



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 10:44 PM EDT

PDB ID : 6GPK
Title : Crystal structure of human GDP-D-mannose 4,6-dehydratase (E157Q) in complex with GDP-Man
Authors : Pfeiffer, M.; Krojer, T.; Johansson, C.; von Delft, F.; Bountra, C.; Arrow-smith, C.H.; Edwards, A.; Nidetzky, B.; Oppermann, U.; Structural Genomics Consortium (SGC)
Deposited on : 2018-06-06
Resolution : 1.47 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](#) ①) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

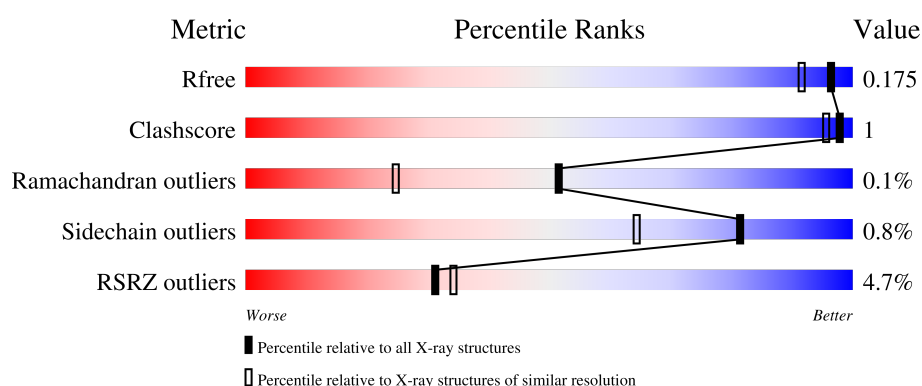
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.47 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	4690 (1.50-1.46)
Clashscore	141614	4955 (1.50-1.46)
Ramachandran outliers	138981	4846 (1.50-1.46)
Sidechain outliers	138945	4844 (1.50-1.46)
RSRZ outliers	127900	4614 (1.50-1.46)

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	373	<div> <div>3%</div> <div>91%</div> <div>6%</div> </div>
1	B	373	<div> <div>2%</div> <div>92%</div> <div>6%</div> </div>
1	C	373	<div> <div>2%</div> <div>88%</div> <div>8%</div> </div>
1	D	373	<div> <div>11%</div> <div>91%</div> <div>8%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12284 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 GDP-mannose 4,6 dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	4	0
			2796	1782	480	523	11			
1	B	350	Total	C	N	O	S	0	1	0
			2783	1776	478	519	10			
1	C	342	Total	C	N	O	S	0	2	0
			2704	1728	465	500	11			
1	D	344	Total	C	N	O	S	0	1	0
			2677	1707	457	502	11			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP O60547
A	1	HIS	-	expression tag	UNP O60547
A	2	HIS	-	expression tag	UNP O60547
A	3	HIS	-	expression tag	UNP O60547
A	4	HIS	-	expression tag	UNP O60547
A	5	HIS	-	expression tag	UNP O60547
A	6	HIS	-	expression tag	UNP O60547
A	7	SER	-	expression tag	UNP O60547
A	8	SER	-	expression tag	UNP O60547
A	9	GLY	-	expression tag	UNP O60547
A	10	VAL	-	expression tag	UNP O60547
A	11	ASP	-	expression tag	UNP O60547
A	12	LEU	-	expression tag	UNP O60547
A	13	GLY	-	expression tag	UNP O60547
A	14	THR	-	expression tag	UNP O60547
A	15	GLU	-	expression tag	UNP O60547
A	16	ASN	-	expression tag	UNP O60547
A	17	LEU	-	expression tag	UNP O60547
A	18	TYR	-	expression tag	UNP O60547
A	19	PHE	-	expression tag	UNP O60547
A	20	GLN	-	expression tag	UNP O60547

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Chain	Residue	Modelled	Actual	Comment	Reference
A	21	SER	-	expression tag	UNP O60547
A	22	MET	-	expression tag	UNP O60547
A	157	GLN	GLU	engineered mutation	UNP O60547
B	0	MET	-	initiating methionine	UNP O60547
B	1	HIS	-	expression tag	UNP O60547
B	2	HIS	-	expression tag	UNP O60547
B	3	HIS	-	expression tag	UNP O60547
B	4	HIS	-	expression tag	UNP O60547
B	5	HIS	-	expression tag	UNP O60547
B	6	HIS	-	expression tag	UNP O60547
B	7	SER	-	expression tag	UNP O60547
B	8	SER	-	expression tag	UNP O60547
B	9	GLY	-	expression tag	UNP O60547
B	10	VAL	-	expression tag	UNP O60547
B	11	ASP	-	expression tag	UNP O60547
B	12	LEU	-	expression tag	UNP O60547
B	13	GLY	-	expression tag	UNP O60547
B	14	THR	-	expression tag	UNP O60547
B	15	GLU	-	expression tag	UNP O60547
B	16	ASN	-	expression tag	UNP O60547
B	17	LEU	-	expression tag	UNP O60547
B	18	TYR	-	expression tag	UNP O60547
B	19	PHE	-	expression tag	UNP O60547
B	20	GLN	-	expression tag	UNP O60547
B	21	SER	-	expression tag	UNP O60547
B	22	MET	-	expression tag	UNP O60547
B	157	GLN	GLU	engineered mutation	UNP O60547
C	0	MET	-	initiating methionine	UNP O60547
C	1	HIS	-	expression tag	UNP O60547
C	2	HIS	-	expression tag	UNP O60547
C	3	HIS	-	expression tag	UNP O60547
C	4	HIS	-	expression tag	UNP O60547
C	5	HIS	-	expression tag	UNP O60547
C	6	HIS	-	expression tag	UNP O60547
C	7	SER	-	expression tag	UNP O60547
C	8	SER	-	expression tag	UNP O60547
C	9	GLY	-	expression tag	UNP O60547
C	10	VAL	-	expression tag	UNP O60547
C	11	ASP	-	expression tag	UNP O60547
C	12	LEU	-	expression tag	UNP O60547
C	13	GLY	-	expression tag	UNP O60547
C	14	THR	-	expression tag	UNP O60547

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Chain	Residue	Modelled	Actual	Comment	Reference
C	15	GLU	-	expression tag	UNP O60547
C	16	ASN	-	expression tag	UNP O60547
C	17	LEU	-	expression tag	UNP O60547
C	18	TYR	-	expression tag	UNP O60547
C	19	PHE	-	expression tag	UNP O60547
C	20	GLN	-	expression tag	UNP O60547
C	21	SER	-	expression tag	UNP O60547
C	22	MET	-	expression tag	UNP O60547
C	157	GLN	GLU	engineered mutation	UNP O60547
D	0	MET	-	initiating methionine	UNP O60547
D	1	HIS	-	expression tag	UNP O60547
D	2	HIS	-	expression tag	UNP O60547
D	3	HIS	-	expression tag	UNP O60547
D	4	HIS	-	expression tag	UNP O60547
D	5	HIS	-	expression tag	UNP O60547
D	6	HIS	-	expression tag	UNP O60547
D	7	SER	-	expression tag	UNP O60547
D	8	SER	-	expression tag	UNP O60547
D	9	GLY	-	expression tag	UNP O60547
D	10	VAL	-	expression tag	UNP O60547
D	11	ASP	-	expression tag	UNP O60547
D	12	LEU	-	expression tag	UNP O60547
D	13	GLY	-	expression tag	UNP O60547
D	14	THR	-	expression tag	UNP O60547
D	15	GLU	-	expression tag	UNP O60547
D	16	ASN	-	expression tag	UNP O60547
D	17	LEU	-	expression tag	UNP O60547
D	18	TYR	-	expression tag	UNP O60547
D	19	PHE	-	expression tag	UNP O60547
D	20	GLN	-	expression tag	UNP O60547
D	21	SER	-	expression tag	UNP O60547
D	22	MET	-	expression tag	UNP O60547
D	157	GLN	GLU	engineered mutation	UNP O60547

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



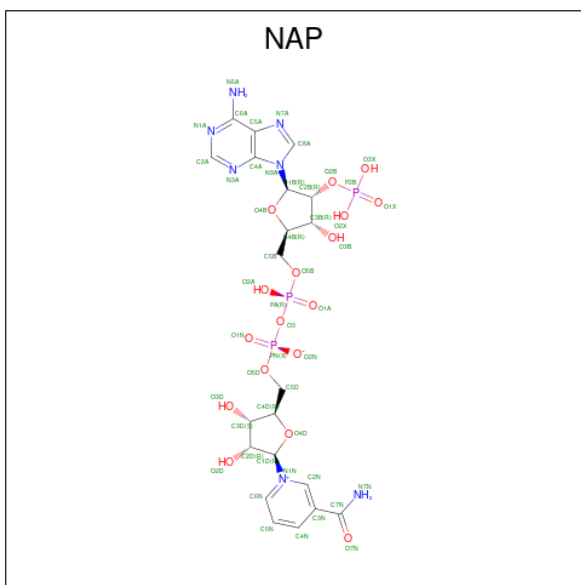
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

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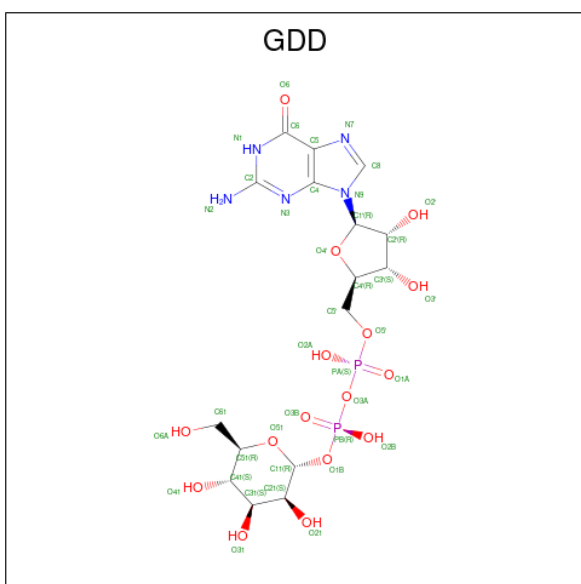
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



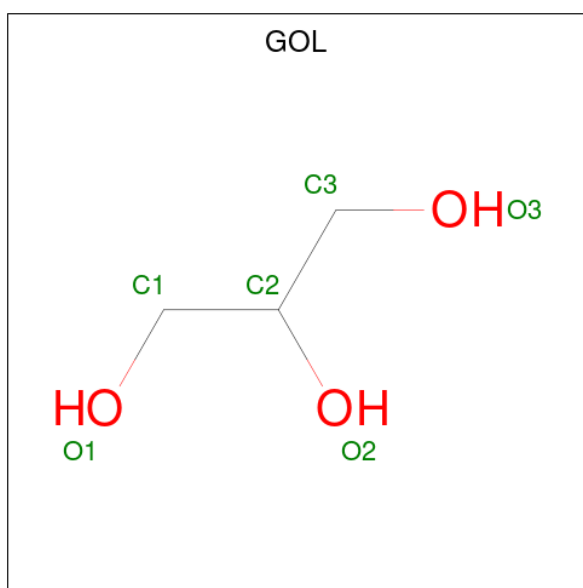
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	C	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	D	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE-ALPHA-D-MANNOSE (three-letter code: GDD) (formula: $\text{C}_{16}\text{H}_{25}\text{N}_5\text{O}_{16}\text{P}_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			39	16	5	16	2		
4	B	1	Total	C	N	O	P	0	0
			39	16	5	16	2		
4	C	1	Total	C	N	O	P	0	0
			39	16	5	16	2		
4	D	1	Total	C	N	O	P	0	0
			39	16	5	16	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			6	3	3		

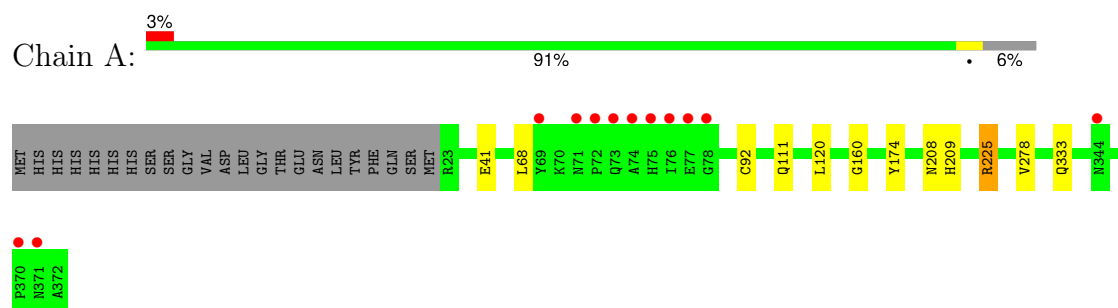
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	263	Total	O	0	0
			263	263		
6	B	257	Total	O	0	0
			257	257		
6	C	193	Total	O	0	0
			193	193		
6	D	145	Total	O	0	0
			145	145		

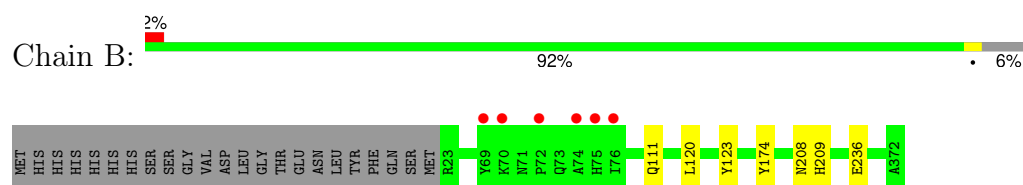
3 Residue-property plots [i](#)

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.

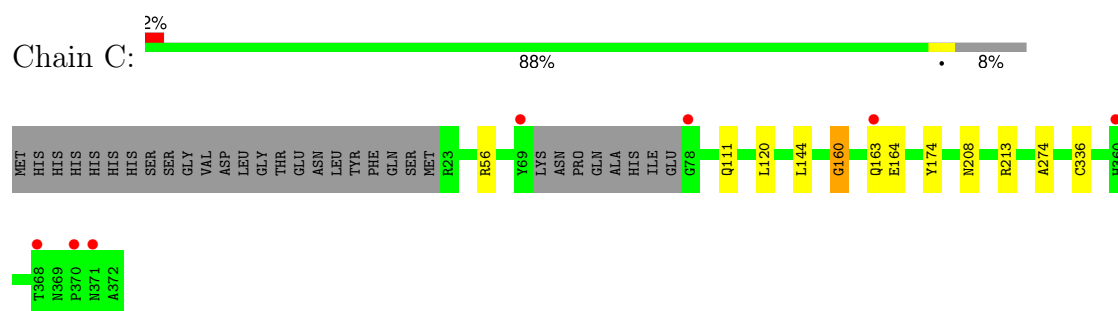
- Molecule 1: GDP-mannose 4,6 dehydratase



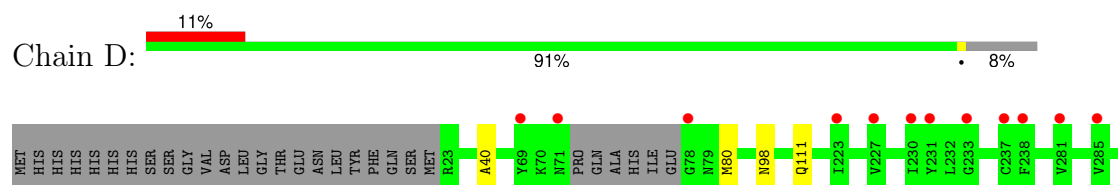
- Molecule 1: GDP-mannose 4,6 dehydratase



- Molecule 1: GDP-mannose 4,6 dehydratase



- Molecule 1: GDP-mannose 4,6 dehydratase



F289	L290	H291	I292	G293	K294	T295	I296	V297	W298	E308	C309	K310	E311	T312	G313	K314	V315	H316	V317	T318	V319	Y324	F351	D352	V355	R356	E357	N358	V359	H360	V363	T368	N369	P370	N371	A372
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.73Å 114.53Å 140.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	88.66 – 1.47 88.66 – 1.47	Depositor EDS
% Data completeness (in resolution range)	100.0 (88.66-1.47) 100.0 (88.66-1.47)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 1.47Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.141 , 0.174 0.141 , 0.175	Depositor DCC
R_{free} test set	12794 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	17.6	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 57.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	12284	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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 30.57 % 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 1.2787e-03. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDD, NAP, EDO, GOL

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	0.69	0/2859	0.72	1/3880 (0.0%)
1	B	0.69	1/2846 (0.0%)	0.70	0/3860
1	C	0.67	0/2764	0.74	3/3749 (0.1%)
1	D	0.62	0/2737	0.67	0/3720
All	All	0.67	1/11206 (0.0%)	0.71	4/15209 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	236	GLU	CD-OE1	-5.66	1.19	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	213	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	C	56	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	A	225	ARG	NE-CZ-NH1	6.03	123.32	120.30
1	C	56	ARG	NE-CZ-NH2	-5.11	117.75	120.30

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	2796	0	2712	6	0
1	B	2783	0	2711	3	0
1	C	2704	0	2615	5	0
1	D	2677	0	2542	1	0
2	A	52	0	78	0	0
2	B	28	0	42	0	0
2	C	20	0	30	0	0
2	D	12	0	18	0	0
3	A	48	0	25	2	0
3	B	48	0	25	2	0
3	C	48	0	25	1	0
3	D	48	0	25	0	0
4	A	39	0	23	0	0
4	B	39	0	23	0	0
4	C	39	0	23	0	0
4	D	39	0	23	0	0
5	C	6	0	8	0	0
6	A	263	0	0	1	0
6	B	257	0	0	1	0
6	C	193	0	0	0	0
6	D	145	0	0	1	0
All	All	12284	0	10948	15	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 1.

All (15) 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:163:GLN:O	1:C:164:GLU:HG3	1.93	0.67
1:A:225:ARG:NH1	6:A:503:HOH:O	2.42	0.51
1:D:40:ALA:HB1	1:D:80:MET:HE1	1.95	0.48
1:C:120:LEU:HD11	6:D:571:HOH:O	2.13	0.48
1:C:274:ALA:N	1:C:336[B]:CYS:SG	2.87	0.48
1:B:209:HIS:H	3:B:408:NAP:H72N	1.64	0.46
1:A:209:HIS:H	3:A:414:NAP:H72N	1.64	0.45
1:A:41:GLU:HG2	1:A:68:LEU:HD21	1.98	0.45
1:A:208:ASN:HA	3:A:414:NAP:H71N	1.82	0.44
1:B:120:LEU:HG	1:B:123:TYR:HB3	2.00	0.42
1:C:208:ASN:HA	3:C:407:NAP:H71N	1.85	0.41
1:A:278[B]:VAL:HG11	1:A:333:GLN:HB2	2.02	0.41
1:C:160:GLY:HA3	1:C:174:TYR:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:LEU:HD11	6:B:604:HOH:O	2.21	0.40
1:B:208:ASN:HA	3:B:408:NAP:H71N	1.87	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	352/373 (94%)	345 (98%)	6 (2%)	1 (0%)	41	18
1	B	349/373 (94%)	342 (98%)	7 (2%)	0	100	100
1	C	340/373 (91%)	332 (98%)	7 (2%)	1 (0%)	41	18
1	D	341/373 (91%)	335 (98%)	6 (2%)	0	100	100
All	All	1382/1492 (93%)	1354 (98%)	26 (2%)	2 (0%)	51	25

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	160	GLY
1	A	160	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	296/323 (92%)	293 (99%)	3 (1%)	76	54
1	B	294/323 (91%)	292 (99%)	2 (1%)	84	68
1	C	281/323 (87%)	279 (99%)	2 (1%)	84	68
1	D	275/323 (85%)	273 (99%)	2 (1%)	84	68
All	All	1146/1292 (89%)	1137 (99%)	9 (1%)	81	64

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	CYS
1	A	111	GLN
1	A	174	TYR
1	B	111	GLN
1	B	174	TYR
1	C	111	GLN
1	C	144	LEU
1	D	98	ASN
1	D	111	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

37 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	EDO	C	403	-	3,3,3	0.50	0	2,2,2	0.19	0
2	EDO	B	405	-	3,3,3	0.44	0	2,2,2	0.24	0
2	EDO	A	403	-	3,3,3	0.45	0	2,2,2	0.50	0
2	EDO	B	402	-	3,3,3	0.56	0	2,2,2	0.28	0
3	NAP	D	404	-	46,52,52	1.33	6 (13%)	61,80,80	1.37	6 (9%)
5	GOL	C	406	-	5,5,5	0.41	0	5,5,5	0.50	0
2	EDO	A	410	-	3,3,3	0.38	0	2,2,2	0.66	0
2	EDO	A	409	-	3,3,3	0.46	0	2,2,2	0.40	0
2	EDO	A	407	-	3,3,3	0.84	0	2,2,2	0.28	0
2	EDO	B	406	-	3,3,3	0.45	0	2,2,2	0.32	0
2	EDO	A	404	-	3,3,3	0.48	0	2,2,2	0.26	0
2	EDO	A	411	-	3,3,3	0.45	0	2,2,2	0.31	0
2	EDO	C	401	-	3,3,3	0.48	0	2,2,2	0.44	0
4	GDD	A	415	-	37,42,42	0.87	1 (2%)	47,65,65	0.67	0
2	EDO	A	412	-	3,3,3	0.51	0	2,2,2	0.23	0
2	EDO	A	405	-	3,3,3	0.32	0	2,2,2	0.14	0
2	EDO	C	402	-	3,3,3	0.49	0	2,2,2	0.40	0
2	EDO	B	407	-	3,3,3	0.43	0	2,2,2	0.69	0
2	EDO	B	401	-	3,3,3	0.40	0	2,2,2	0.58	0
2	EDO	A	408	-	3,3,3	0.52	0	2,2,2	0.24	0
3	NAP	C	407	-	46,52,52	1.52	7 (15%)	61,80,80	1.38	6 (9%)
2	EDO	A	402	-	3,3,3	0.77	0	2,2,2	0.60	0
4	GDD	D	405	-	37,42,42	0.90	2 (5%)	47,65,65	0.75	1 (2%)
2	EDO	C	405	-	3,3,3	0.36	0	2,2,2	0.18	0
2	EDO	B	403	-	3,3,3	0.42	0	2,2,2	0.24	0
2	EDO	A	413	-	3,3,3	0.41	0	2,2,2	0.30	0
4	GDD	C	408	-	37,42,42	0.96	1 (2%)	47,65,65	0.69	0
2	EDO	D	402	-	3,3,3	0.35	0	2,2,2	0.25	0
3	NAP	B	408	-	46,52,52	1.45	8 (17%)	61,80,80	1.40	7 (11%)
2	EDO	D	401	-	3,3,3	0.57	0	2,2,2	0.49	0
2	EDO	D	403	-	3,3,3	0.29	0	2,2,2	0.17	0
2	EDO	B	404	-	3,3,3	0.41	0	2,2,2	0.07	0
2	EDO	C	404	-	3,3,3	0.41	0	2,2,2	0.28	0
2	EDO	A	401	-	3,3,3	0.43	0	2,2,2	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	A	414	-	46,52,52	1.58	7 (15%)	61,80,80	1.38	8 (13%)
4	GDD	B	409	-	37,42,42	0.97	3 (8%)	47,65,65	0.67	0
2	EDO	A	406	-	3,3,3	0.57	0	2,2,2	0.44	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	EDO	C	403	-	-	0/1/1/1	-
2	EDO	B	405	-	-	0/1/1/1	-
2	EDO	A	403	-	-	0/1/1/1	-
2	EDO	B	402	-	-	0/1/1/1	-
3	NAP	D	404	-	-	7/31/67/67	0/5/5/5
5	GOL	C	406	-	-	4/4/4/4	-
2	EDO	A	410	-	-	0/1/1/1	-
2	EDO	A	409	-	-	1/1/1/1	-
2	EDO	A	407	-	-	0/1/1/1	-
2	EDO	B	406	-	-	1/1/1/1	-
2	EDO	A	404	-	-	0/1/1/1	-
2	EDO	A	411	-	-	0/1/1/1	-
2	EDO	C	401	-	-	0/1/1/1	-
4	GDD	A	415	-	-	2/19/59/59	0/4/4/4
2	EDO	A	412	-	-	0/1/1/1	-
2	EDO	A	405	-	-	0/1/1/1	-
2	EDO	C	402	-	-	0/1/1/1	-
2	EDO	B	407	-	-	1/1/1/1	-
2	EDO	B	401	-	-	0/1/1/1	-
2	EDO	A	408	-	-	1/1/1/1	-
3	NAP	C	407	-	-	4/31/67/67	0/5/5/5
2	EDO	A	402	-	-	1/1/1/1	-
4	GDD	D	405	-	-	2/19/59/59	0/4/4/4
2	EDO	C	405	-	-	0/1/1/1	-
2	EDO	B	403	-	-	0/1/1/1	-
2	EDO	A	413	-	-	0/1/1/1	-
4	GDD	C	408	-	-	4/19/59/59	0/4/4/4
2	EDO	D	402	-	-	0/1/1/1	-
3	NAP	B	408	-	-	6/31/67/67	0/5/5/5
2	EDO	D	401	-	-	0/1/1/1	-
2	EDO	D	403	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	B	404	-	-	0/1/1/1	-
2	EDO	C	404	-	-	0/1/1/1	-
2	EDO	A	401	-	-	0/1/1/1	-
3	NAP	A	414	-	-	4/31/67/67	0/5/5/5
4	GDD	B	409	-	-	3/19/59/59	0/4/4/4
2	EDO	A	406	-	-	0/1/1/1	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	414	NAP	O4D-C1D	5.06	1.47	1.40
3	C	407	NAP	PN-O3	4.55	1.64	1.59
3	B	408	NAP	O4D-C1D	4.50	1.46	1.40
3	C	407	NAP	O4D-C1D	4.28	1.46	1.40
3	A	414	NAP	C4N-C3N	4.11	1.45	1.39
3	B	408	NAP	PN-O3	4.04	1.63	1.59
3	D	404	NAP	O4D-C1D	4.01	1.46	1.40
3	A	414	NAP	PN-O3	3.91	1.63	1.59
3	A	414	NAP	PA-O3	3.61	1.63	1.59
3	B	408	NAP	C4N-C3N	3.35	1.44	1.39
3	C	407	NAP	C2A-N3A	3.30	1.37	1.32
3	D	404	NAP	PN-O3	3.21	1.63	1.59
3	C	407	NAP	PA-O3	3.14	1.62	1.59
3	C	407	NAP	C4N-C3N	3.06	1.44	1.39
4	C	408	GDD	PB-O1B	2.95	1.68	1.59
3	D	404	NAP	C2A-N3A	2.85	1.36	1.32
3	D	404	NAP	P2B-O3X	-2.84	1.44	1.54
4	B	409	GDD	PB-O3A	2.83	1.62	1.59
4	D	405	GDD	PB-O1B	2.80	1.67	1.59
3	B	408	NAP	O7N-C7N	2.68	1.29	1.24
3	C	407	NAP	P2B-O2B	2.68	1.64	1.59
3	A	414	NAP	O7N-C7N	2.55	1.28	1.24
3	B	408	NAP	C7N-N7N	-2.51	1.28	1.33
3	A	414	NAP	P2B-O2B	2.49	1.63	1.59
4	B	409	GDD	PB-O1B	2.44	1.66	1.59
3	D	404	NAP	C4N-C3N	2.43	1.43	1.39
3	B	408	NAP	C2A-N3A	2.29	1.35	1.32
3	C	407	NAP	O7N-C7N	2.29	1.28	1.24
4	A	415	GDD	PA-O3A	2.23	1.61	1.59
3	B	408	NAP	PA-O3	2.21	1.61	1.59
3	A	414	NAP	C2A-N3A	2.12	1.35	1.32
4	B	409	GDD	C8-N7	-2.11	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	408	NAP	P2B-O2B	2.11	1.63	1.59
4	D	405	GDD	C8-N7	-2.03	1.31	1.34
3	D	404	NAP	O7N-C7N	2.01	1.27	1.24

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	408	NAP	O7N-C7N-C3N	5.02	125.73	119.60
3	C	407	NAP	N3A-C2A-N1A	-4.99	121.90	128.67
3	D	404	NAP	N3A-C2A-N1A	-4.51	122.55	128.67
3	A	414	NAP	C5N-C4N-C3N	-4.31	116.13	120.36
3	D	404	NAP	O7N-C7N-C3N	4.27	124.82	119.60
3	C	407	NAP	O7N-C7N-C3N	3.98	124.46	119.60
3	B	408	NAP	N3A-C2A-N1A	-3.90	123.38	128.67
3	A	414	NAP	O7N-C7N-C3N	3.74	124.18	119.60
3	A	414	NAP	N3A-C2A-N1A	-3.71	123.64	128.67
3	B	408	NAP	C5N-C4N-C3N	-3.36	117.06	120.36
3	D	404	NAP	O2N-PN-O1N	3.03	126.55	112.44
3	C	407	NAP	C5N-C4N-C3N	-3.03	117.39	120.36
3	B	408	NAP	O7N-C7N-N7N	-2.87	118.47	122.62
3	A	414	NAP	C6N-N1N-C2N	-2.59	119.67	121.88
3	D	404	NAP	C2D-C3D-C4D	2.50	107.43	102.61
3	D	404	NAP	N6A-C6A-N1A	2.33	123.31	118.33
3	C	407	NAP	C1B-N9A-C4A	-2.33	122.56	126.64
3	A	414	NAP	C3B-C2B-C1B	-2.30	98.40	102.81
3	C	407	NAP	O4B-C1B-N9A	2.29	111.78	108.75
3	D	404	NAP	C3B-C2B-C1B	-2.26	98.48	102.81
3	A	414	NAP	C4D-O4D-C1D	2.24	111.97	109.92
3	B	408	NAP	C3B-C2B-C1B	-2.23	98.55	102.81
3	A	414	NAP	C2N-C3N-C4N	2.17	120.78	118.26
3	B	408	NAP	O2B-P2B-O1X	-2.09	101.87	109.33
3	C	407	NAP	O7N-C7N-N7N	-2.06	119.64	122.62
3	A	414	NAP	O2N-PN-O1N	2.04	121.95	112.44
3	B	408	NAP	C6N-N1N-C2N	-2.03	120.15	121.88
4	D	405	GDD	O1B-C11-C21	2.03	112.09	108.38

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	414	NAP	O4D-C1D-N1N-C2N
3	A	414	NAP	O4D-C1D-N1N-C6N

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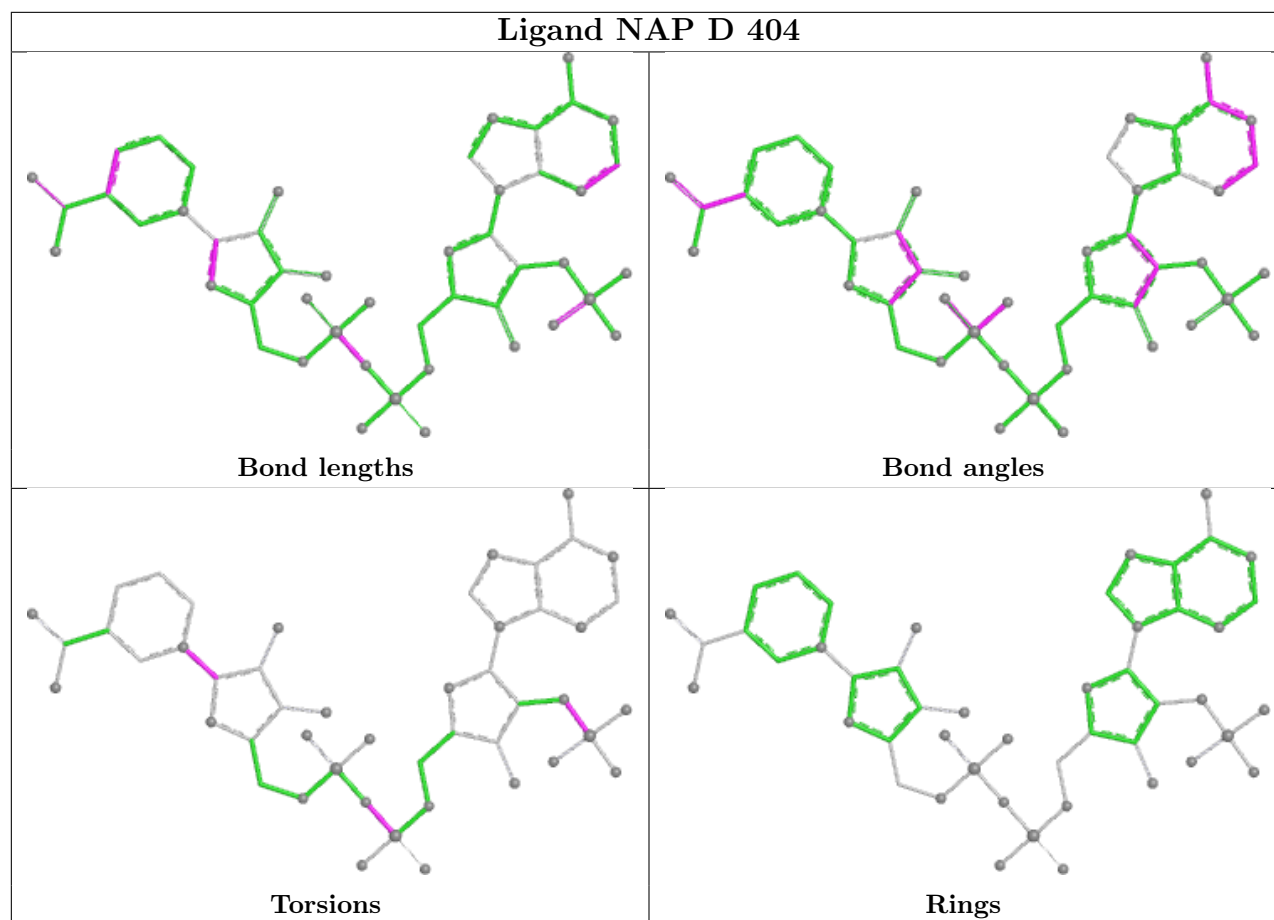
Mol	Chain	Res	Type	Atoms
3	A	414	NAP	C2D-C1D-N1N-C6N
3	B	408	NAP	O4D-C1D-N1N-C2N
3	B	408	NAP	O4D-C1D-N1N-C6N
3	B	408	NAP	C2D-C1D-N1N-C6N
3	C	407	NAP	O4D-C1D-N1N-C2N
3	C	407	NAP	O4D-C1D-N1N-C6N
3	C	407	NAP	C2D-C1D-N1N-C6N
3	D	404	NAP	O4D-C1D-N1N-C2N
3	D	404	NAP	O4D-C1D-N1N-C6N
3	D	404	NAP	C2D-C1D-N1N-C6N
4	A	415	GDD	PB-O3A-PA-O5'
4	B	409	GDD	PB-O3A-PA-O5'
4	C	408	GDD	PB-O3A-PA-O5'
4	D	405	GDD	PB-O3A-PA-O5'
5	C	406	GOL	O1-C1-C2-C3
5	C	406	GOL	C1-C2-C3-O3
2	A	402	EDO	O1-C1-C2-O2
5	C	406	GOL	O2-C2-C3-O3
2	A	409	EDO	O1-C1-C2-O2
2	B	407	EDO	O1-C1-C2-O2
5	C	406	GOL	O1-C1-C2-O2
3	A	414	NAP	C2B-O2B-P2B-O2X
3	B	408	NAP	C2B-O2B-P2B-O3X
3	D	404	NAP	C2B-O2B-P2B-O2X
3	B	408	NAP	C2D-C1D-N1N-C2N
3	B	408	NAP	C2B-O2B-P2B-O1X
3	D	404	NAP	C2B-O2B-P2B-O1X
2	B	406	EDO	O1-C1-C2-O2
4	A	415	GDD	PA-O3A-PB-O3B
4	B	409	GDD	PA-O3A-PB-O3B
4	C	408	GDD	PA-O3A-PB-O2B
4	C	408	GDD	PA-O3A-PB-O3B
4	D	405	GDD	PA-O3A-PB-O3B
3	D	404	NAP	C2B-O2B-P2B-O3X
2	A	408	EDO	O1-C1-C2-O2
4	C	408	GDD	C41-C51-C61-O6A
3	C	407	NAP	PN-O3-PA-O2A
3	D	404	NAP	PN-O3-PA-O2A
4	B	409	GDD	PA-O3A-PB-O2B

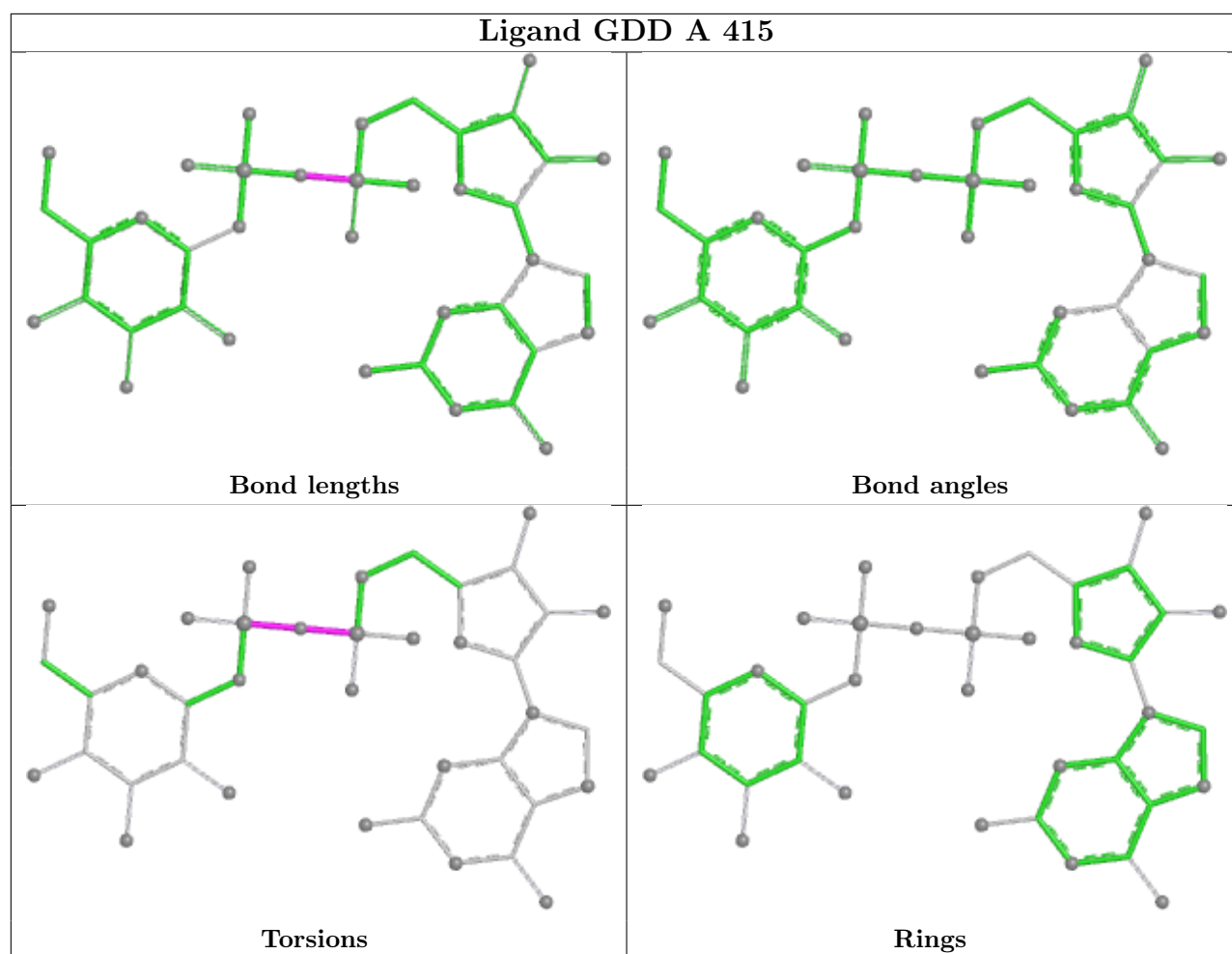
There are no ring outliers.

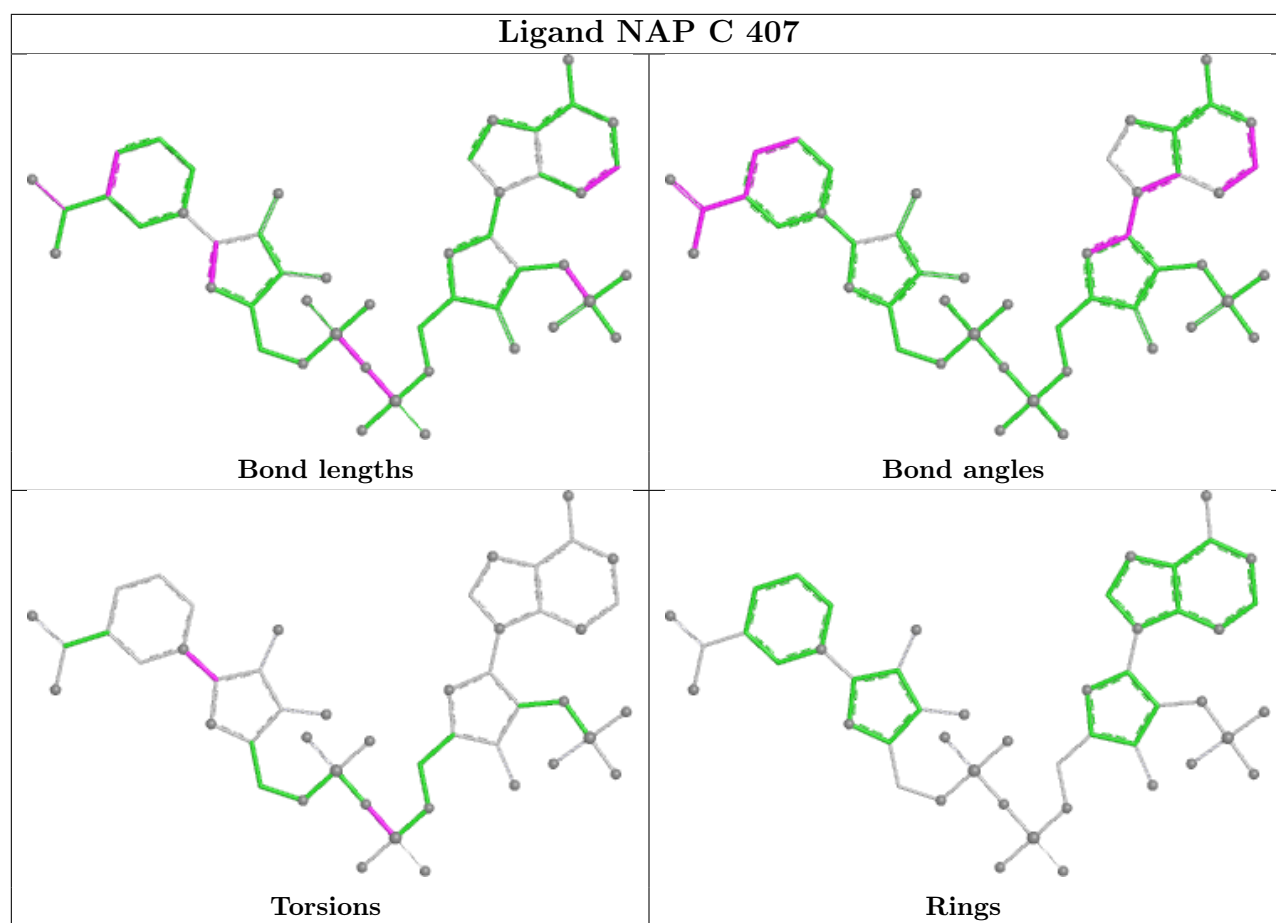
3 monomers are involved in 5 short contacts:

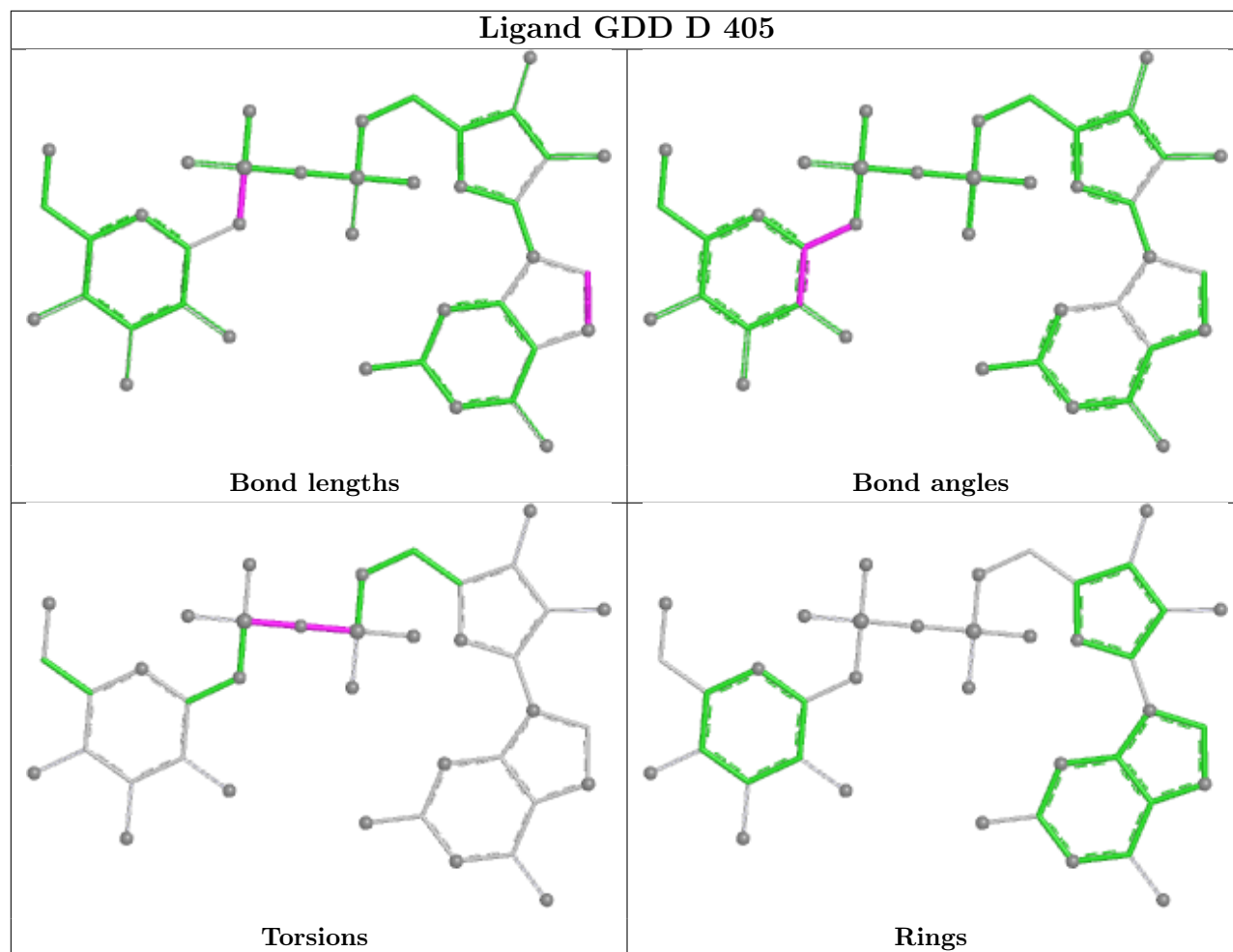
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	407	NAP	1	0
3	B	408	NAP	2	0
3	A	414	NAP	2	0

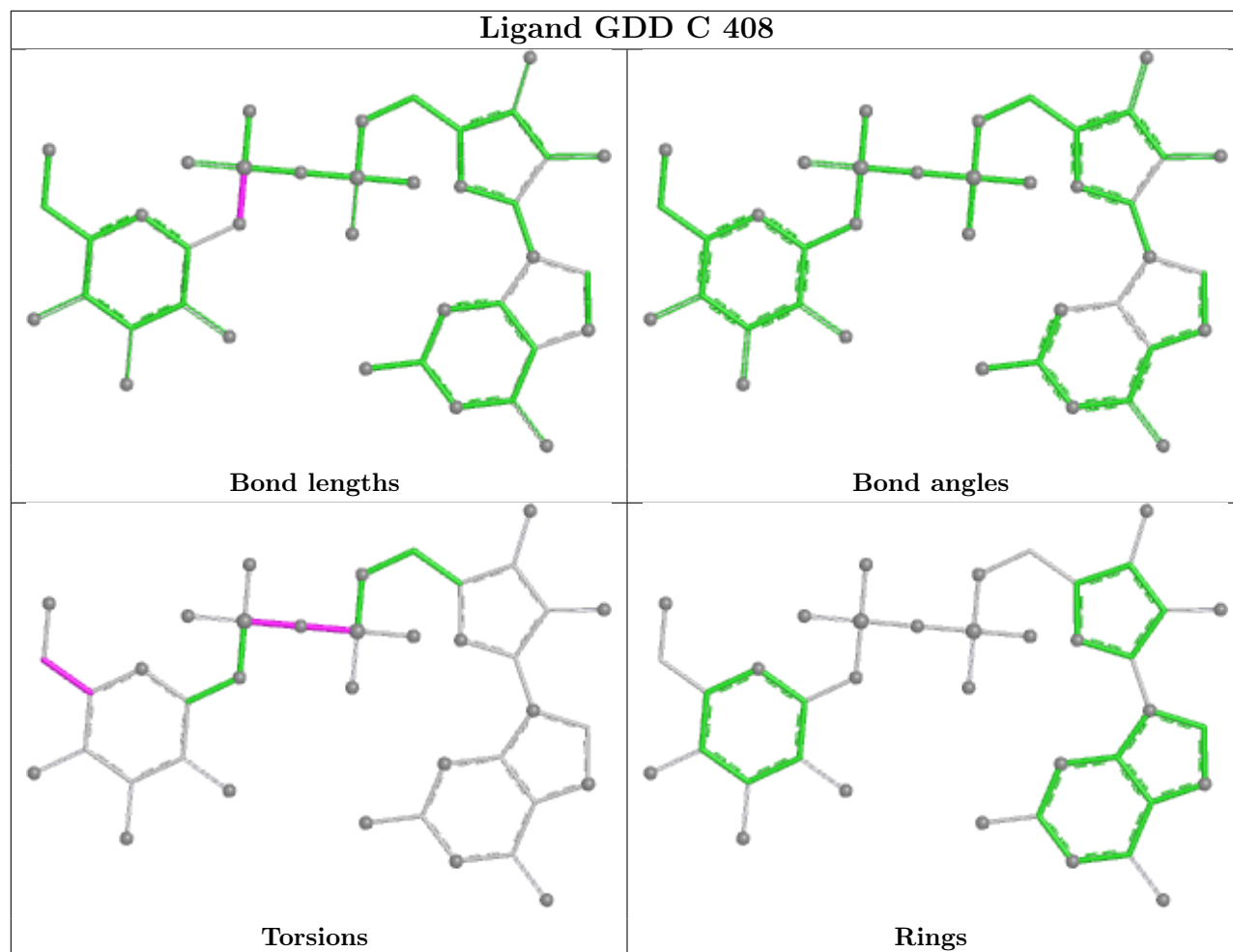
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

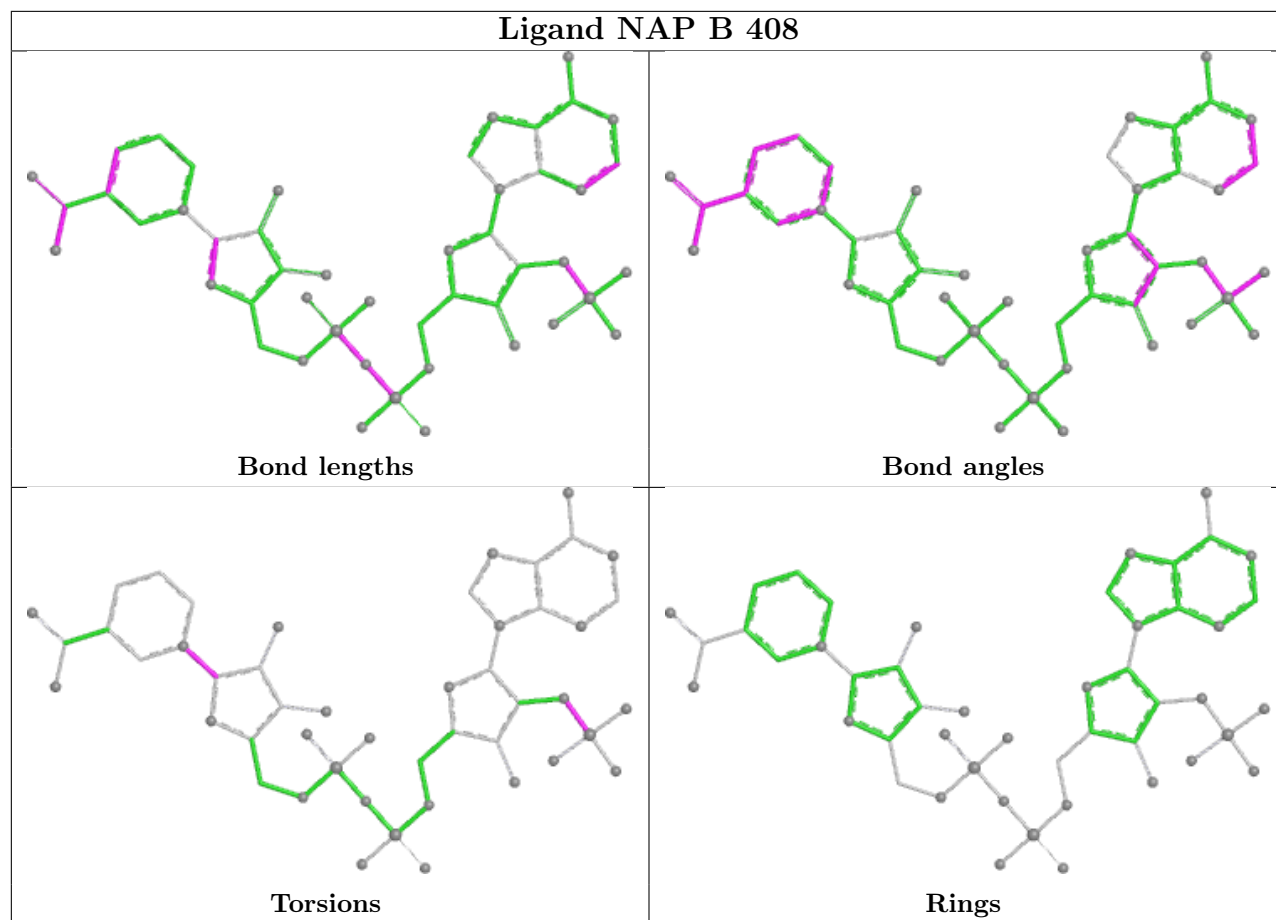


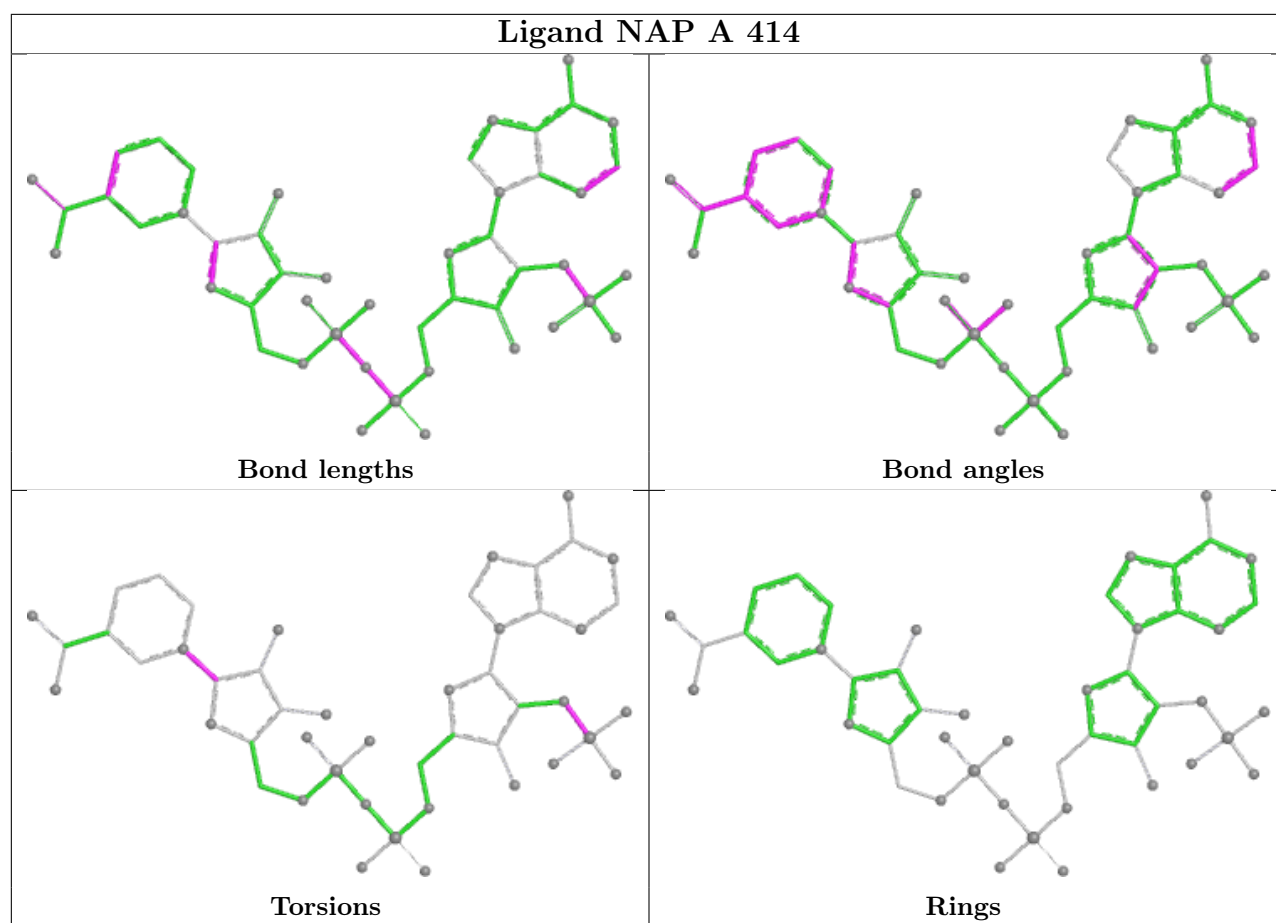


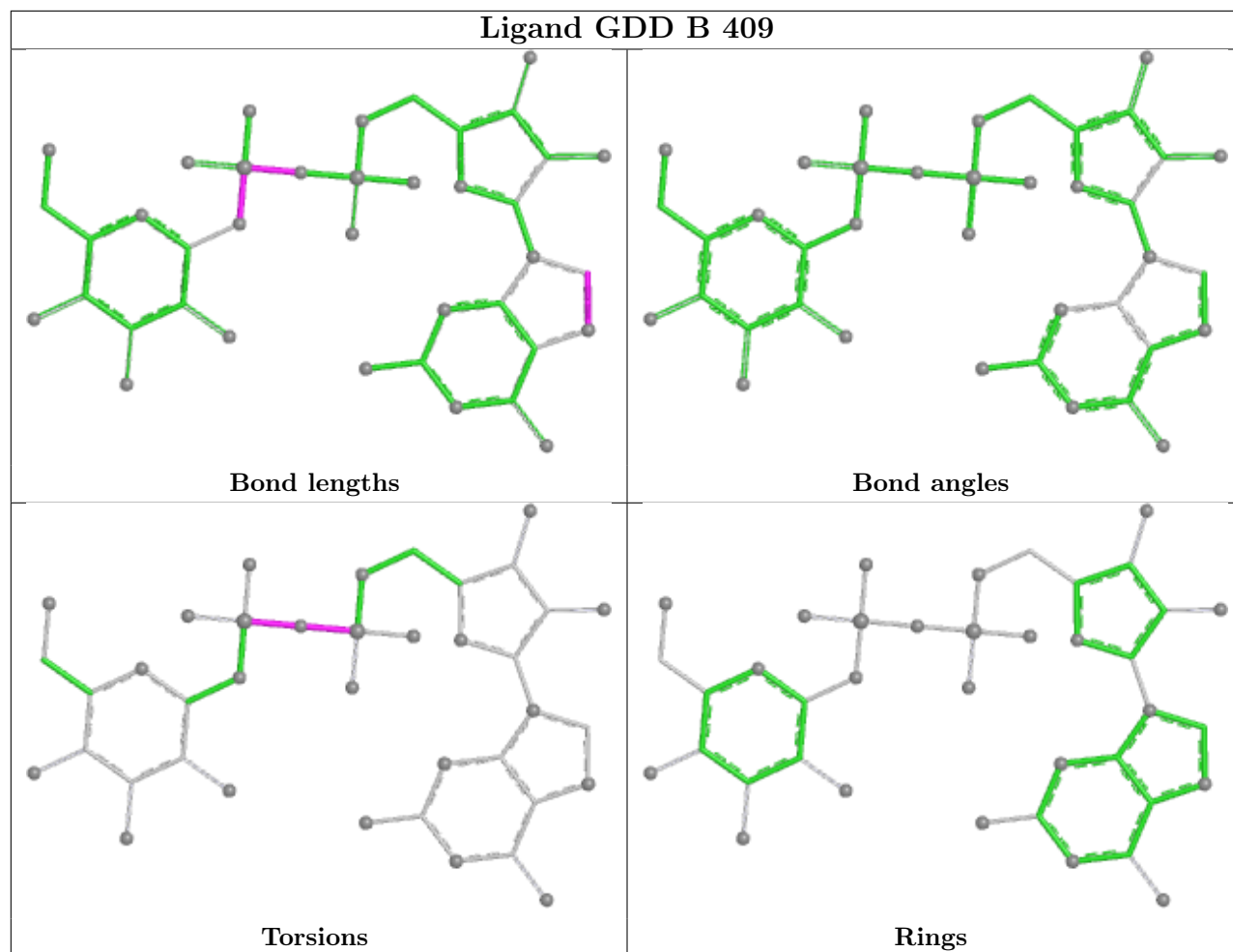












5.7 Other polymers [i](#)

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	350/373 (93%)	-0.11	12 (3%) 45 49	13, 19, 36, 59	0
1	B	350/373 (93%)	-0.20	6 (1%) 70 73	13, 18, 33, 49	0
1	C	342/373 (91%)	-0.23	7 (2%) 65 69	14, 22, 36, 74	0
1	D	344/373 (92%)	0.53	40 (11%) 4 4	15, 29, 52, 76	0
All	All	1386/1492 (92%)	-0.00	65 (4%) 31 34	13, 22, 44, 76	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	69	TYR	7.7
1	D	227	VAL	6.8
1	D	223	ILE	6.7
1	D	230	ILE	6.4
1	D	231	TYR	6.4
1	A	72	PRO	6.1
1	A	76	ILE	5.7
1	A	74	ALA	5.7
1	D	69	TYR	5.5
1	A	75	HIS	5.4
1	D	297	VAL	5.1
1	D	313	GLY	4.9
1	D	290	LEU	4.8
1	D	237	CYS	4.6
1	B	76	ILE	4.2
1	A	78	GLY	4.2
1	D	292	ILE	4.1
1	D	315	VAL	4.1
1	B	69	TYR	4.1
1	D	368	THR	4.0
1	D	358[A]	MET	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	78	GLY	3.8
1	D	233	GLY	3.7
1	D	293	GLY	3.7
1	D	295	THR	3.6
1	C	368	THR	3.5
1	D	319	VAL	3.4
1	A	73	GLN	3.4
1	A	71	ASN	3.3
1	C	371	ASN	3.3
1	B	74	ALA	3.3
1	D	289	PHE	3.3
1	D	312	THR	3.2
1	D	296	ILE	3.1
1	D	310	LYS	3.1
1	D	351	PHE	3.0
1	D	363	VAL	3.0
1	D	372	ALA	3.0
1	D	298	TRP	3.0
1	A	371	ASN	3.0
1	D	355	VAL	2.9
1	B	75	HIS	2.9
1	B	72	PRO	2.8
1	D	324	TYR	2.7
1	D	317	VAL	2.6
1	B	70	LYS	2.4
1	D	285	VAL	2.4
1	D	356	ARG	2.4
1	D	281	VAL	2.3
1	D	238	PHE	2.3
1	A	69	TYR	2.3
1	A	77	GLU	2.2
1	A	370	PRO	2.2
1	C	370	PRO	2.2
1	D	370	PRO	2.2
1	C	163	GLN	2.2
1	D	309	CYS	2.1
1	D	352	ASP	2.1
1	D	360	HIS	2.1
1	C	360	HIS	2.1
1	D	308	ARG	2.1
1	D	294	LYS	2.1
1	C	78	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	71	ASN	2.0
1	A	344	ASN	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 monosaccharides 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.

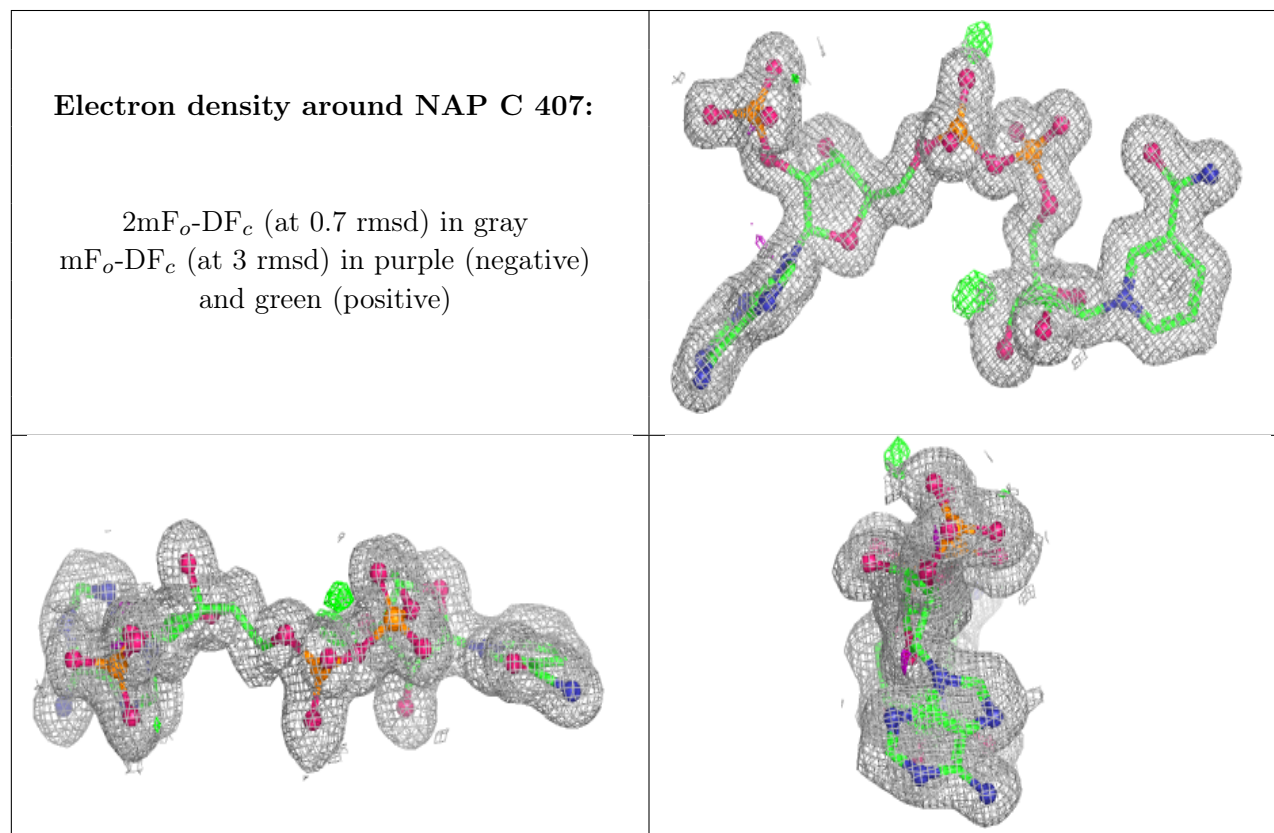
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	EDO	C	402	4/4	0.71	0.28	53,53,53,54	0
2	EDO	A	410	4/4	0.76	0.19	46,46,47,49	0
2	EDO	A	408	4/4	0.78	0.18	43,47,48,49	0
2	EDO	B	406	4/4	0.82	0.13	45,49,50,55	0
5	GOL	C	406	6/6	0.85	0.17	38,41,47,49	0
2	EDO	D	401	4/4	0.86	0.14	29,32,38,48	0
2	EDO	C	401	4/4	0.86	0.30	44,51,57,61	0
2	EDO	A	409	4/4	0.87	0.20	38,48,51,60	0
2	EDO	A	402	4/4	0.90	0.14	22,23,26,28	0
2	EDO	A	407	4/4	0.92	0.09	24,25,27,27	0
2	EDO	B	407	4/4	0.93	0.13	28,30,35,47	0
2	EDO	A	411	4/4	0.94	0.11	26,31,34,34	0
2	EDO	D	402	4/4	0.94	0.10	24,29,34,35	0
2	EDO	C	403	4/4	0.94	0.08	28,29,30,31	0
2	EDO	A	413	4/4	0.95	0.17	20,22,27,29	0
2	EDO	D	403	4/4	0.95	0.09	27,29,30,35	0
2	EDO	B	405	4/4	0.95	0.11	22,27,30,31	0
2	EDO	C	404	4/4	0.96	0.07	23,28,29,29	0
2	EDO	C	405	4/4	0.96	0.07	28,29,30,33	0
2	EDO	B	401	4/4	0.96	0.14	25,26,27,28	0
2	EDO	B	402	4/4	0.96	0.06	21,22,23,24	0

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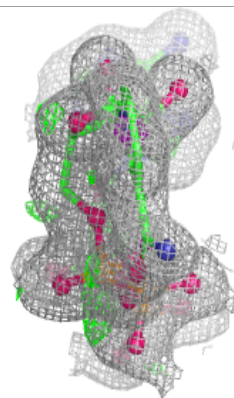
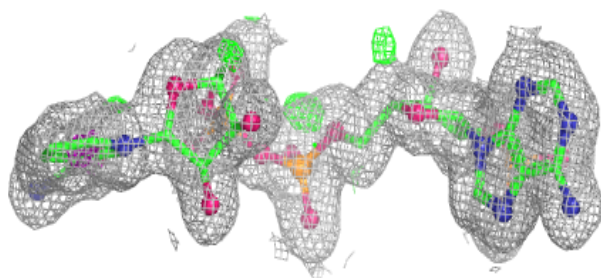
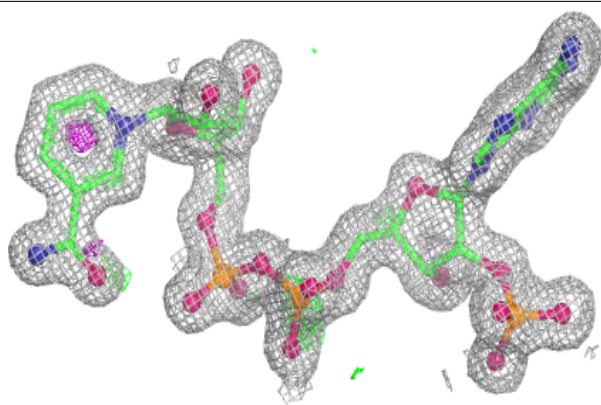
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	EDO	A	405	4/4	0.96	0.09	26,26,26,30	0
2	EDO	A	406	4/4	0.96	0.06	21,22,22,24	0
2	EDO	A	404	4/4	0.97	0.05	23,23,23,25	0
2	EDO	A	403	4/4	0.97	0.07	23,26,29,33	0
2	EDO	A	412	4/4	0.97	0.06	21,22,24,24	0
3	NAP	C	407	48/48	0.97	0.07	16,18,20,21	0
3	NAP	D	404	48/48	0.97	0.07	18,21,26,27	0
4	GDD	D	405	39/39	0.97	0.07	20,24,29,30	0
2	EDO	B	404	4/4	0.97	0.05	21,22,23,25	0
2	EDO	A	401	4/4	0.98	0.10	19,19,20,20	0
2	EDO	B	403	4/4	0.98	0.06	17,18,18,19	0
4	GDD	A	415	39/39	0.98	0.07	13,14,15,15	0
4	GDD	C	408	39/39	0.98	0.06	15,16,18,19	0
3	NAP	A	414	48/48	0.98	0.08	14,16,18,19	0
3	NAP	B	408	48/48	0.98	0.09	13,15,18,19	0
4	GDD	B	409	39/39	0.99	0.07	12,13,15,15	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.

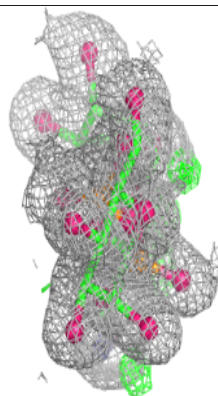
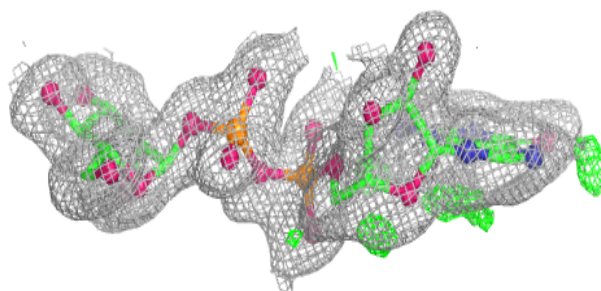
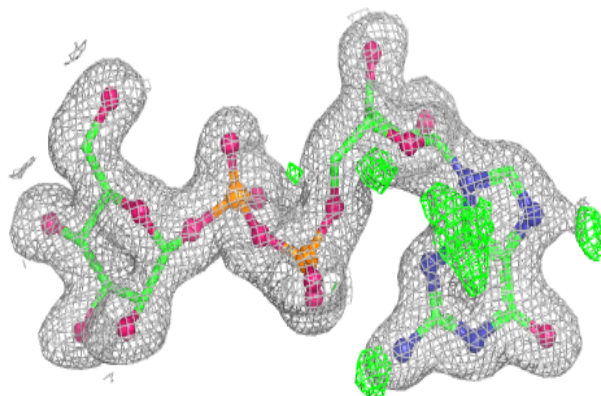


Electron density around NAP D 404:

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

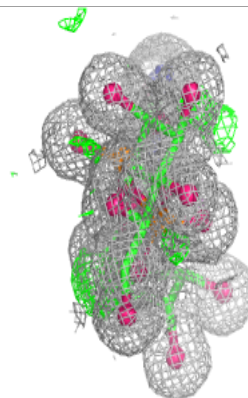
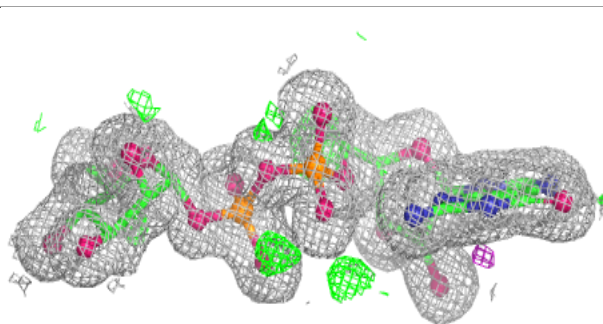
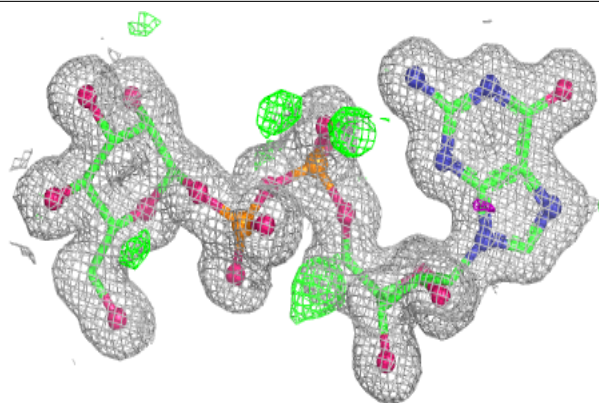
**Electron density around GDD D 405:**

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

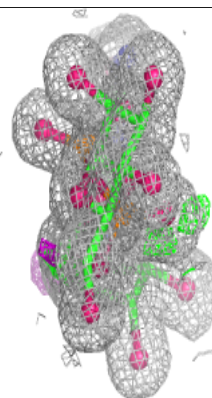
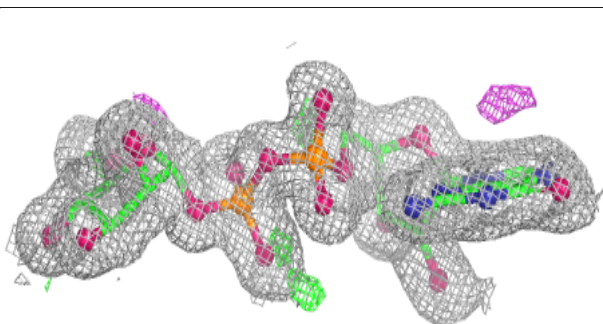
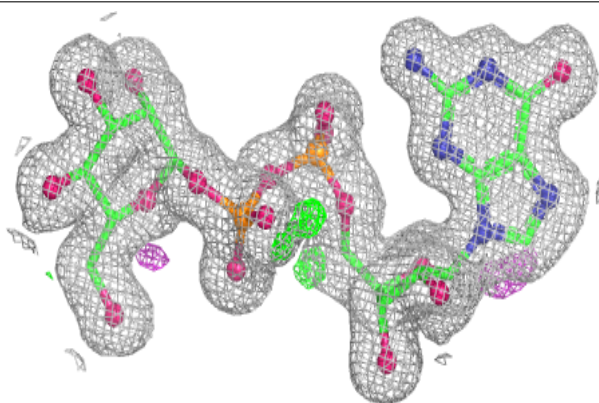


Electron density around GDD A 415:

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

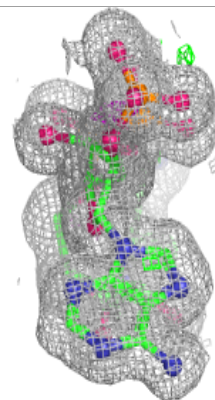
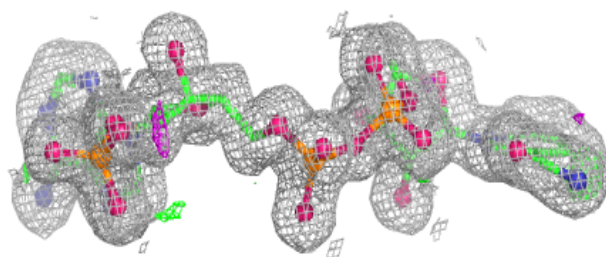
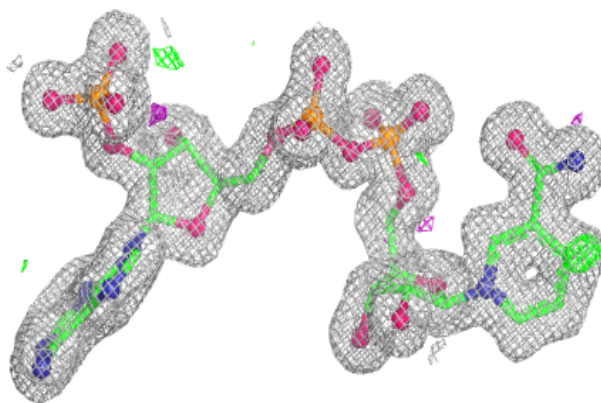
**Electron density around GDD C 408:**

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

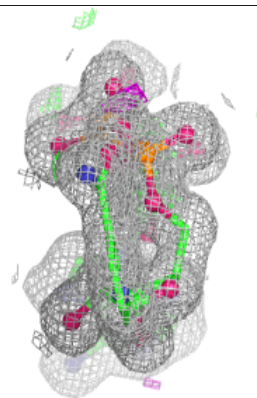
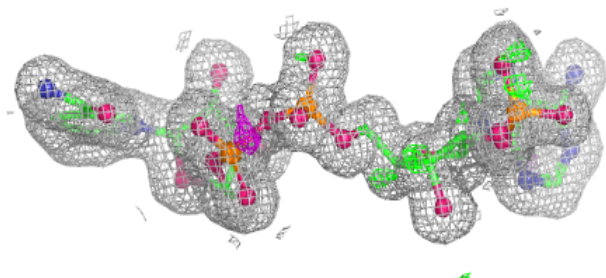
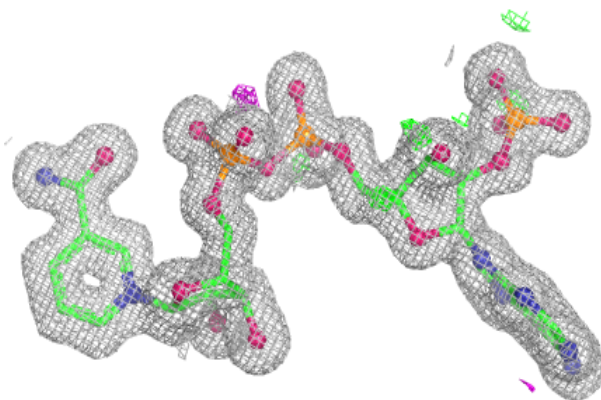


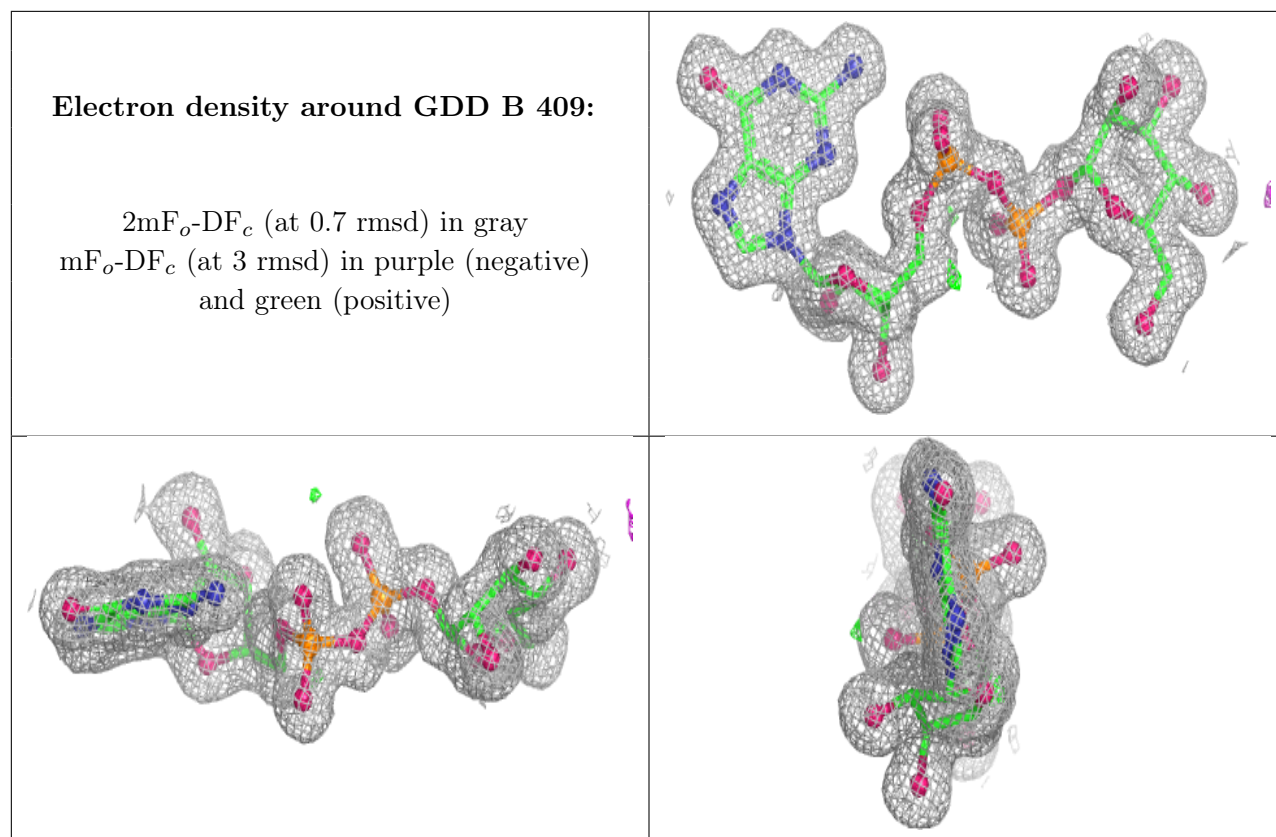
Electron density around NAP A 414:

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

**Electron density around NAP B 408:**

$2mF_o-DF_c$ (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.