%)	17	3
1	C	171/184 (93%)	160 (94%)	11 (6%)	17	3
1	D	171/184 (93%)	160 (94%)	11 (6%)	17	3
1	E	173/184 (94%)	163 (94%)	10 (6%)	20	4
1	F	170/184 (92%)	162 (95%)	8 (5%)	26	7
1	G	170/184 (92%)	162 (95%)	8 (5%)	26	7
1	H	170/184 (92%)	165 (97%)	5 (3%)	42	19
All	All	1367/1472 (93%)	1291 (94%)	76 (6%)	21	5

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	55	ASN
1	A	59	ILE
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
1	A	193	LEU
1	B	7	PRO
1	B	113	GLU
1	B	114	ASN
1	B	127	LYS
1	B	132	LYS
1	B	134	LYS
1	B	140	ARG

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Mol	Chain	Res	Type
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	69	GLN
1	C	72	PHE
1	C	95	ARG
1	C	107	ASP
1	C	112	CYS
1	C	134	LYS
1	C	193	LEU
1	C	205	GLN
1	D	50	LEU
1	D	55	ASN
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	95	ARG
1	E	99	LYS
1	E	106	ARG
1	E	127	LYS
1	E	134	LYS
1	E	143	ASN
1	E	179	MET
1	E	193	LEU
1	F	9	VAL
1	F	55	ASN
1	F	56	ARG
1	F	108	LEU
1	F	127	LYS
1	F	140	ARG

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Mol	Chain	Res	Type
1	F	141	LYS
1	F	196	GLN
1	G	15	LEU
1	G	56	ARG
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	59	ILE
1	H	71	LYS
1	H	193	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) 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	A	199	HIS
1	B	8	GLN
1	B	48	HIS
1	B	53	HIS
1	B	55	ASN
1	B	62	ASN
1	B	84	GLN
1	B	114	ASN
1	C	10	GLN
1	C	48	HIS
1	C	53	HIS
1	C	55	ASN
1	C	62	ASN
1	C	114	ASN

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Mol	Chain	Res	Type
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	145	GLN
1	D	199	HIS
1	E	10	GLN
1	E	48	HIS
1	E	55	ASN
1	E	62	ASN
1	E	143	ASN
1	E	199	HIS
1	F	10	GLN
1	F	48	HIS
1	F	55	ASN
1	F	62	ASN
1	F	103	ASN
1	G	10	GLN
1	G	48	HIS
1	G	53	HIS
1	G	55	ASN
1	G	62	ASN
1	G	103	ASN
1	G	139	HIS
1	G	199	HIS
1	H	48	HIS
1	H	53	HIS
1	H	55	ASN
1	H	62	ASN
1	H	103	ASN

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 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	D	301	3	24,30,30	1.59	5 (20%)	31,47,47	1.83	8 (25%)
2	GDP	F	301	3	24,30,30	1.22	2 (8%)	31,47,47	1.78	6 (19%)
2	GDP	B	301	3	24,30,30	1.57	5 (20%)	31,47,47	1.69	8 (25%)
2	GDP	E	301	3	24,30,30	1.53	3 (12%)	31,47,47	2.00	7 (22%)
2	GDP	G	301	3	24,30,30	1.35	3 (12%)	31,47,47	2.08	7 (22%)
2	GDP	A	301	3	24,30,30	1.13	2 (8%)	31,47,47	1.64	7 (22%)
4	PO4	C	304	3	4,4,4	0.48	0	6,6,6	0.80	0
2	GDP	C	301	3	24,30,30	1.50	4 (16%)	31,47,47	1.73	9 (29%)
2	GDP	H	301	3	24,30,30	1.17	2 (8%)	31,47,47	1.89	6 (19%)
4	PO4	B	304	3	4,4,4	0.78	0	6,6,6	0.90	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GDP	D	301	3	-	2/12/32/32	0/3/3/3
2	GDP	F	301	3	-	0/12/32/32	0/3/3/3
2	GDP	B	301	3	-	0/12/32/32	0/3/3/3
2	GDP	E	301	3	-	2/12/32/32	0/3/3/3
2	GDP	G	301	3	-	0/12/32/32	0/3/3/3
2	GDP	A	301	3	-	0/12/32/32	0/3/3/3
2	GDP	C	301	3	-	1/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GDP	H	301	3	-	2/12/32/32	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	GDP	C6-C5	4.72	1.49	1.41
2	B	301	GDP	O4'-C1'	4.63	1.47	1.41
2	G	301	GDP	C6-C5	4.30	1.48	1.41
2	C	301	GDP	C6-C5	4.22	1.48	1.41
2	D	301	GDP	O4'-C1'	4.01	1.46	1.41
2	F	301	GDP	C6-C5	3.66	1.47	1.41
2	A	301	GDP	C6-N1	3.16	1.38	1.33
2	E	301	GDP	C6-N1	3.12	1.38	1.33
2	H	301	GDP	C6-N1	2.98	1.38	1.33
2	F	301	GDP	C5-C4	2.93	1.48	1.40
2	B	301	GDP	C6-C5	2.91	1.46	1.41
2	D	301	GDP	C6-C5	2.90	1.46	1.41
2	C	301	GDP	C6-N1	2.88	1.38	1.33
2	G	301	GDP	C5-C4	2.75	1.48	1.40
2	B	301	GDP	C4-N3	2.74	1.39	1.35
2	E	301	GDP	C5-C4	2.73	1.48	1.40
2	D	301	GDP	C5-C4	2.71	1.48	1.40
2	A	301	GDP	C5-C4	2.46	1.47	1.40
2	C	301	GDP	C5-C4	2.44	1.47	1.40
2	D	301	GDP	C6-N1	2.36	1.37	1.33
2	D	301	GDP	PA-O2A	-2.18	1.45	1.55
2	H	301	GDP	C5-C4	2.17	1.46	1.40
2	B	301	GDP	C6-N1	2.15	1.36	1.33
2	B	301	GDP	C5-C4	2.12	1.46	1.40
2	C	301	GDP	O6-C6	2.04	1.29	1.24
2	G	301	GDP	C6-N1	2.03	1.36	1.33

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	301	GDP	C6-C5-C4	-6.15	114.92	120.80
2	H	301	GDP	C6-C5-C4	-5.17	115.86	120.80
2	D	301	GDP	C5-C6-N1	-5.00	116.60	123.43
2	C	301	GDP	C5-C6-N1	-4.75	116.94	123.43
2	B	301	GDP	C6-C5-C4	-4.64	116.36	120.80
2	E	301	GDP	C6-C5-C4	-4.64	116.37	120.80
2	E	301	GDP	C6-N1-C2	4.51	123.10	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	GDP	C6-C5-C4	-4.43	116.57	120.80
2	F	301	GDP	C5-C6-N1	-4.40	117.42	123.43
2	A	301	GDP	C6-C5-C4	-4.33	116.66	120.80
2	E	301	GDP	C5-C6-N1	-4.31	117.54	123.43
2	G	301	GDP	C6-N1-C2	4.28	122.72	115.93
2	G	301	GDP	C2-N3-C4	4.22	120.17	115.36
2	E	301	GDP	N3-C2-N1	-4.12	121.73	127.22
2	D	301	GDP	C6-N1-C2	4.09	122.43	115.93
2	H	301	GDP	C6-N1-C2	3.97	122.25	115.93
2	F	301	GDP	C6-N1-C2	3.97	122.24	115.93
2	G	301	GDP	C5-C6-N1	-3.77	118.28	123.43
2	C	301	GDP	C6-N1-C2	3.63	121.69	115.93
2	A	301	GDP	C5-C6-N1	-3.59	118.52	123.43
2	G	301	GDP	N3-C2-N1	-3.51	122.54	127.22
2	H	301	GDP	C5-C6-N1	-3.51	118.63	123.43
2	E	301	GDP	C2-N3-C4	3.47	119.32	115.36
2	G	301	GDP	O4'-C1'-C2'	-3.44	101.90	106.93
2	F	301	GDP	C2-N3-C4	3.42	119.26	115.36
2	D	301	GDP	C6-C5-C4	-3.21	117.73	120.80
2	H	301	GDP	N3-C2-N1	-3.19	122.97	127.22
2	B	301	GDP	C6-N1-C2	3.11	120.86	115.93
2	A	301	GDP	C6-N1-C2	3.03	120.75	115.93
2	C	301	GDP	C2-N3-C4	2.95	118.72	115.36
2	F	301	GDP	C4-C5-N7	-2.91	106.36	109.40
2	B	301	GDP	C2-N3-C4	2.85	118.61	115.36
2	B	301	GDP	C5-C6-N1	-2.83	119.56	123.43
2	G	301	GDP	C4-C5-N7	-2.82	106.46	109.40
2	E	301	GDP	O4'-C1'-C2'	-2.82	102.81	106.93
2	H	301	GDP	C1'-N9-C4	-2.80	121.71	126.64
2	D	301	GDP	C4-C5-N7	-2.77	106.52	109.40
2	D	301	GDP	O2B-PB-O3A	2.74	113.81	104.64
2	C	301	GDP	N3-C2-N1	-2.69	123.63	127.22
2	A	301	GDP	O2A-PA-O1A	2.52	124.70	112.24
2	B	301	GDP	C4-C5-N7	-2.45	106.84	109.40
2	B	301	GDP	N3-C2-N1	-2.41	124.00	127.22
2	C	301	GDP	O4'-C1'-C2'	-2.37	103.46	106.93
2	B	301	GDP	O3'-C3'-C2'	-2.33	104.30	111.82
2	C	301	GDP	O2B-PB-O3A	-2.32	96.86	104.64
2	A	301	GDP	O3B-PB-O2B	2.31	116.47	107.64
2	F	301	GDP	N3-C2-N1	-2.30	124.16	127.22
2	B	301	GDP	C2'-C3'-C4'	2.24	107.00	102.64
2	C	301	GDP	O3'-C3'-C2'	-2.21	104.66	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	GDP	O4'-C1'-C2'	-2.20	103.72	106.93
2	C	301	GDP	C6-C5-C4	-2.17	118.72	120.80
2	D	301	GDP	O3'-C3'-C2'	-2.14	104.91	111.82
2	H	301	GDP	C2-N3-C4	2.13	117.79	115.36
2	D	301	GDP	O4'-C4'-C5'	2.10	116.29	109.37
2	D	301	GDP	PA-O3A-PB	-2.09	125.66	132.83
2	E	301	GDP	O3B-PB-O2B	2.07	115.55	107.64
2	C	301	GDP	O5'-PA-O1A	2.05	117.09	109.07
2	A	301	GDP	O3'-C3'-C4'	-2.02	105.20	111.05

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	D	301	GDP	PA-O3A-PB-O1B
2	D	301	GDP	PA-O3A-PB-O2B
2	C	301	GDP	C5'-O5'-PA-O1A

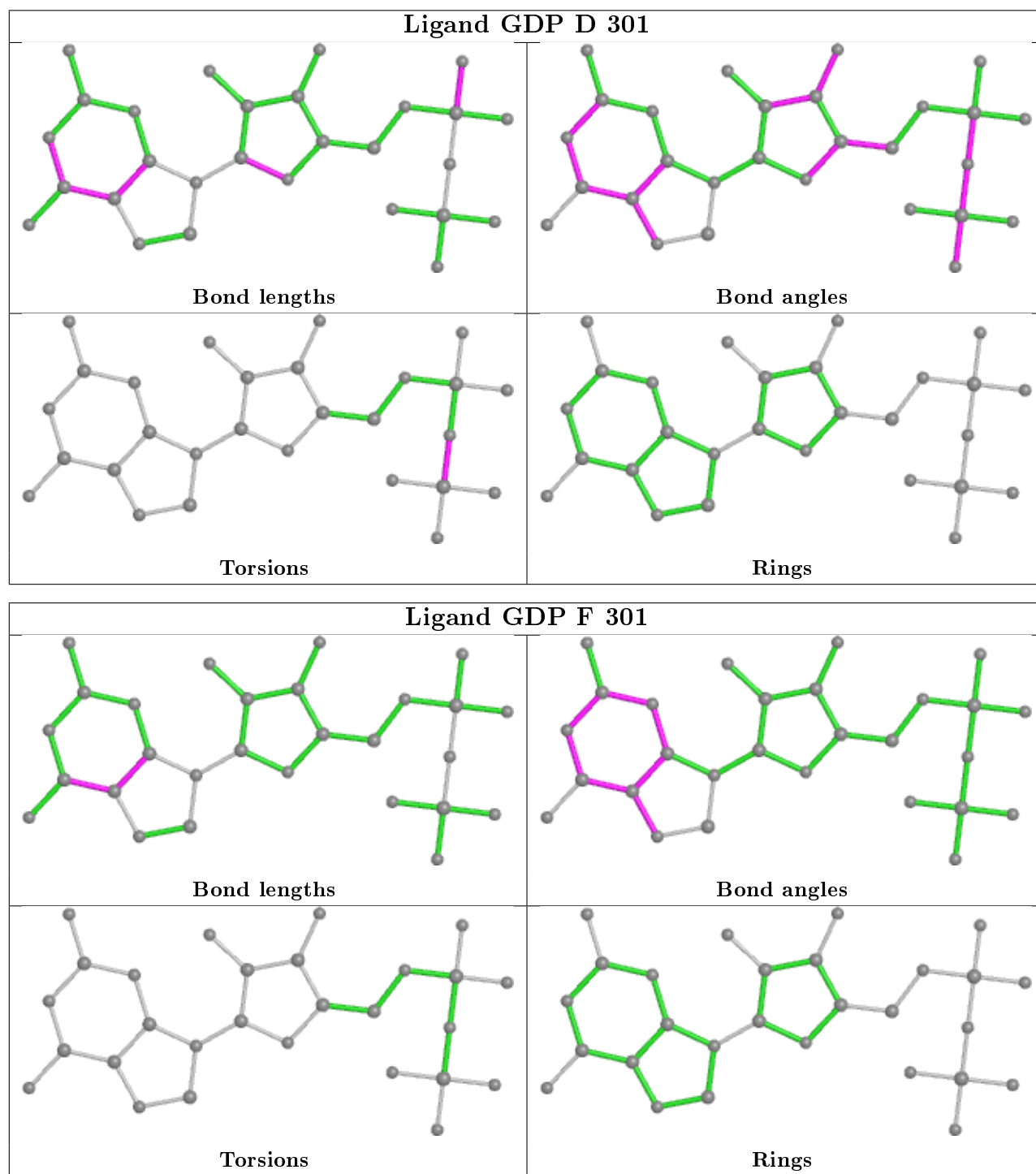
There are no ring outliers.

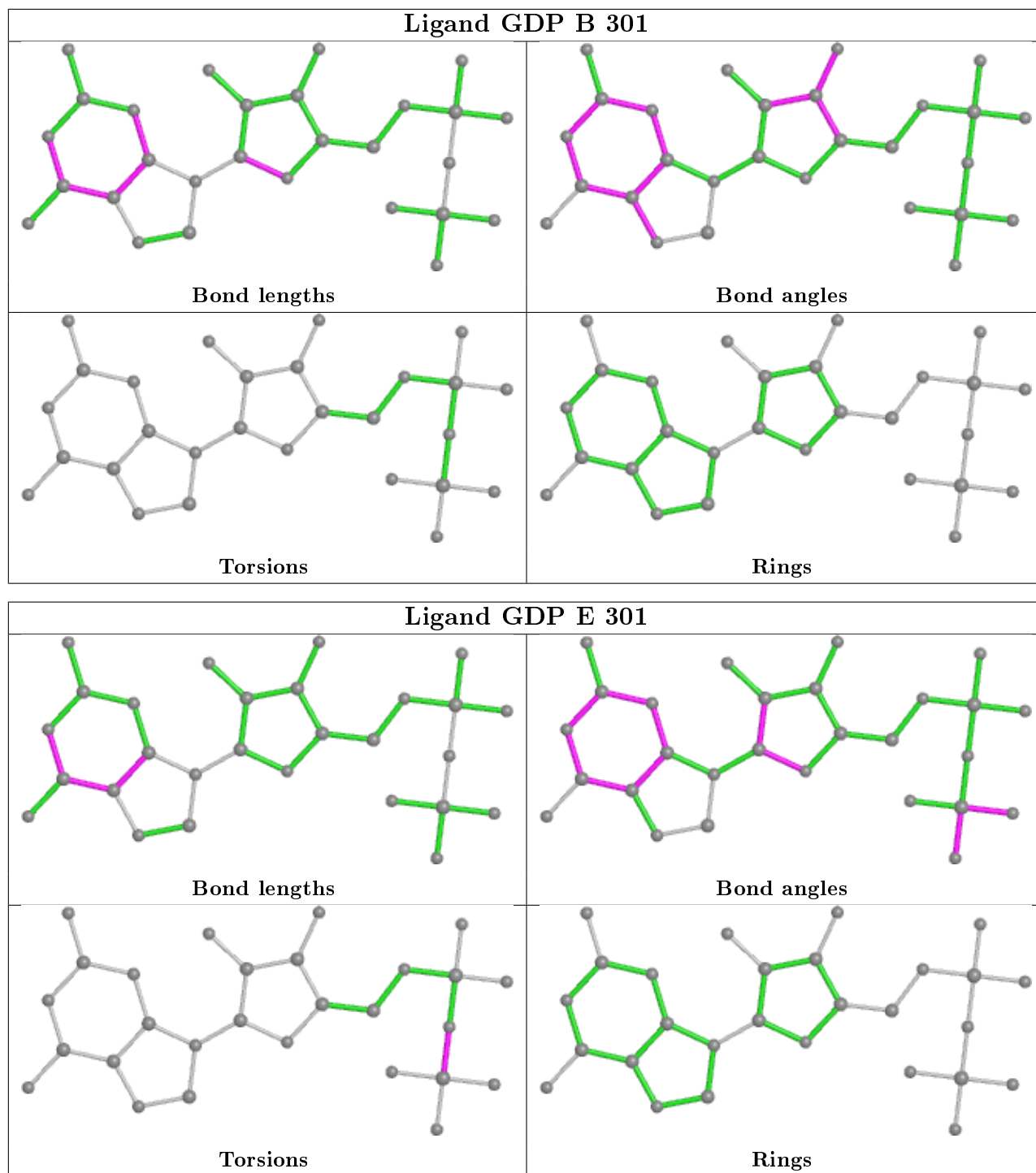
5 monomers are involved in 11 short contacts:

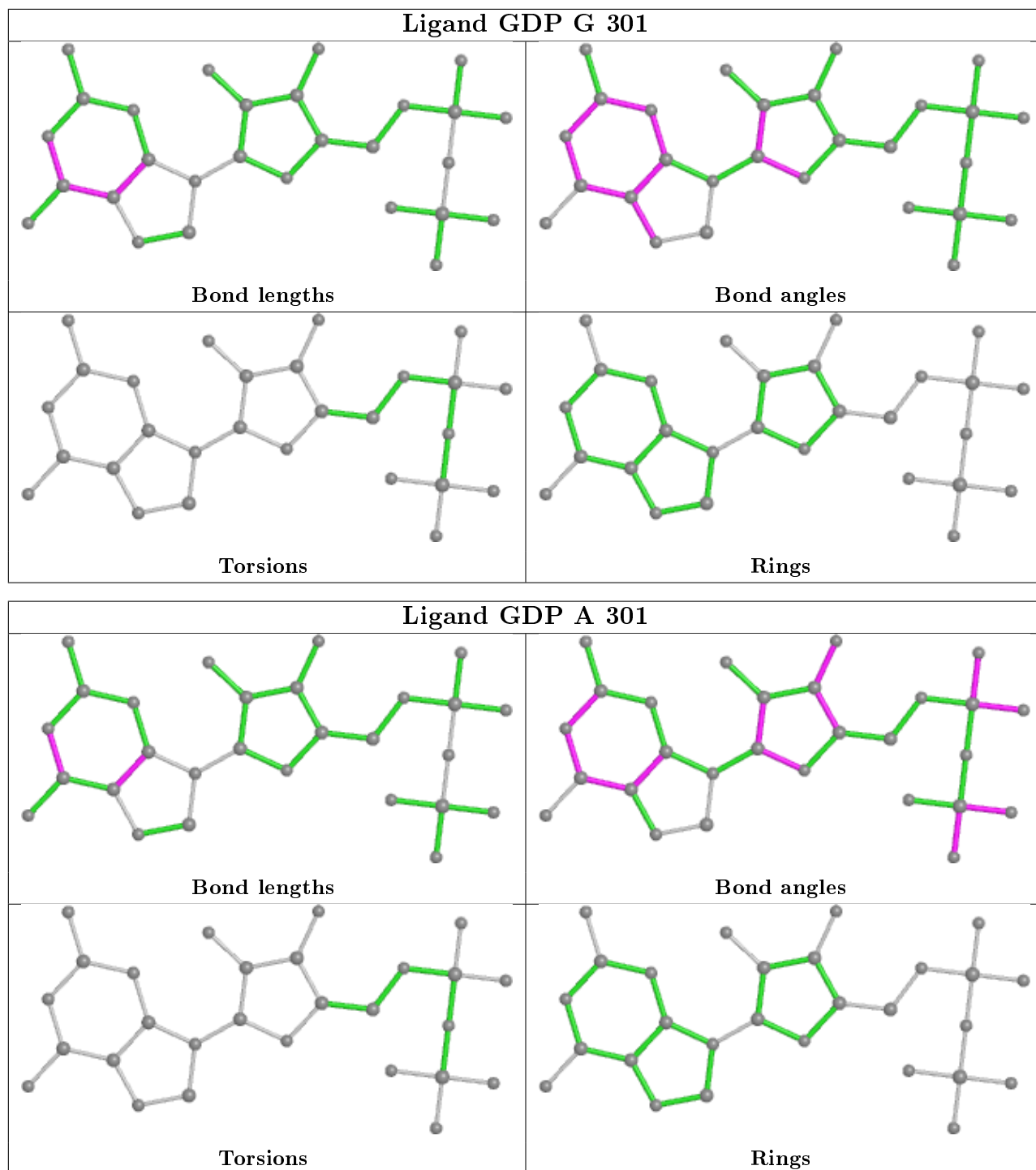
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	GDP	2	0
2	F	301	GDP	1	0
2	G	301	GDP	4	0
2	A	301	GDP	2	0
2	H	301	GDP	2	0

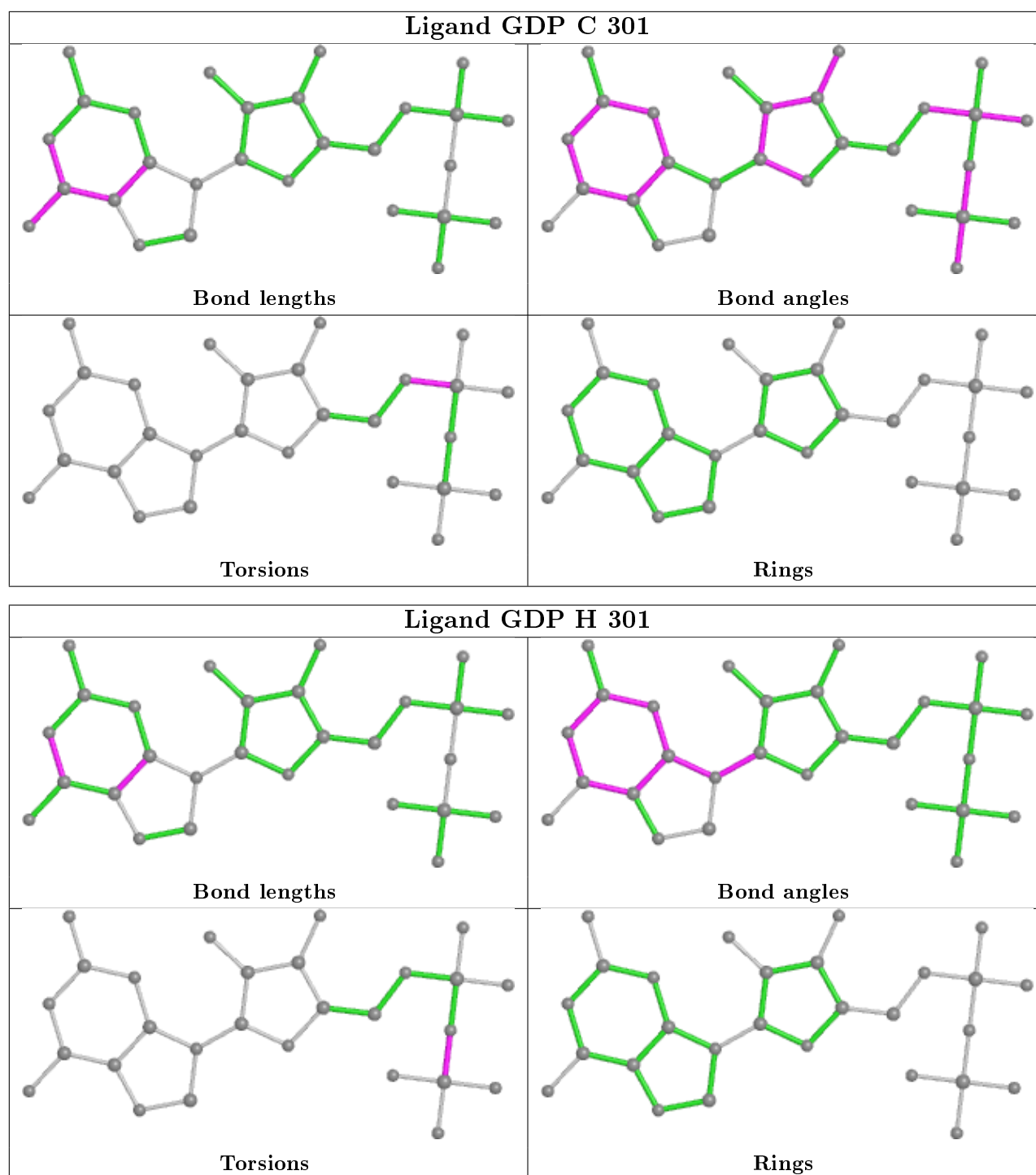
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	197/216 (91%)	0.42	13 (6%) 18 24	17, 28, 54, 77	0
1	B	199/216 (92%)	0.21	5 (2%) 57 63	13, 20, 44, 63	0
1	C	198/216 (91%)	0.55	19 (9%) 8 10	16, 26, 55, 69	0
1	D	198/216 (91%)	0.21	5 (2%) 57 63	12, 20, 42, 58	0
1	E	200/216 (92%)	0.37	10 (5%) 28 34	15, 26, 55, 67	0
1	F	197/216 (91%)	0.51	15 (7%) 13 18	14, 29, 51, 75	0
1	G	197/216 (91%)	0.45	12 (6%) 21 26	14, 30, 51, 81	0
1	H	197/216 (91%)	0.60	18 (9%) 9 11	16, 28, 52, 69	0
All	All	1583/1728 (91%)	0.41	97 (6%) 21 26	12, 26, 52, 81	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	73	GLY	7.9
1	C	75	LEU	6.1
1	E	72	PHE	5.4
1	A	114	ASN	4.9
1	C	144	LEU	4.7
1	E	41	ALA	4.4
1	G	109	VAL	4.2
1	G	140	ARG	4.2
1	H	140	ARG	4.1
1	G	138	PHE	4.1
1	F	141	LYS	4.0
1	F	73	GLY	4.0
1	E	73	GLY	3.9
1	H	203	VAL	3.8
1	E	114	ASN	3.8
1	E	140	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	75	LEU	3.8
1	C	74	GLY	3.8
1	H	144	LEU	3.7
1	C	76	ARG	3.7
1	C	140	ARG	3.6
1	G	170	GLY	3.5
1	F	144	LEU	3.4
1	H	99	LYS	3.4
1	F	138	PHE	3.3
1	C	143	ASN	3.3
1	A	201	LEU	3.2
1	H	137	VAL	3.2
1	D	137	VAL	3.1
1	C	72	PHE	3.1
1	G	143	ASN	3.0
1	F	143	ASN	3.0
1	C	141	LYS	3.0
1	B	143	ASN	3.0
1	B	188	VAL	3.0
1	H	101	VAL	2.9
1	A	113	GLU	2.9
1	E	42	THR	2.9
1	H	109	VAL	2.9
1	H	114	ASN	2.9
1	G	72	PHE	2.8
1	F	72	PHE	2.8
1	H	141	LYS	2.8
1	F	106	ARG	2.7
1	F	137	VAL	2.7
1	H	133	ALA	2.7
1	D	141	LYS	2.7
1	D	200	ASP	2.6
1	H	127	LYS	2.6
1	B	138	PHE	2.6
1	H	143	ASN	2.6
1	C	205	GLN	2.6
1	F	41	ALA	2.6
1	H	73	GLY	2.5
1	A	173	ASN	2.5
1	F	81	ILE	2.5
1	C	109	VAL	2.5
1	C	43	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	142	LYS	2.5
1	A	144	LEU	2.5
1	A	174	LEU	2.5
1	F	74	GLY	2.5
1	C	9	VAL	2.4
1	H	59	ILE	2.4
1	E	67	ALA	2.4
1	G	144	LEU	2.3
1	H	72	PHE	2.3
1	A	98	TYR	2.3
1	A	140	ARG	2.3
1	H	134	LYS	2.3
1	E	81	ILE	2.3
1	A	141	LYS	2.3
1	F	115	ILE	2.3
1	G	113	GLU	2.3
1	G	98	TYR	2.3
1	F	114	ASN	2.3
1	H	96	VAL	2.2
1	C	108	LEU	2.2
1	H	108	LEU	2.2
1	A	143	ASN	2.2
1	G	188	VAL	2.2
1	A	204	ALA	2.2
1	C	113	GLU	2.1
1	B	140	ARG	2.1
1	D	7	PRO	2.1
1	A	189	MET	2.1
1	C	42	THR	2.1
1	C	106	ARG	2.1
1	A	104	TRP	2.1
1	E	170	GLY	2.1
1	B	199	HIS	2.1
1	C	102	PRO	2.0
1	G	204	ALA	2.0
1	F	75	LEU	2.0
1	F	134	LYS	2.0
1	D	143	ASN	2.0
1	G	141	LYS	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](#)

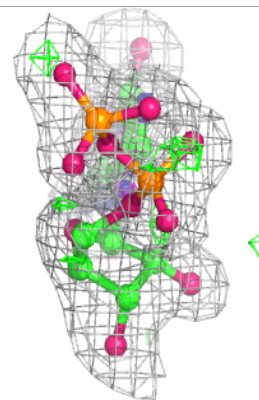
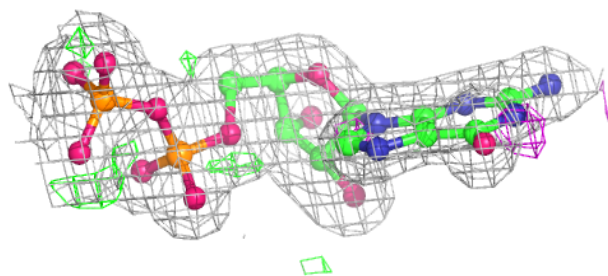
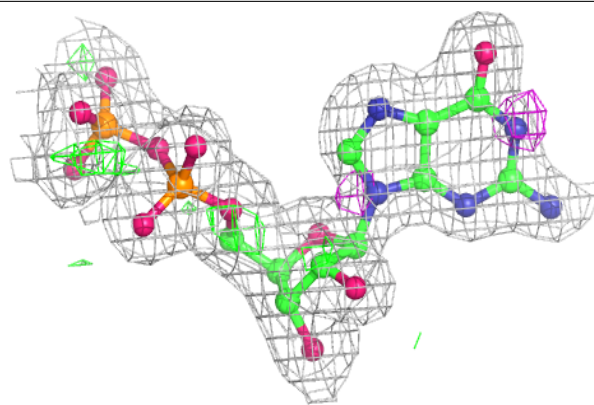
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	B	303	1/1	0.91	0.09	26,26,26,26	0
2	GDP	G	301	28/28	0.95	0.11	20,24,28,33	0
2	GDP	H	301	28/28	0.96	0.10	19,23,26,27	0
4	PO4	B	304	5/5	0.96	0.09	24,25,28,28	0
3	MG	B	305	1/1	0.96	0.10	25,25,25,25	0
2	GDP	D	301	28/28	0.97	0.09	12,16,20,24	0
3	MG	G	302	1/1	0.97	0.08	23,23,23,23	0
2	GDP	E	301	28/28	0.97	0.09	17,19,25,31	0
2	GDP	A	301	28/28	0.97	0.08	19,25,27,28	0
3	MG	F	302	1/1	0.97	0.05	23,23,23,23	0
4	PO4	C	304	5/5	0.97	0.08	23,25,26,26	0
2	GDP	C	301	28/28	0.97	0.08	16,20,25,33	0
3	MG	E	302	1/1	0.98	0.04	20,20,20,20	0
3	MG	C	305	1/1	0.98	0.08	25,25,25,25	0
3	MG	C	303	1/1	0.98	0.07	26,26,26,26	0
2	GDP	B	301	28/28	0.98	0.09	13,16,20,23	0
3	MG	D	302	1/1	0.98	0.05	14,14,14,14	0
2	GDP	F	301	28/28	0.98	0.09	19,24,30,34	0
3	MG	C	302	1/1	0.98	0.05	19,19,19,19	0
3	MG	H	302	1/1	0.99	0.05	24,24,24,24	0
3	MG	A	302	1/1	0.99	0.06	23,23,23,23	0
3	MG	B	302	1/1	0.99	0.12	15,15,15,15	0

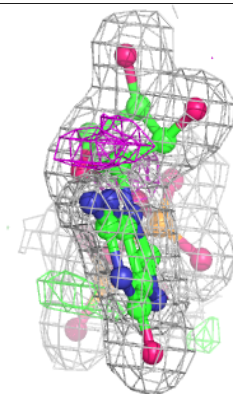
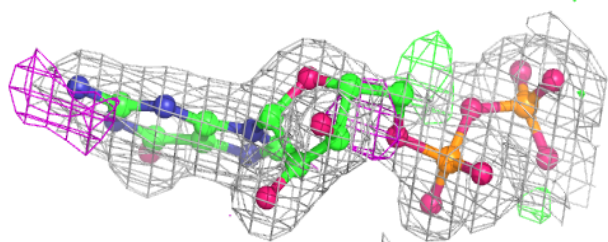
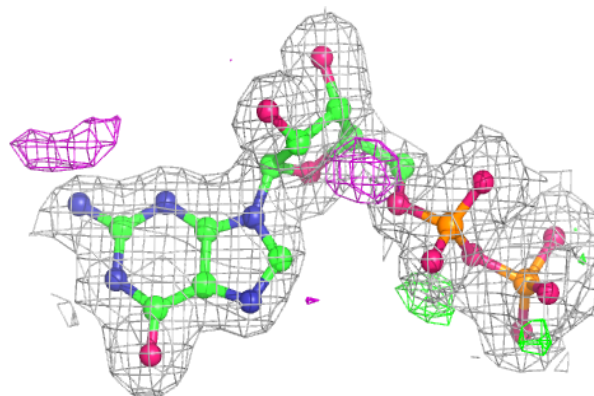
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP 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)

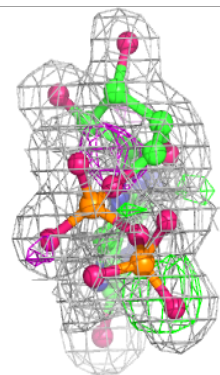
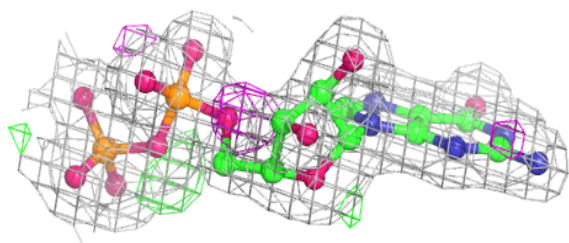
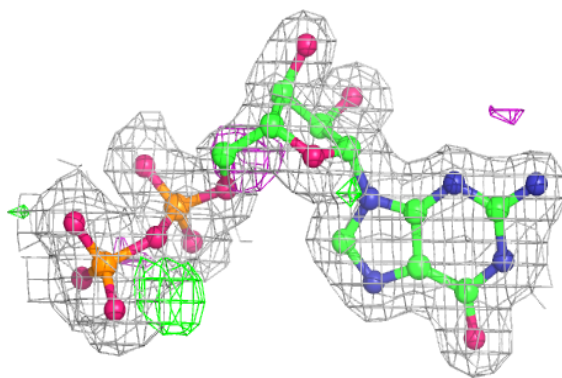
**Electron density around GDP H 301:**

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

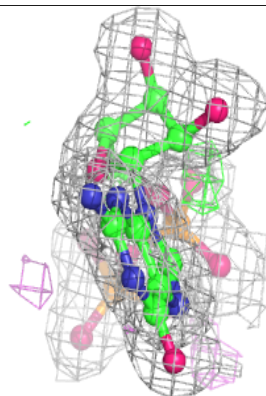
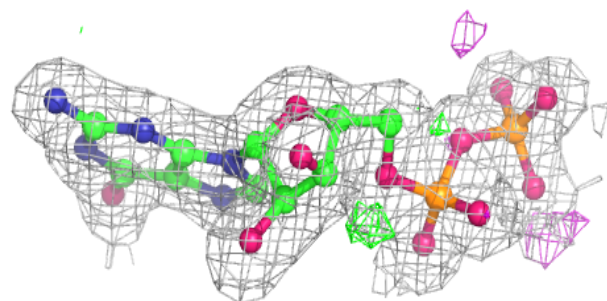
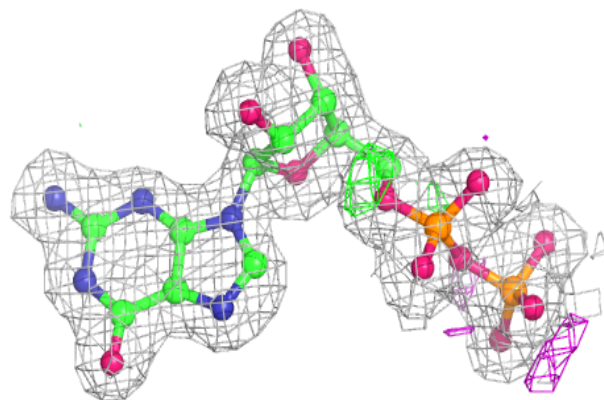


Electron density around GDP D 301:

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

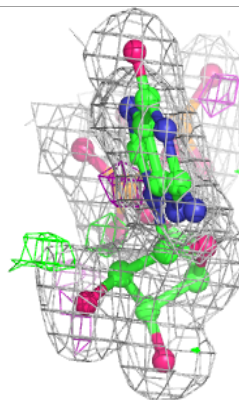
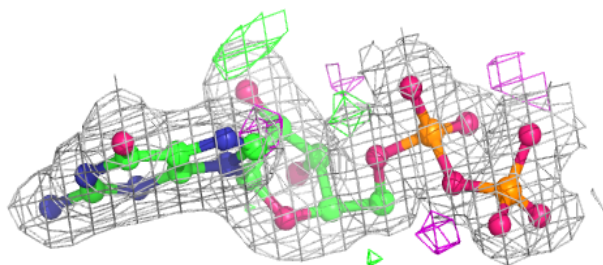
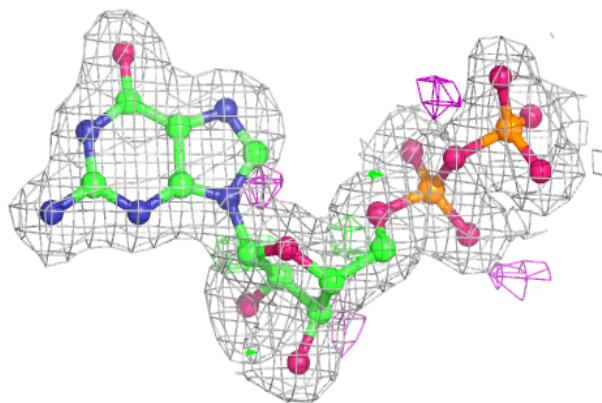
**Electron density around GDP E 301:**

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

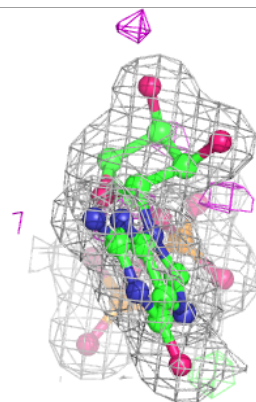
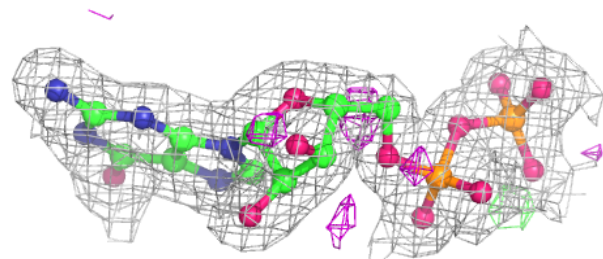
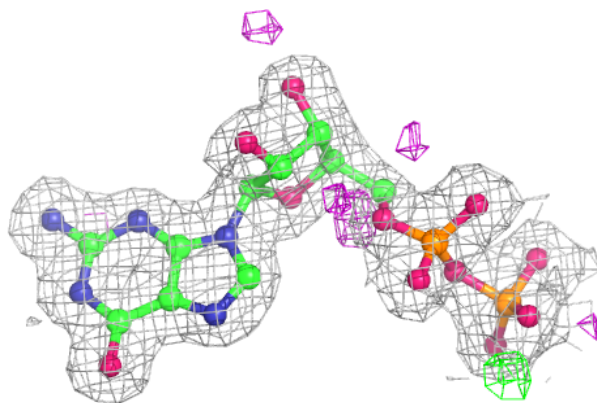


Electron density around GDP A 301:

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

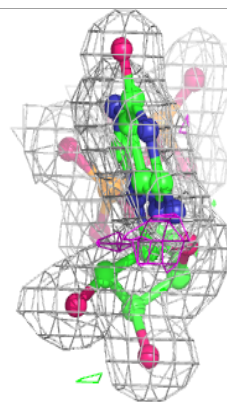
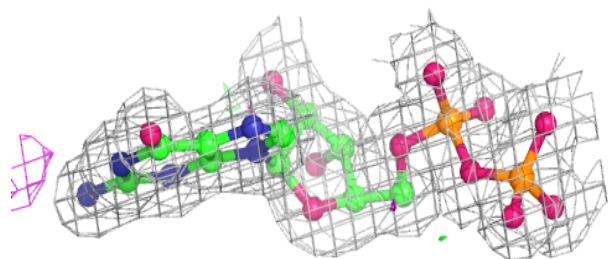
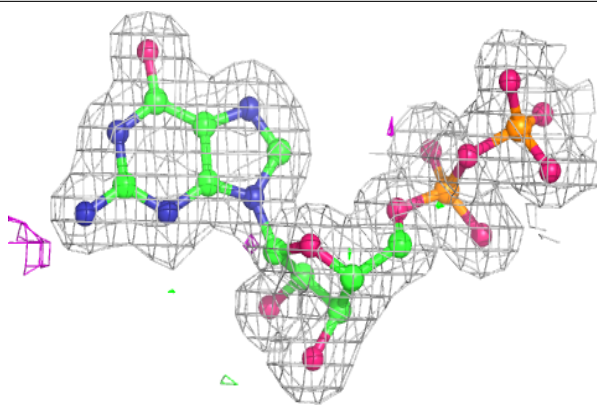
**Electron density around GDP C 301:**

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

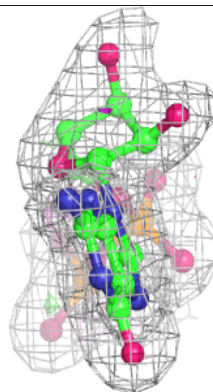
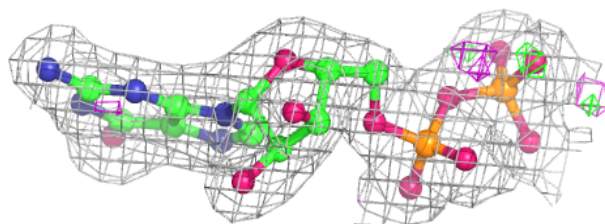
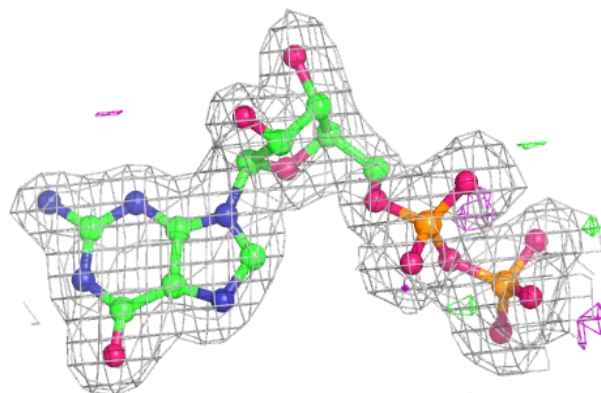


Electron density around GDP B 301:

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

**Electron density around GDP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.