



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:22 AM UTC

PDB ID : 1VG8 / pdb_00001vg8
Title : GPPNHP-Bound Rab7
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Deposited on : 2004-04-23
Resolution : 1.70 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

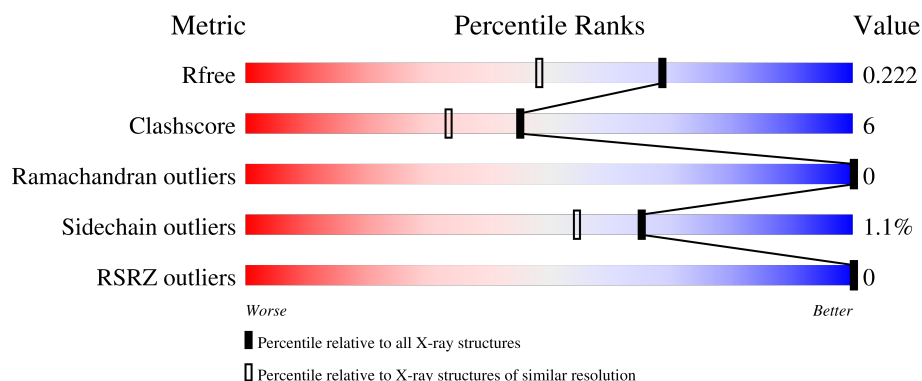
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	207	 75% 13% 11%
1	B	207	 76% 10% 14%
1	C	207	 78% 8% 14%
1	D	207	 74% 14% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6679 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 Ras-related protein Rab-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	184	Total	C	N	O	S	0	2	0
			1488	950	249	283	6			
1	B	179	Total	C	N	O	S	0	1	0
			1438	917	242	272	7			
1	C	178	Total	C	N	O	S	0	2	0
			1434	913	241	274	6			
1	D	184	Total	C	N	O	S	0	1	0
			1481	946	247	282	6			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	B	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	C	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	D	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 4 is water.

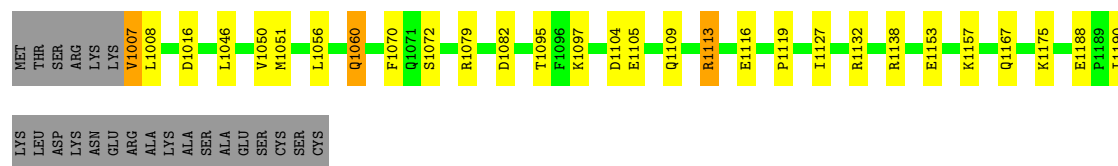
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	176	Total	O	0	0
			176	176		
4	B	182	Total	O	0	0
			182	182		
4	C	177	Total	O	0	0
			177	177		
4	D	171	Total	O	0	0
			171	171		

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.

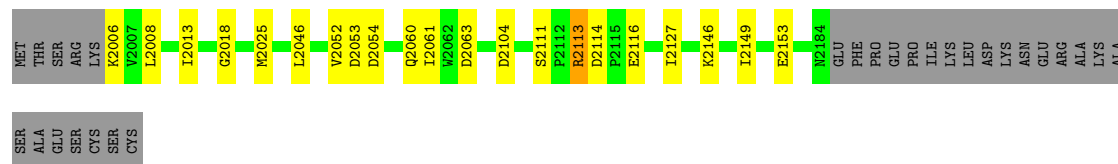
• Molecule 1: Ras-related protein Rab-7

Chain A: 



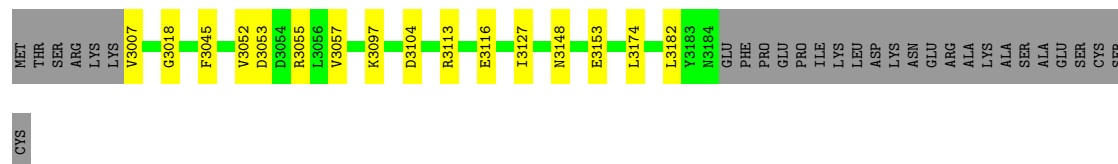
• Molecule 1: Ras-related protein Rab-7

Chain B: 



• Molecule 1: Ras-related protein Rab-7

Chain C: 



• Molecule 1: Ras-related protein Rab-7

Chain D: 



L4174	L4190
LYS	LYS
LEU	ASP
LYS	LYS
ASN	GLU
ARG	ALA
LYS	LYS
ALA	ALA
SER	ALA
GLU	SER
CYS	CYS
SER	SER
CYS	CYS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.06Å 57.07Å 74.31Å 71.73° 71.69° 77.65°	Depositor
Resolution (Å)	19.56 – 1.70 19.56 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.2 (19.56-1.70) 96.2 (19.56-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 1.70Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.198 , 0.224 0.196 , 0.222	Depositor DCC
R_{free} test set	4440 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.469 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6679	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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 37.03 % 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 4.5615e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, 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	0.94	0/1526	1.09	4/2068 (0.2%)
1	B	0.98	0/1469	1.13	7/1988 (0.4%)
1	C	0.99	0/1469	1.13	4/1990 (0.2%)
1	D	0.95	0/1515	1.10	5/2054 (0.2%)
All	All	0.96	0/5979	1.11	20/8100 (0.2%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1060	GLN	OE1-CD-NE2	-10.35	112.25	122.60
1	B	2060	GLN	OE1-CD-NE2	-10.16	112.44	122.60
1	D	4060	GLN	OE1-CD-NE2	-9.35	113.25	122.60
1	C	3113	ARG	N-CA-C	8.83	120.90	111.28
1	B	2113	ARG	N-CA-C	7.30	119.87	111.11
1	D	4060	GLN	CG-CD-NE2	6.78	126.56	116.40
1	A	1060	GLN	CG-CD-NE2	6.71	126.46	116.40
1	B	2060	GLN	CG-CD-NE2	6.46	126.09	116.40
1	D	4113	ARG	N-CA-C	6.08	117.91	111.28
1	C	3045	PHE	N-CA-C	6.07	118.92	109.52
1	D	4054	ASP	N-CA-C	6.05	119.91	111.74
1	B	2111	SER	CB-CA-C	-5.66	107.18	111.20
1	A	1113	ARG	N-CA-C	-5.64	102.54	110.50
1	B	2149	ILE	CA-C-N	5.56	125.49	119.76
1	B	2149	ILE	C-N-CA	5.56	125.49	119.76
1	C	3148	ASN	N-CA-C	5.43	118.62	111.28
1	B	2046	LEU	N-CA-C	-5.34	101.42	109.85
1	D	4118	PHE	CA-CB-CG	-5.12	108.68	113.80
1	A	1046	LEU	N-CA-C	-5.04	101.65	109.72
1	C	3097	LYS	N-CA-C	5.02	117.65	111.82

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	1488	0	1464	26	0
1	B	1438	0	1425	16	0
1	C	1434	0	1411	12	0
1	D	1481	0	1457	21	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	32	0	13	0	0
3	B	32	0	13	1	0
3	C	32	0	13	1	0
3	D	32	0	13	0	0
4	A	176	0	0	6	0
4	B	182	0	0	1	0
4	C	177	0	0	1	0
4	D	171	0	0	0	0
All	All	6679	0	5809	69	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 6.

All (69) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1051:MET:HE1	1:A:1056:LEU:HB3	1.63	0.81
1:B:2127:ILE:HG21	1:B:2153:GLU:HB3	1.74	0.69
1:C:3007:VAL:HG22	1:C:3057:VAL:HG12	1.78	0.66
1:D:4038:LYS:HE2	1:D:4039:ALA:N	2.12	0.65
1:D:4164:GLN:NE2	1:D:4164:GLN:H	1.95	0.64
1:B:2025[A]:MET:HE2	1:B:2061:ILE:HG22	1.78	0.63
1:D:4052:VAL:HG21	1:D:4174:LEU:HD22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1097:LYS:HG2	4:A:5481:HOH:O	1.98	0.62
1:C:3127:ILE:HG21	1:C:3153:GLU:HB3	1.80	0.62
1:D:4161:ASN:HA	1:D:4164:GLN:HE21	1.63	0.62
1:A:1056:LEU:HD23	1:A:1056:LEU:H	1.65	0.61
1:C:3055:ARG:HD3	1:C:3174:LEU:HD21	1.81	0.61
1:A:1056:LEU:O	1:A:1056:LEU:HG	2.00	0.61
1:A:1008:LEU:HD21	1:A:1060:GLN:HB2	1.84	0.60
1:D:4109:GLN:HE21	1:D:4109:GLN:HA	1.67	0.59
1:A:1097:LYS:NZ	1:A:1138:ARG:HH22	2.01	0.58
1:B:2013:ILE:HD12	1:B:2025[A]:MET:HE2	1.85	0.57
1:A:1116:GLU:OE2	1:D:4104:ASP:OD2	2.23	0.57
1:A:1104:ASP:OD2	1:D:4116:GLU:OE2	2.23	0.57
1:A:1157:LYS:NZ	4:A:5652:HOH:O	2.37	0.57
1:A:1007:VAL:HA	4:A:5644:HOH:O	2.05	0.56
1:B:2008:LEU:HD13	4:B:5704:HOH:O	2.05	0.56
1:A:1051:MET:CE	1:A:1056:LEU:HB3	2.35	0.56
1:B:2025[A]:MET:HE1	1:B:2063:ASP:HB2	1.88	0.55
1:B:2104:ASP:OD2	1:C:3116:GLU:OE1	2.25	0.55
1:A:1070:PHE:CZ	1:C:3182:LEU:HB3	2.42	0.54
1:B:2116:GLU:OE2	1:C:3104:ASP:OD2	2.25	0.54
1:D:4051:MET:HE3	1:D:4055:ARG:C	2.33	0.54
1:A:1097:LYS:HZ2	1:A:1138:ARG:HH22	1.57	0.53
1:B:2025[A]:MET:CE	1:B:2063:ASP:HB2	2.41	0.51
1:A:1190:ILE:HG23	1:D:4068:GLU:OE1	2.11	0.51
1:C:3052:VAL:O	1:C:3053:ASP:C	2.54	0.50
1:D:4047:THR:HG23	1:D:4058:THR:CG2	2.41	0.50
1:A:1109:GLN:HE21	1:A:1109:GLN:HA	1.76	0.50
1:A:1079:ARG:NH1	4:A:5669:HOH:O	2.44	0.49
1:D:4047:THR:CG2	1:D:4058:THR:HG23	2.43	0.49
1:D:4052:VAL:O	1:D:4052:VAL:HG23	2.12	0.49
1:B:2013:ILE:HD12	1:B:2025[A]:MET:CE	2.43	0.48
1:A:1050:VAL:HG22	1:A:1051:MET:N	2.28	0.47
1:D:4161:ASN:HA	1:D:4164:GLN:NE2	2.28	0.47
1:A:1175:LYS:HE3	4:A:5082:HOH:O	2.13	0.47
1:D:4047:THR:HG23	1:D:4058:THR:HG23	1.97	0.47
1:D:4127:ILE:HG21	1:D:4153:GLU:HB3	1.96	0.47
1:A:1016:ASP:OD1	1:A:1095:THR:HA	2.15	0.47
1:C:3007:VAL:CG2	1:C:3057:VAL:HG12	2.44	0.46
1:A:1105:GLU:O	1:A:1109:GLN:HG2	2.15	0.46
1:B:2113:ARG:HG3	1:B:2114:ASP:N	2.31	0.46
1:D:4136:THR:O	1:D:4140[B]:GLN:HG3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1113:ARG:HB3	1:A:1113:ARG:CZ	2.45	0.45
1:B:2018:GLY:H	3:B:2400:GNP:HNB3	1.65	0.45
1:D:4016:ASP:OD1	1:D:4095:THR:HA	2.16	0.45
1:A:1008:LEU:C	1:A:1008:LEU:HD23	2.42	0.45
1:A:1127:ILE:HG21	1:A:1153:GLU:HB3	1.98	0.45
1:A:1097:LYS:NZ	1:A:1138:ARG:NH2	2.63	0.45
1:B:2006:LYS:HA	1:B:2006:LYS:HD3	1.71	0.44
1:A:1167:GLN:HG3	4:A:5697:HOH:O	2.17	0.44
1:B:2053:ASP:O	1:B:2054:ASP:HB2	2.17	0.43
1:D:4105:GLU:OE2	1:D:4109:GLN:HG3	2.19	0.43
1:C:3052:VAL:HG23	1:C:3057:VAL:HG22	2.00	0.43
1:D:4052:VAL:CG2	1:D:4174:LEU:HD22	2.47	0.42
1:B:2146:LYS:HA	1:B:2146:LYS:HD3	1.92	0.42
1:C:3055:ARG:NH1	4:C:5371:HOH:O	2.52	0.42
1:C:3182:LEU:HD23	1:C:3182:LEU:HA	1.88	0.42
1:B:2025[A]:MET:CE	1:B:2061:ILE:HG22	2.48	0.42
1:D:4050:VAL:HG22	1:D:4051:MET:N	2.35	0.41
1:C:3018:GLY:H	3:C:3400:GNP:HNB3	1.69	0.41
1:A:1082:ASP:O	1:A:1119:PRO:HG2	2.21	0.41
1:B:2052:VAL:O	1:B:2053:ASP:C	2.65	0.40
1:D:4149:ILE:HA	1:D:4150:PRO:HD3	1.93	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	184/207 (89%)	179 (97%)	5 (3%)	0	100	100
1	B	178/207 (86%)	171 (96%)	7 (4%)	0	100	100
1	C	178/207 (86%)	173 (97%)	5 (3%)	0	100	100
1	D	183/207 (88%)	179 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	723/828 (87%)	702 (97%)	21 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	163/181 (90%)	158 (97%)	5 (3%)	35	18
1	B	157/181 (87%)	157 (100%)	0	100	100
1	C	157/181 (87%)	157 (100%)	0	100	100
1	D	162/181 (90%)	159 (98%)	3 (2%)	50	34
All	All	639/724 (88%)	631 (99%)	8 (1%)	65	48

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1007	VAL
1	A	1072	SER
1	A	1132[A]	ARG
1	A	1132[B]	ARG
1	A	1188	GLU
1	D	4038	LYS
1	D	4072	SER
1	D	4075	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1026	ASN
1	A	1109	GLN
1	A	1125	ASN
1	A	1148	ASN

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Mol	Chain	Res	Type
1	A	1164	GLN
1	B	2026	ASN
1	B	2109	GLN
1	B	2125	ASN
1	C	3026	ASN
1	C	3140	GLN
1	C	3161	ASN
1	C	3184	ASN
1	D	4071	GLN
1	D	4094	ASN
1	D	4109	GLN
1	D	4125	ASN
1	D	4164	GLN
1	D	4167	GLN
1	D	4172	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GNP	C	3400	2	34,34,34	2.17	10 (29%)	47,54,54	1.83	8 (17%)
3	GNP	D	4400	2	34,34,34	2.30	11 (32%)	47,54,54	1.95	8 (17%)
3	GNP	B	2400	2	34,34,34	2.32	11 (32%)	47,54,54	1.84	9 (19%)
3	GNP	A	1400	2	34,34,34	2.28	11 (32%)	47,54,54	1.82	8 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GNP	C	3400	2	-	3/18/38/38	0/3/3/3
3	GNP	D	4400	2	-	3/18/38/38	0/3/3/3
3	GNP	B	2400	2	-	3/18/38/38	0/3/3/3
3	GNP	A	1400	2	-	3/18/38/38	0/3/3/3

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1400	GNP	PG-O1G	6.02	1.55	1.46
3	D	4400	GNP	PG-N3B	5.92	1.78	1.63
3	B	2400	GNP	C2-N2	5.60	1.47	1.34
3	A	1400	GNP	C2-N2	5.31	1.46	1.34
3	C	3400	GNP	C2-N2	5.13	1.46	1.34
3	D	4400	GNP	C2-N2	4.91	1.45	1.34
3	D	4400	GNP	PG-O1G	4.91	1.53	1.46
3	A	1400	GNP	PG-N3B	4.88	1.76	1.63
3	C	3400	GNP	C8-N9	4.62	1.47	1.37
3	D	4400	GNP	C8-N9	4.51	1.47	1.37
3	A	1400	GNP	C8-N9	4.51	1.47	1.37
3	C	3400	GNP	PG-N3B	4.48	1.75	1.63
3	B	2400	GNP	PG-N3B	4.48	1.75	1.63
3	B	2400	GNP	PB-O2B	-4.32	1.45	1.56
3	B	2400	GNP	PG-O1G	4.20	1.52	1.46
3	B	2400	GNP	C5-N7	4.07	1.47	1.39
3	C	3400	GNP	PB-O2B	-3.98	1.46	1.56
3	C	3400	GNP	C5-N7	3.95	1.47	1.39
3	D	4400	GNP	PB-O2B	-3.88	1.46	1.56
3	B	2400	GNP	C8-N9	3.86	1.46	1.37
3	C	3400	GNP	PG-O1G	3.85	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2400	GNP	PB-O3A	3.29	1.63	1.59
3	B	2400	GNP	PA-O3A	-2.96	1.56	1.59
3	D	4400	GNP	PB-N3B	2.84	1.70	1.63
3	D	4400	GNP	C5-N7	2.80	1.44	1.39
3	A	1400	GNP	PB-O2B	-2.77	1.49	1.56
3	A	1400	GNP	PB-N3B	2.76	1.70	1.63
3	B	2400	GNP	PB-N3B	2.70	1.70	1.63
3	C	3400	GNP	O6-C6	-2.69	1.18	1.23
3	A	1400	GNP	C5-N7	2.62	1.44	1.39
3	A	1400	GNP	PG-O2G	-2.58	1.50	1.56
3	B	2400	GNP	PG-O3G	-2.57	1.50	1.56
3	C	3400	GNP	PB-N3B	2.47	1.69	1.63
3	C	3400	GNP	PG-O2G	-2.46	1.50	1.56
3	D	4400	GNP	PG-O2G	-2.41	1.50	1.56
3	A	1400	GNP	O6-C6	-2.41	1.19	1.23
3	D	4400	GNP	C2-N1	2.39	1.43	1.37
3	B	2400	GNP	O6-C6	-2.32	1.19	1.23
3	A	1400	GNP	C2-N1	2.25	1.43	1.37
3	D	4400	GNP	C2-N3	-2.12	1.28	1.33
3	D	4400	GNP	O6-C6	-2.08	1.19	1.23
3	A	1400	GNP	C2-N3	-2.06	1.28	1.33
3	C	3400	GNP	C3'-C4'	2.02	1.58	1.53

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3400	GNP	O1G-PG-N3B	-7.59	100.59	111.77
3	D	4400	GNP	O1G-PG-N3B	-7.51	100.71	111.77
3	B	2400	GNP	O1G-PG-N3B	-7.04	101.40	111.77
3	A	1400	GNP	N1-C2-N3	5.68	133.72	123.32
3	D	4400	GNP	N1-C2-N3	5.43	133.26	123.32
3	A	1400	GNP	O1G-PG-N3B	-5.43	103.77	111.77
3	B	2400	GNP	N1-C2-N3	4.96	132.40	123.32
3	C	3400	GNP	N1-C2-N3	4.82	132.15	123.32
3	D	4400	GNP	O2B-PB-O1B	4.48	119.49	109.87
3	A	1400	GNP	O2B-PB-O1B	4.32	119.14	109.87
3	B	2400	GNP	O2B-PB-O1B	4.11	118.69	109.87
3	C	3400	GNP	O2B-PB-O1B	3.71	117.82	109.87
3	A	1400	GNP	C2-N3-C4	-3.23	106.73	112.30
3	D	4400	GNP	C2-N3-C4	-3.14	106.88	112.30
3	A	1400	GNP	C2-N1-C6	-3.12	119.45	125.11
3	D	4400	GNP	C2-N1-C6	-3.04	119.59	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2400	GNP	C2-N3-C4	-2.92	107.26	112.30
3	C	3400	GNP	C2-N1-C6	-2.90	119.84	125.11
3	B	2400	GNP	C2-N1-C6	-2.82	119.99	125.11
3	C	3400	GNP	O2G-PG-O3G	2.82	115.16	107.59
3	D	4400	GNP	N2-C2-N1	-2.76	110.93	116.76
3	A	1400	GNP	N2-C2-N1	-2.65	111.17	116.76
3	C	3400	GNP	C2-N3-C4	-2.57	107.87	112.30
3	C	3400	GNP	N2-C2-N1	-2.56	111.35	116.76
3	D	4400	GNP	O1B-PB-N3B	-2.42	108.21	111.77
3	B	2400	GNP	O3A-PB-N3B	-2.40	99.95	106.59
3	B	2400	GNP	N2-C2-N1	-2.35	111.81	116.76
3	A	1400	GNP	N2-C2-N3	-2.34	115.11	119.67
3	A	1400	GNP	O2G-PG-O3G	2.17	113.43	107.59
3	C	3400	GNP	O3A-PA-O1A	2.16	117.21	110.70
3	B	2400	GNP	O2G-PG-O3G	2.04	113.06	107.59
3	B	2400	GNP	O3G-PG-O1G	-2.03	108.35	113.45
3	D	4400	GNP	N9-C8-N7	-2.01	109.67	113.40

There are no chirality outliers.

All (12) torsion outliers are listed below:

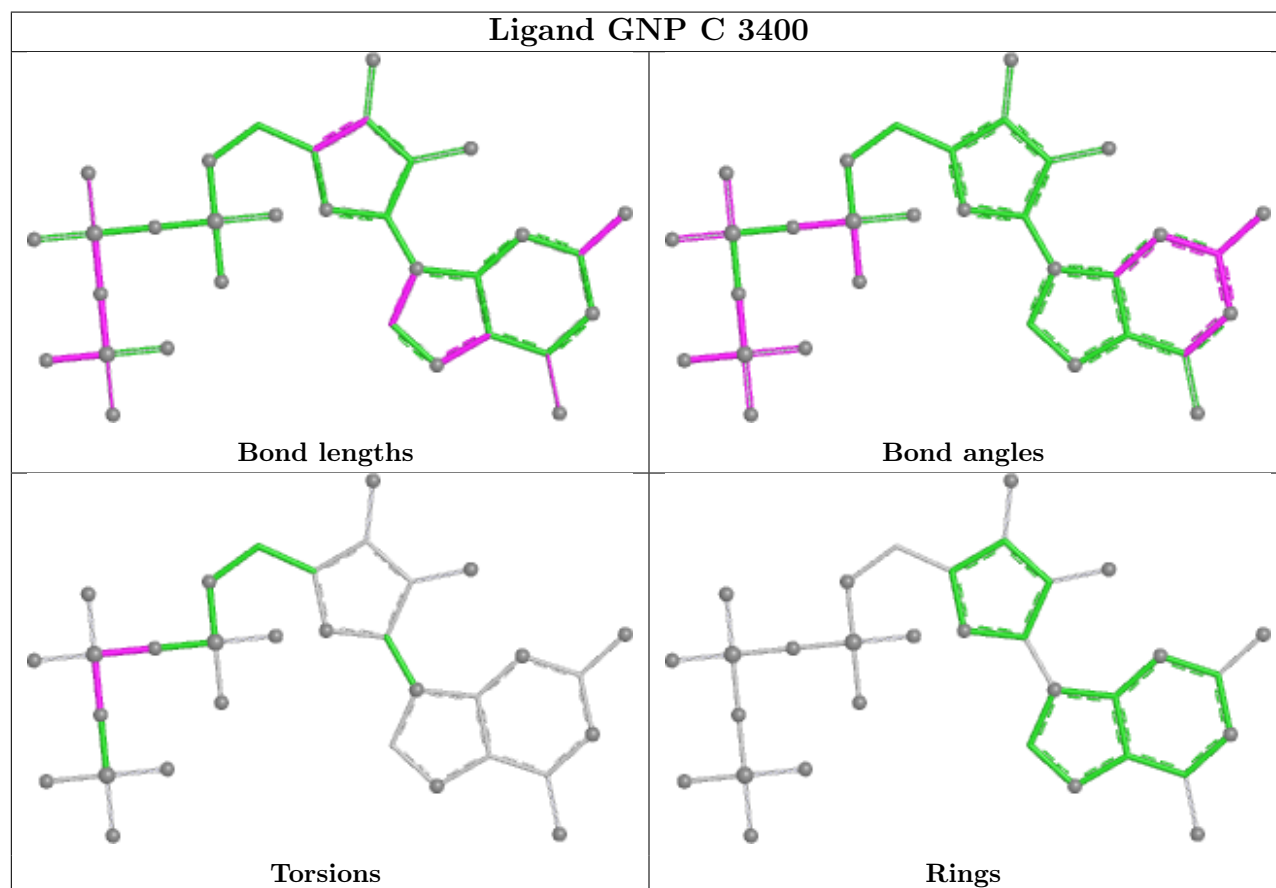
Mol	Chain	Res	Type	Atoms
3	A	1400	GNP	PG-N3B-PB-O1B
3	A	1400	GNP	PA-O3A-PB-O2B
3	B	2400	GNP	PG-N3B-PB-O1B
3	B	2400	GNP	PA-O3A-PB-O2B
3	C	3400	GNP	PG-N3B-PB-O1B
3	C	3400	GNP	PA-O3A-PB-O2B
3	D	4400	GNP	PG-N3B-PB-O1B
3	D	4400	GNP	PA-O3A-PB-O2B
3	A	1400	GNP	PA-O3A-PB-O1B
3	B	2400	GNP	PA-O3A-PB-O1B
3	C	3400	GNP	PA-O3A-PB-O1B
3	D	4400	GNP	PA-O3A-PB-O1B

There are no ring outliers.

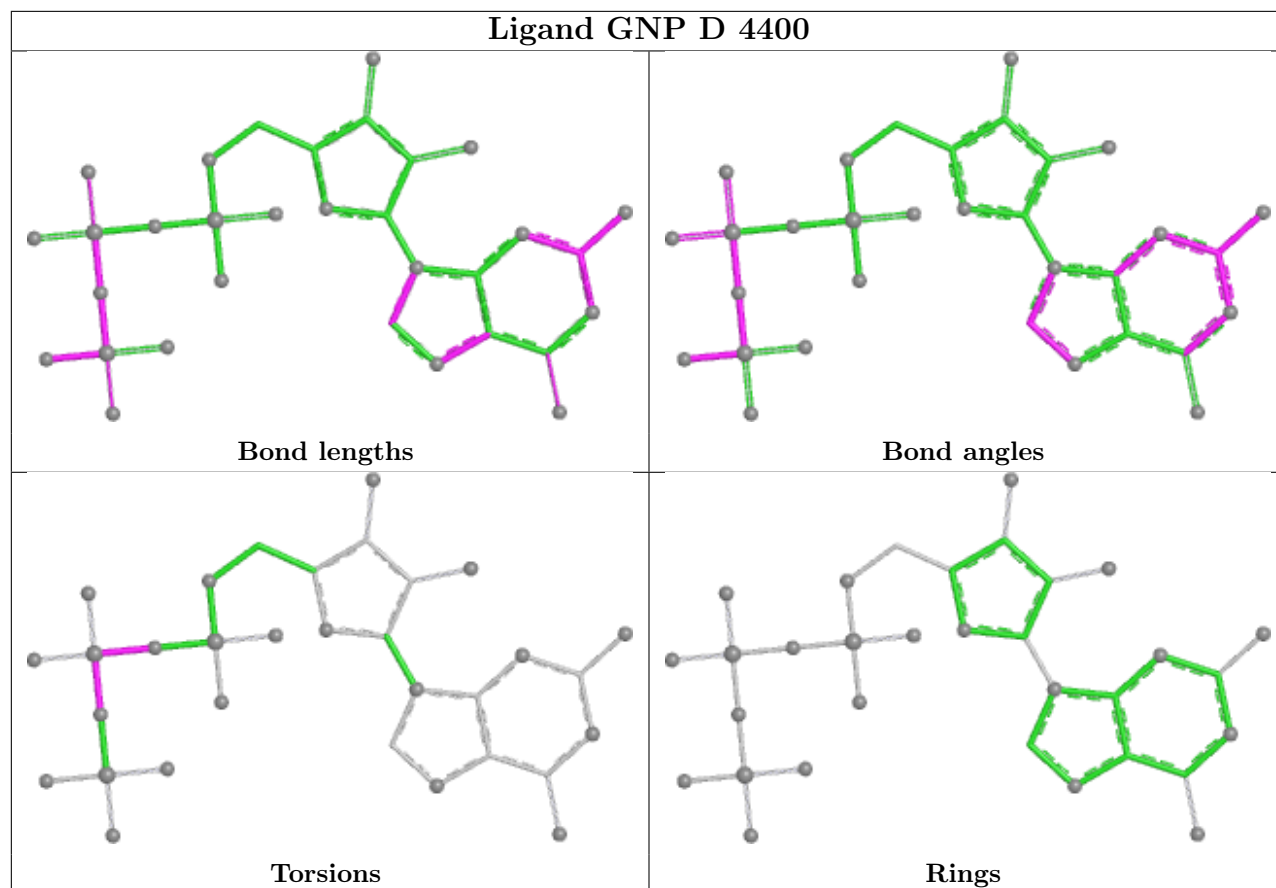
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3400	GNP	1	0
3	B	2400	GNP	1	0

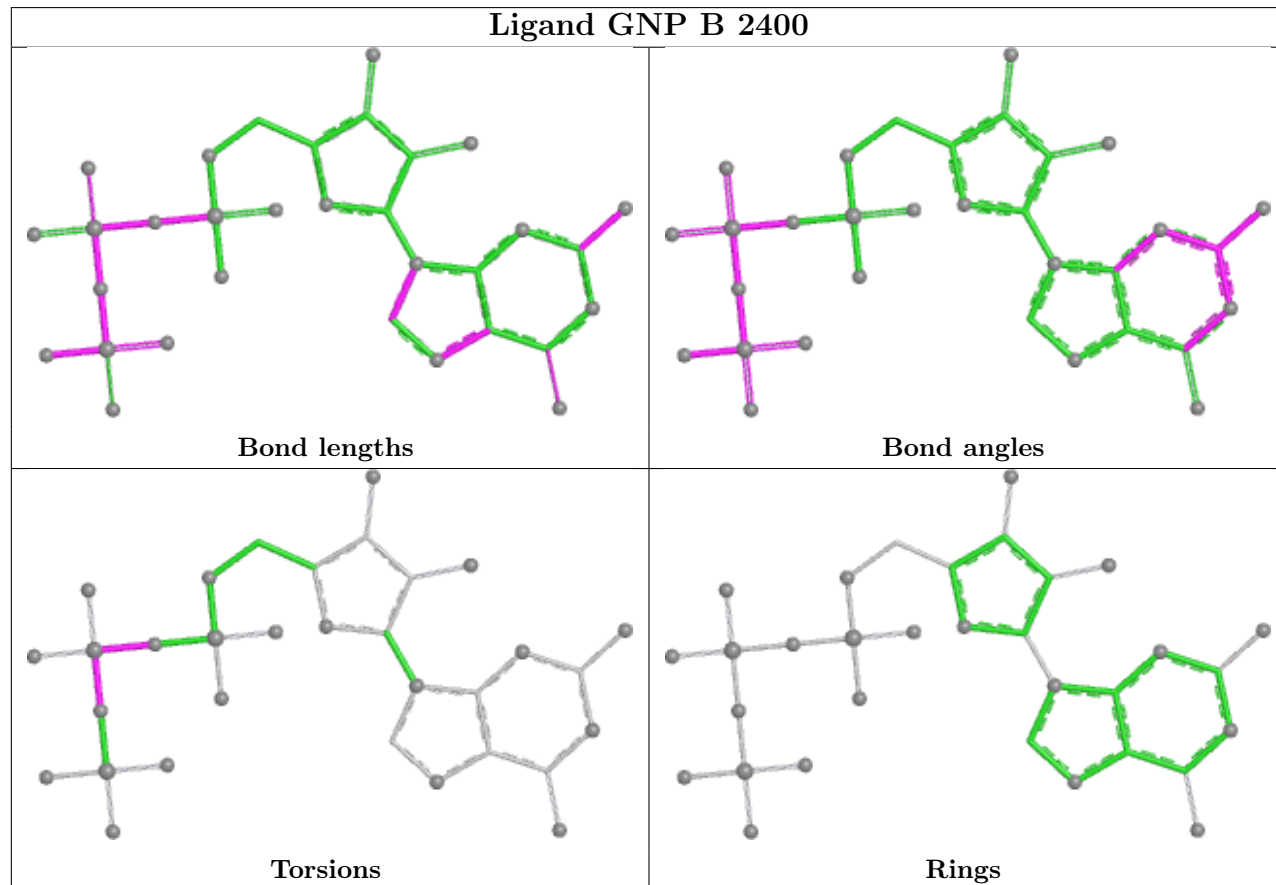
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

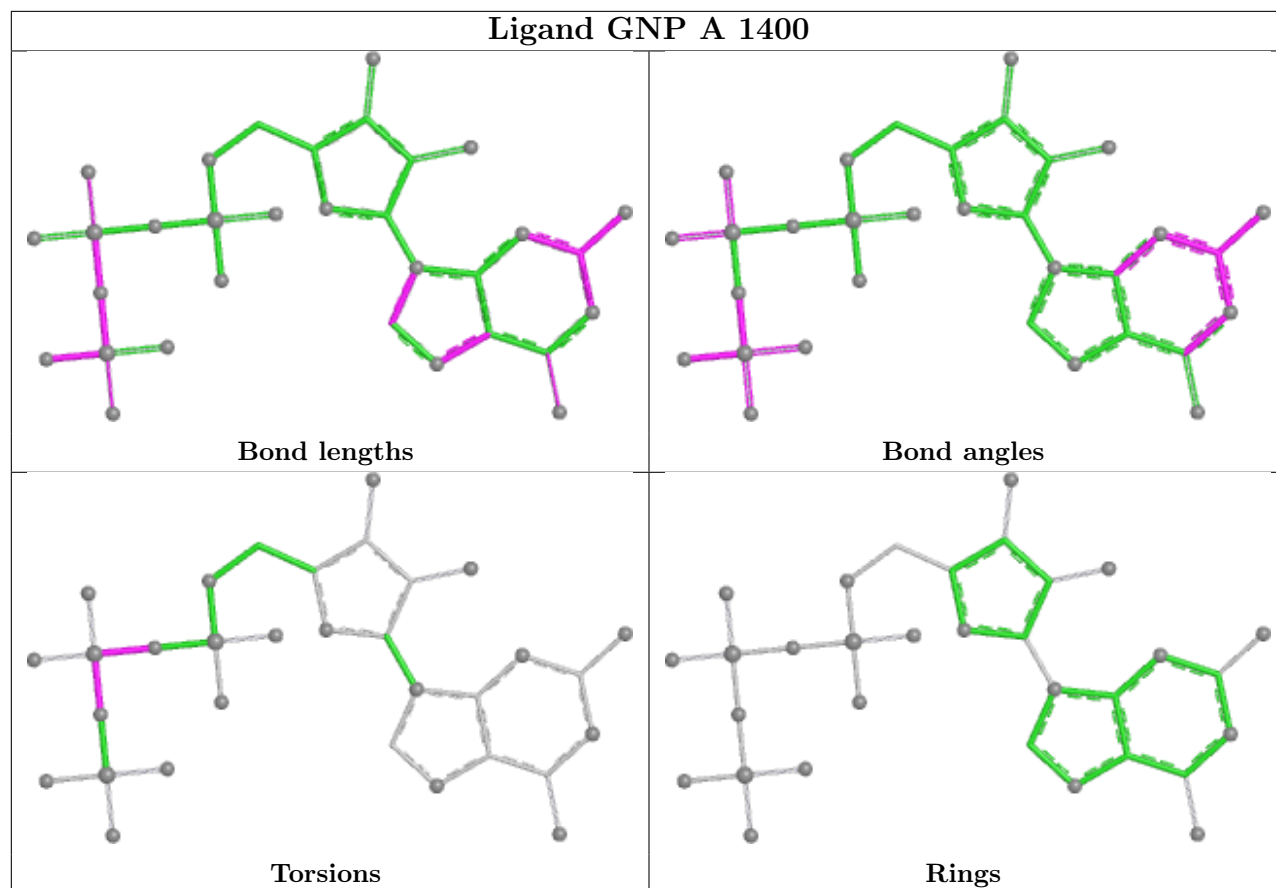


Ligand GNP D 4400



Ligand GNP B 2400





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	184/207 (88%)	-1.18	0 100 100	14, 25, 42, 49	2 (1%)
1	B	179/207 (86%)	-1.21	0 100 100	14, 23, 45, 51	1 (0%)
1	C	178/207 (85%)	-1.18	0 100 100	14, 23, 43, 51	2 (1%)
1	D	184/207 (88%)	-1.16	0 100 100	15, 25, 41, 49	1 (0%)
All	All	725/828 (87%)	-1.18	0 100 100	14, 24, 43, 51	6 (0%)

There are no RSRZ outliers to report.

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 [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	A	1401	1/1	0.99	0.02	16,16,16,16	0
2	MG	B	2401	1/1	1.00	0.01	15,15,15,15	0
2	MG	C	3401	1/1	1.00	0.02	16,16,16,16	0
2	MG	D	4401	1/1	1.00	0.01	15,15,15,15	0

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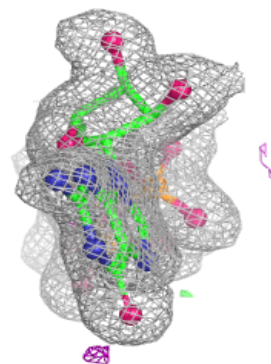
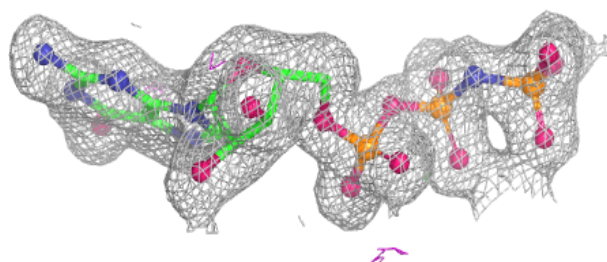
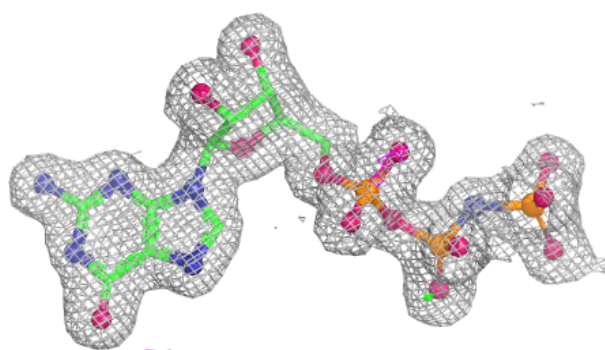
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GNP	A	1400	32/32	1.00	0.02	13,20,24,24	0
3	GNP	B	2400	32/32	1.00	0.03	13,18,21,24	0
3	GNP	C	3400	32/32	1.00	0.02	13,19,21,25	0
3	GNP	D	4400	32/32	1.00	0.02	13,19,23,24	0

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.

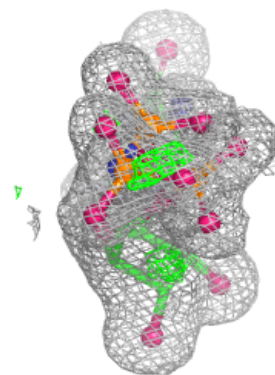
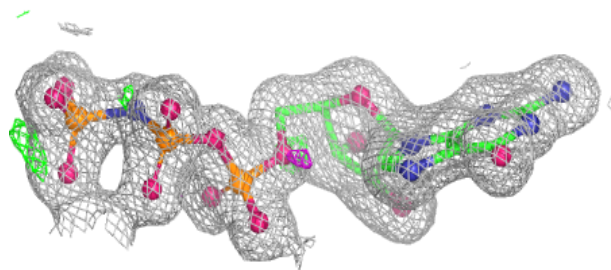
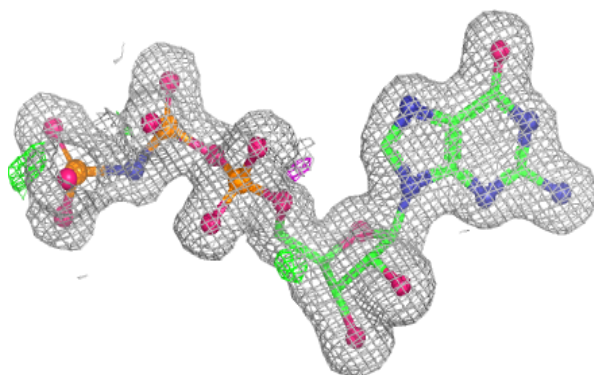
Electron density around GNP A 1400:

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

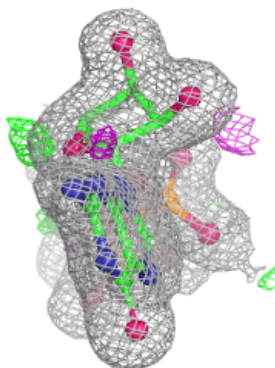
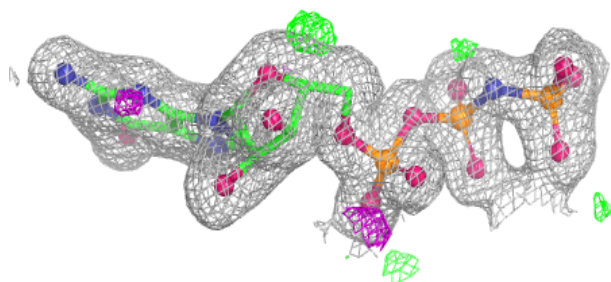
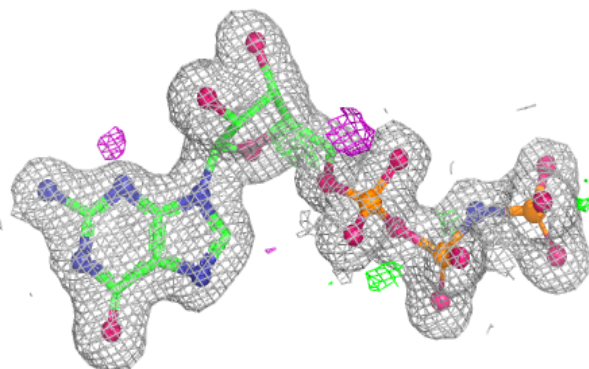


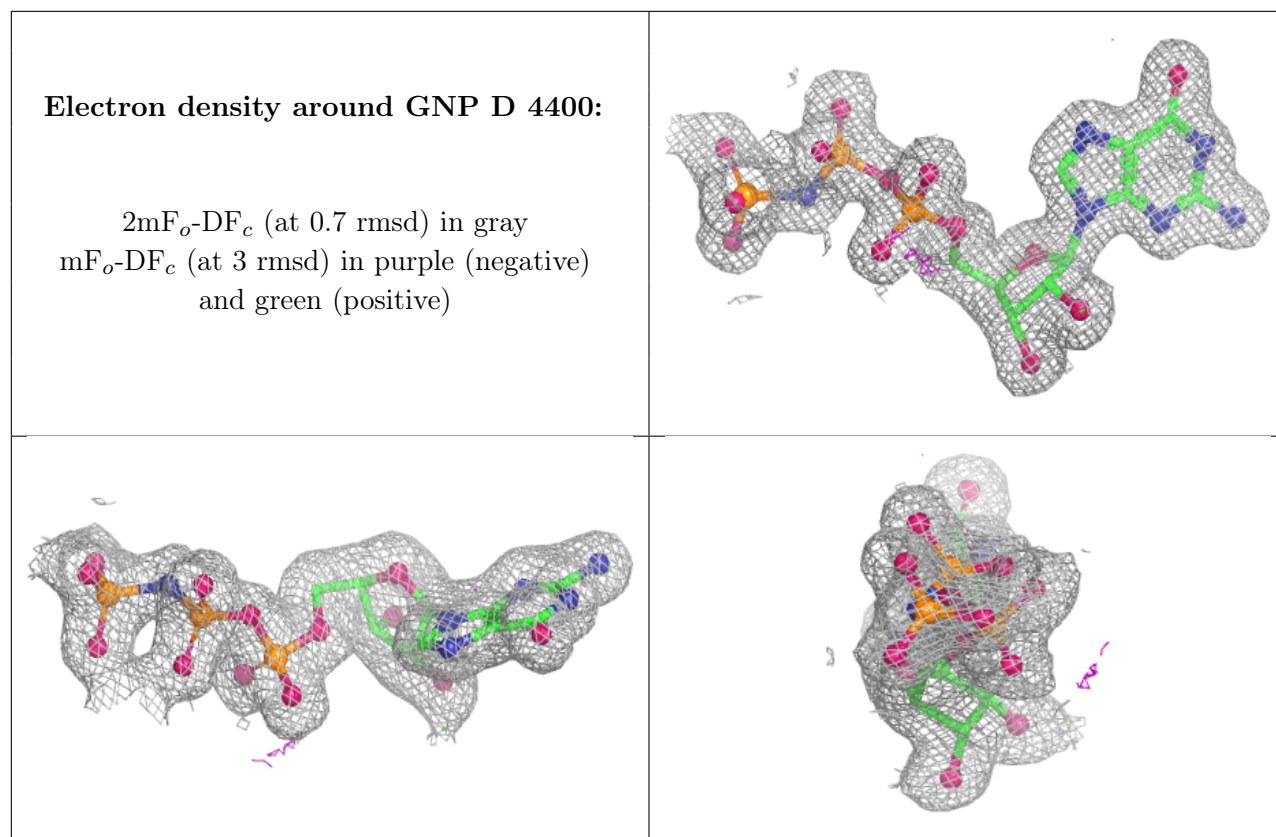
Electron density around GNP B 2400:

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

**Electron density around GNP C 3400:**

$2mF_o-DF_c$ (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.