



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2024 – 12:36 AM EST

PDB ID : 3RHJ  
Title : Crystal structure of the E673A mutant of the C-terminal domain of RAT 10 'FORMYLTETRAHYDROFOLATE DEHYDROGENASE in complex with co-purified NADP  
Authors : Tsybovsky, Y.  
Deposited on : 2011-04-11  
Resolution : 1.89 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](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

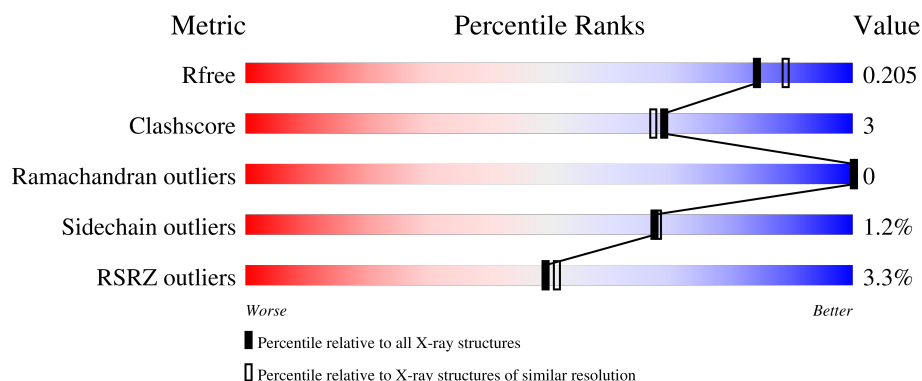
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.89 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))
$R_{free}$	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

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  $\geq 3$ , 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	517	<div> <div>4%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div>.</div> </div> </div>
1	B	517	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>7%</div> <div>.</div> </div> </div>
1	C	517	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>7%</div> <div>.</div> </div> </div>
1	D	517	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>7%</div> <div>.</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17396 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 Aldehyde dehydrogenase 1 family, member L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	23	0
			3901	2485	660	734	22			
1	B	498	Total	C	N	O	S	0	23	0
			3908	2484	669	733	22			
1	C	498	Total	C	N	O	S	0	20	0
			3893	2476	669	726	22			
1	D	498	Total	C	N	O	S	0	21	0
			3903	2482	667	732	22			

There are 48 discrepancies between the modelled and reference sequences:

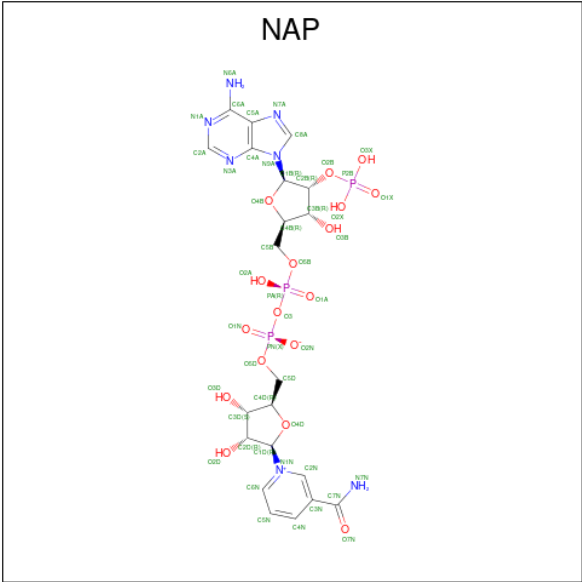
Chain	Residue	Modelled	Actual	Comment	Reference
A	386	MET	-	expression tag	UNP Q5HQB2
A	387	ARG	-	expression tag	UNP Q5HQB2
A	388	GLY	-	expression tag	UNP Q5HQB2
A	389	SER	-	expression tag	UNP Q5HQB2
A	390	HIS	-	expression tag	UNP Q5HQB2
A	391	HIS	-	expression tag	UNP Q5HQB2
A	392	HIS	-	expression tag	UNP Q5HQB2
A	393	HIS	-	expression tag	UNP Q5HQB2
A	394	HIS	-	expression tag	UNP Q5HQB2
A	395	THR	-	expression tag	UNP Q5HQB2
A	396	THR	-	expression tag	UNP Q5HQB2
A	673	ALA	GLU	engineered mutation	UNP Q5HQB2
B	386	MET	-	expression tag	UNP Q5HQB2
B	387	ARG	-	expression tag	UNP Q5HQB2
B	388	GLY	-	expression tag	UNP Q5HQB2
B	389	SER	-	expression tag	UNP Q5HQB2
B	390	HIS	-	expression tag	UNP Q5HQB2
B	391	HIS	-	expression tag	UNP Q5HQB2
B	392	HIS	-	expression tag	UNP Q5HQB2
B	393	HIS	-	expression tag	UNP Q5HQB2
B	394	HIS	-	expression tag	UNP Q5HQB2

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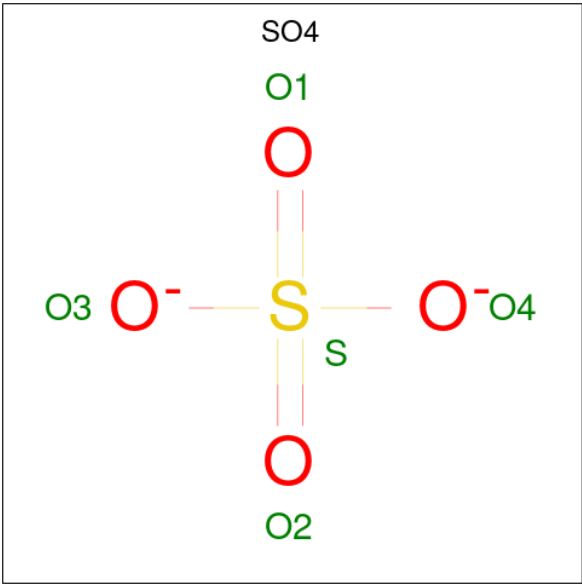
Chain	Residue	Modelled	Actual	Comment	Reference
B	395	THR	-	expression tag	UNP Q5HQB2
B	396	THR	-	expression tag	UNP Q5HQB2
B	673	ALA	GLU	engineered mutation	UNP Q5HQB2
C	386	MET	-	expression tag	UNP Q5HQB2
C	387	ARG	-	expression tag	UNP Q5HQB2
C	388	GLY	-	expression tag	UNP Q5HQB2
C	389	SER	-	expression tag	UNP Q5HQB2
C	390	HIS	-	expression tag	UNP Q5HQB2
C	391	HIS	-	expression tag	UNP Q5HQB2
C	392	HIS	-	expression tag	UNP Q5HQB2
C	393	HIS	-	expression tag	UNP Q5HQB2
C	394	HIS	-	expression tag	UNP Q5HQB2
C	395	THR	-	expression tag	UNP Q5HQB2
C	396	THR	-	expression tag	UNP Q5HQB2
C	673	ALA	GLU	engineered mutation	UNP Q5HQB2
D	386	MET	-	expression tag	UNP Q5HQB2
D	387	ARG	-	expression tag	UNP Q5HQB2
D	388	GLY	-	expression tag	UNP Q5HQB2
D	389	SER	-	expression tag	UNP Q5HQB2
D	390	HIS	-	expression tag	UNP Q5HQB2
D	391	HIS	-	expression tag	UNP Q5HQB2
D	392	HIS	-	expression tag	UNP Q5HQB2
D	393	HIS	-	expression tag	UNP Q5HQB2
D	394	HIS	-	expression tag	UNP Q5HQB2
D	395	THR	-	expression tag	UNP Q5HQB2
D	396	THR	-	expression tag	UNP Q5HQB2
D	673	ALA	GLU	engineered mutation	UNP Q5HQB2

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



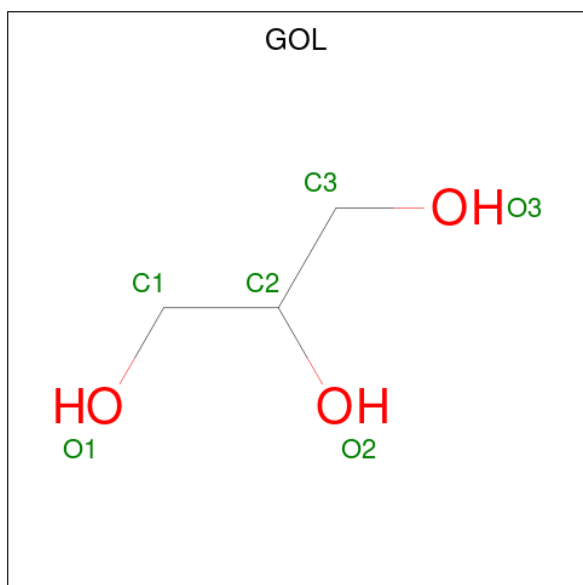
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	349	Total	O	0	1
			349	349		
5	B	345	Total	O	0	3
			345	345		
5	C	409	Total	O	0	3
			409	409		

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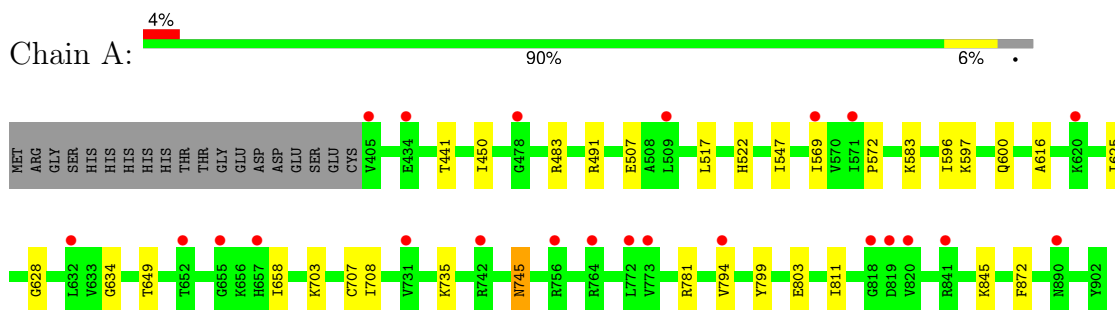
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	352	Total	O	0	2
			352	352		



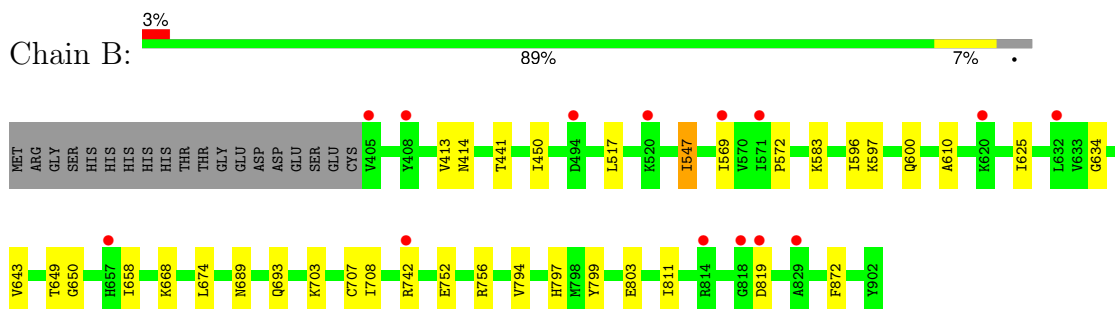
### 3 Residue-property plots

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.

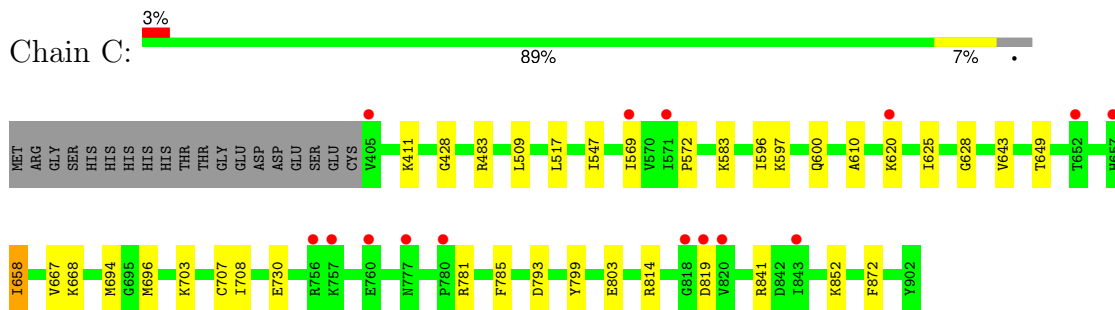
- Molecule 1: Aldehyde dehydrogenase 1 family, member L1



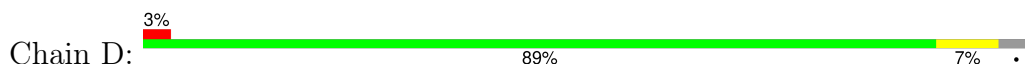
- Molecule 1: Aldehyde dehydrogenase 1 family, member L1

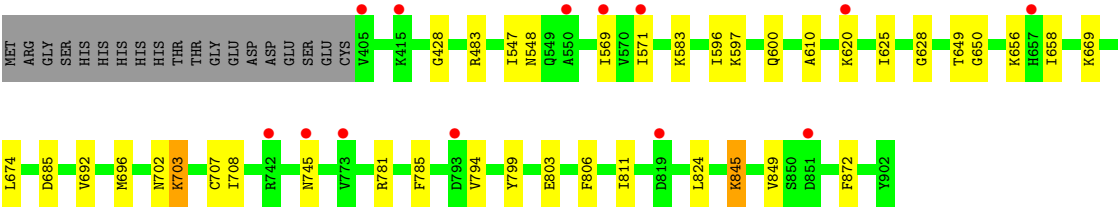


- Molecule 1: Aldehyde dehydrogenase 1 family, member L1



- Molecule 1: Aldehyde dehydrogenase 1 family, member L1





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	259.39Å 194.93Å 97.48Å 90.00° 108.94° 90.00°	Depositor
Resolution (Å)	48.91 – 1.89 48.91 – 1.89	Depositor EDS
% Data completeness (in resolution range)	97.8 (48.91-1.89) 97.8 (48.91-1.89)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.189 , 0.203 0.189 , 0.205	Depositor DCC
$R_{free}$ test set	17875 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.8	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 37.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	17396	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, NAP

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	0.51	0/4075	0.56	0/5512
1	B	0.49	0/4083	0.57	0/5522
1	C	0.55	0/4055	0.61	0/5485
1	D	0.50	0/4064	0.56	0/5497
All	All	0.51	0/16277	0.58	0/22016

There are no bond length outliers.

There are no bond angle outliers.

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	3901	0	3886	24	0
1	B	3908	0	3898	26	0
1	C	3893	0	3880	29	0
1	D	3903	0	3896	31	0
2	A	48	0	25	6	0
2	B	48	0	25	7	0
2	C	48	0	25	5	0
2	D	48	0	25	7	0
3	A	30	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	30	0	0	0	0
3	C	35	0	0	1	0
3	D	25	0	0	1	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	6	0	8	0	0
5	A	349	0	0	4	0
5	B	345	0	0	5	0
5	C	409	0	0	2	0
5	D	352	0	0	2	0
All	All	17396	0	15692	109	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 3.

All (109) 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:D:707[B]:CYS:SG	2:D:101:NAP:C4N	2.12	1.37
1:B:707[B]:CYS:SG	2:B:101:NAP:C4N	2.23	1.26
1:A:707[B]:CYS:SG	2:A:101:NAP:C4N	2.24	1.25
1:C:707[B]:CYS:SG	2:C:101:NAP:C4N	2.34	1.15
1:C:841[B]:ARG:HG2	1:C:841[B]:ARG:HH11	1.11	1.09
1:A:707[B]:CYS:SG	5:A:1348:HOH:O	2.01	1.07
1:C:707[B]:CYS:SG	5:C:1330:HOH:O	2.18	1.00
1:B:707[B]:CYS:SG	5:B:1344:HOH:O	2.26	0.92
1:A:707[B]:CYS:SG	2:A:101:NAP:C3N	2.62	0.88
1:D:707[B]:CYS:SG	2:D:101:NAP:C3N	2.63	0.85
1:C:597:LYS:HE2	1:C:628:GLY:O	1.79	0.83
1:D:707[B]:CYS:SG	2:D:101:NAP:C5N	2.66	0.82
1:B:707[B]:CYS:SG	2:B:101:NAP:C3N	2.68	0.81
1:D:707[B]:CYS:SG	2:D:101:NAP:H4N	2.16	0.80
1:D:707[B]:CYS:SG	5:D:1351:HOH:O	2.19	0.79
1:C:799:TYR:CE2	1:C:803[A]:GLU:HG3	2.20	0.77
1:B:707[B]:CYS:SG	2:B:101:NAP:H4N	2.23	0.76
1:C:841[B]:ARG:HG2	1:C:841[B]:ARG:NH1	1.91	0.75
1:A:781[A]:ARG:NH1	3:A:106:SO4:O2	2.16	0.75
1:A:569:ILE:HD11	1:A:596:ILE:HG12	1.70	0.74
1:A:799:TYR:CE2	1:A:803[A]:GLU:HG3	2.26	0.71
1:A:707[B]:CYS:SG	2:A:101:NAP:H4N	2.30	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:707[B]:CYS:SG	2:C:101:NAP:C3N	2.79	0.70
1:B:799:TYR:CE2	1:B:803[B]:GLU:HG3	2.27	0.69
1:D:597:LYS:HE2	1:D:628:GLY:O	1.92	0.69
1:C:707[B]:CYS:SG	2:C:101:NAP:H4N	2.32	0.69
1:D:569:ILE:HD12	1:D:571:ILE:HD11	1.76	0.68
1:C:428:GLY:HA3	1:C:620[B]:LYS:HG3	1.74	0.68
1:B:707[B]:CYS:SG	2:B:101:NAP:C5N	2.82	0.67
1:A:658:ILE:HD11	2:A:101:NAP:C2A	2.26	0.65
1:A:707[B]:CYS:SG	2:A:101:NAP:C5N	2.84	0.65
1:D:658:ILE:HD11	2:D:101:NAP:C2A	2.28	0.63
1:C:610:ALA:HB2	1:C:625:ILE:HD12	1.82	0.61
1:D:799:TYR:CE2	1:D:803[A]:GLU:HG3	2.35	0.61
1:B:600:GLN:NE2	5:B:1143:HOH:O	2.32	0.60
1:B:658:ILE:HD11	2:B:101:NAP:C2A	2.32	0.60
1:C:707[B]:CYS:SG	2:C:101:NAP:C5N	2.92	0.58
1:A:707[A]:CYS:SG	5:A:1348:HOH:O	2.51	0.57
1:C:793:ASP:OD2	1:C:814:ARG:NH2	2.38	0.57
1:A:597:LYS:HE2	1:A:628:GLY:O	2.05	0.56
1:B:799:TYR:CZ	1:B:803[B]:GLU:HG3	2.41	0.55
1:B:610:ALA:HB2	1:B:625:ILE:HD12	1.87	0.55
1:C:658:ILE:HD11	2:C:101:NAP:C2A	2.37	0.55
1:D:692:VAL:O	1:D:696:MET:HG2	2.06	0.55
1:A:708:ILE:HG21	1:A:872:PHE:HE1	1.72	0.54
1:A:491:ARG:HD2	1:A:616:ALA:O	2.07	0.54
1:D:708:ILE:HG21	1:D:872:PHE:HE1	1.73	0.53
1:A:600:GLN:NE2	5:A:1166:HOH:O	2.35	0.53
1:D:428:GLY:HA3	1:D:620[B]:LYS:HD2	1.90	0.53
1:D:708:ILE:CG2	1:D:872:PHE:HE1	2.22	0.52
1:C:583:LYS:HE2	1:C:649:THR:OG1	2.09	0.52
1:D:781[B]:ARG:HD2	1:D:785:PHE:CD2	2.44	0.52
1:A:572:PRO:HD3	1:A:649:THR:HB	1.90	0.52
1:B:752:GLU:O	1:B:756[A]:ARG:HG3	2.09	0.51
1:D:610:ALA:HB2	1:D:625:ILE:HD12	1.93	0.51
1:C:708:ILE:HG21	1:C:872:PHE:HE1	1.75	0.51
1:B:597:LYS:HG3	1:B:597:LYS:O	2.10	0.51
1:C:852:LYS:NZ	3:C:102:SO4:O3	2.34	0.51
1:D:794:VAL:HG21	1:D:811:ILE:HG23	1.94	0.50
1:B:689:ASN:O	1:B:693[B]:GLN:HG2	2.12	0.49
1:D:658:ILE:CD1	2:D:101:NAP:C2A	2.90	0.49
1:A:583:LYS:HE2	1:A:649:THR:OG1	2.13	0.49
1:A:569:ILE:CD1	1:A:596:ILE:HG12	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1010:HOH:O	1:C:483:ARG:HD3	2.13	0.49
1:B:414:ASN:OD1	1:B:742:ARG:NH2	2.38	0.49
1:A:794:VAL:HG21	1:A:811:ILE:HG23	1.95	0.48
1:C:600:GLN:NE2	5:C:1133:HOH:O	2.45	0.48
1:B:572:PRO:HD3	1:B:649:THR:HB	1.96	0.48
1:D:685:ASP:OD2	1:D:845:LYS:NZ	2.47	0.48
1:D:583:LYS:HE2	1:D:649:THR:OG1	2.14	0.47
1:A:483:ARG:HB3	1:D:548:ASN:HD21	1.79	0.47
1:C:572:PRO:HD3	1:C:649:THR:HB	1.97	0.47
1:D:669:LYS:NZ	3:D:106:SO4:O2	2.33	0.47
1:B:569:ILE:HD11	1:B:596:ILE:HG12	1.97	0.47
1:D:569:ILE:HG12	1:D:596:ILE:HG12	1.95	0.46
1:D:600:GLN:NE2	5:D:1085:HOH:O	2.48	0.46
1:C:411:LYS:HD3	1:C:509:LEU:HD21	1.96	0.46
1:C:781[B]:ARG:HD2	1:C:785:PHE:CD2	2.51	0.45
1:B:547:ILE:H	1:B:547:ILE:HD13	1.81	0.45
1:B:752:GLU:HG2	1:B:756[A]:ARG:HE	1.82	0.45
1:A:634:GLY:HA3	2:A:101:NAP:C2A	2.47	0.45
1:D:702:ASN:O	1:D:703:LYS:HG2	2.16	0.45
1:B:634:GLY:HA3	2:B:101:NAP:C2A	2.47	0.44
2:B:101:NAP:H8A	5:B:1264:HOH:O	2.16	0.44
1:D:708:ILE:CG2	1:D:872:PHE:CE1	3.00	0.44
1:B:650:GLY:O	1:B:674:LEU:HA	2.16	0.44
1:C:799:TYR:CZ	1:C:803[A]:GLU:HG3	2.53	0.44
1:D:569:ILE:O	1:D:569:ILE:HG13	2.17	0.43
1:C:569:ILE:HD11	1:C:596:ILE:HG12	2.00	0.43
5:B:1008:HOH:O	1:D:483:ARG:HD3	2.19	0.42
1:B:794:VAL:HG21	1:B:811:ILE:HG23	2.00	0.42
1:C:667:VAL:HG13	1:D:656:LYS:HG2	2.01	0.42
1:C:643:VAL:O	1:C:668:LYS:HE3	2.19	0.42
1:D:824:LEU:HD21	1:D:849:VAL:HG13	2.02	0.42
1:B:643:VAL:O	1:B:668:LYS:HE3	2.20	0.42
1:A:441:THR:HG23	1:A:450:ILE:HB	2.02	0.41
1:A:517:LEU:CD2	1:A:522:HIS:CE1	3.03	0.41
1:C:696:MET:SD	1:C:730:GLU:HB2	2.61	0.41
1:D:806:PHE:CE1	2:D:101:NAP:H2D	2.55	0.41
1:B:441:THR:HG23	1:B:450:ILE:HB	2.01	0.41
1:D:650:GLY:O	1:D:674:LEU:HA	2.21	0.41
1:B:708:ILE:CG2	1:B:872:PHE:HE1	2.32	0.41
1:B:797:HIS:HD2	5:B:1214:HOH:O	2.04	0.41
1:A:735:LYS:H	1:A:745:ASN:HD21	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:583:LYS:HE2	1:B:649:THR:OG1	2.21	0.40
1:A:708:ILE:HG21	1:A:872:PHE:CE1	2.55	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	519/517 (100%)	506 (98%)	13 (2%)	0	100	100
1	B	519/517 (100%)	505 (97%)	14 (3%)	0	100	100
1	C	516/517 (100%)	499 (97%)	17 (3%)	0	100	100
1	D	517/517 (100%)	499 (96%)	18 (4%)	0	100	100
All	All	2071/2068 (100%)	2009 (97%)	62 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	423/425 (100%)	417 (99%)	6 (1%)	62	62
1	B	425/425 (100%)	420 (99%)	5 (1%)	67	68
1	C	420/425 (99%)	415 (99%)	5 (1%)	67	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	423/425 (100%)	419 (99%)	4 (1%)	75	77
All	All	1691/1700 (100%)	1671 (99%)	20 (1%)	67	68

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	507	GLU
1	A	547	ILE
1	A	625	ILE
1	A	703	LYS
1	A	745	ASN
1	A	845	LYS
1	B	413	VAL
1	B	517	LEU
1	B	547	ILE
1	B	703	LYS
1	B	819	ASP
1	C	517	LEU
1	C	547	ILE
1	C	658	ILE
1	C	703	LYS
1	C	819	ASP
1	D	547	ILE
1	D	703	LYS
1	D	745	ASN
1	D	845	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	706	ASN
1	A	745	ASN
1	A	750	ASN
1	B	407	ASN
1	B	600	GLN
1	B	706	ASN
1	B	750	ASN
1	C	600	GLN
1	C	706	ASN
1	D	407	ASN
1	D	548	ASN

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Mol	Chain	Res	Type
1	D	600	GLN
1	D	706	ASN
1	D	745	ASN
1	D	750	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](#)

32 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	$\# Z  > 2$
3	SO4	C	106	-	4,4,4	0.23	0	6,6,6	0.20	0
3	SO4	C	103	-	4,4,4	0.22	0	6,6,6	0.20	0
3	SO4	C	105	-	4,4,4	0.26	0	6,6,6	0.09	0
3	SO4	D	102	-	4,4,4	0.22	0	6,6,6	0.12	0
3	SO4	D	104	-	4,4,4	0.26	0	6,6,6	0.09	0
3	SO4	B	105	-	4,4,4	0.26	0	6,6,6	0.16	0
3	SO4	D	103	-	4,4,4	0.22	0	6,6,6	0.17	0
3	SO4	A	105	-	4,4,4	0.22	0	6,6,6	0.14	0
2	NAP	D	101	-	46,52,52	1.76	4 (8%)	61,80,80	1.23	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAP	A	101	-	46,52,52	1.72	4 (8%)	61,80,80	1.22	5 (8%)
3	SO4	B	102	-	4,4,4	0.26	0	6,6,6	0.08	0
3	SO4	B	104	-	4,4,4	0.25	0	6,6,6	0.12	0
3	SO4	A	102	-	4,4,4	0.24	0	6,6,6	0.06	0
3	SO4	C	104	-	4,4,4	0.24	0	6,6,6	0.15	0
4	GOL	D	107	-	5,5,5	0.36	0	5,5,5	0.24	0
3	SO4	A	107	-	4,4,4	0.24	0	6,6,6	0.39	0
4	GOL	A	108	-	5,5,5	0.37	0	5,5,5	0.32	0
3	SO4	D	105	-	4,4,4	0.23	0	6,6,6	0.10	0
3	SO4	D	106	-	4,4,4	0.24	0	6,6,6	0.34	0
3	SO4	A	106	-	4,4,4	0.24	0	6,6,6	0.10	0
4	GOL	C	109	-	5,5,5	0.35	0	5,5,5	0.27	0
3	SO4	B	107	-	4,4,4	0.32	0	6,6,6	0.31	0
3	SO4	B	103	-	4,4,4	0.23	0	6,6,6	0.17	0
3	SO4	C	108	-	4,4,4	0.30	0	6,6,6	0.24	0
3	SO4	B	106	-	4,4,4	0.24	0	6,6,6	0.13	0
2	NAP	B	101	-	46,52,52	1.77	4 (8%)	61,80,80	1.25	3 (4%)
3	SO4	A	103	-	4,4,4	0.23	0	6,6,6	0.30	0
4	GOL	B	108	-	5,5,5	0.32	0	5,5,5	0.30	0
3	SO4	C	102	-	4,4,4	0.24	0	6,6,6	0.08	0
2	NAP	C	101	-	46,52,52	1.78	4 (8%)	61,80,80	1.26	4 (6%)
3	SO4	A	104	-	4,4,4	0.25	0	6,6,6	0.12	0
3	SO4	C	107	-	4,4,4	0.20	0	6,6,6	0.35	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	NAP	B	101	-	-	6/31/67/67	0/5/5/5
4	GOL	B	108	-	-	3/4/4/4	-
4	GOL	C	109	-	-	4/4/4/4	-
2	NAP	D	101	-	-	6/31/67/67	0/5/5/5
2	NAP	C	101	-	-	7/31/67/67	0/5/5/5
2	NAP	A	101	-	-	6/31/67/67	0/5/5/5
4	GOL	D	107	-	-	1/4/4/4	-
4	GOL	A	108	-	-	2/4/4/4	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	101	NAP	O7N-C7N	9.30	1.41	1.24
2	B	101	NAP	O7N-C7N	9.29	1.41	1.24
2	D	101	NAP	O7N-C7N	9.27	1.41	1.24
2	A	101	NAP	O7N-C7N	9.08	1.41	1.24
2	C	101	NAP	C2A-N3A	4.33	1.38	1.32
2	D	101	NAP	C2A-N3A	4.27	1.38	1.32
2	B	101	NAP	C2A-N3A	3.93	1.38	1.32
2	A	101	NAP	C2A-N3A	3.83	1.38	1.32
2	A	101	NAP	C2A-N1A	2.58	1.38	1.33
2	C	101	NAP	C2N-N1N	2.55	1.37	1.35
2	D	101	NAP	C2N-N1N	2.52	1.37	1.35
2	B	101	NAP	C2A-N1A	2.50	1.38	1.33
2	C	101	NAP	C2A-N1A	2.48	1.38	1.33
2	D	101	NAP	C2A-N1A	2.43	1.38	1.33
2	B	101	NAP	C2N-N1N	2.42	1.37	1.35
2	A	101	NAP	C2N-N1N	2.27	1.37	1.35

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	101	NAP	N3A-C2A-N1A	-6.07	120.43	128.67
2	A	101	NAP	N3A-C2A-N1A	-5.92	120.64	128.67
2	B	101	NAP	N3A-C2A-N1A	-5.87	120.71	128.67
2	C	101	NAP	N3A-C2A-N1A	-5.84	120.75	128.67
2	B	101	NAP	O4B-C1B-N9A	4.49	114.70	108.75
2	C	101	NAP	O4B-C1B-N9A	4.33	114.49	108.75
2	D	101	NAP	O4B-C1B-N9A	4.00	114.05	108.75
2	A	101	NAP	O4B-C1B-N9A	3.74	113.71	108.75
2	C	101	NAP	C3N-C7N-N7N	2.23	120.48	117.74
2	A	101	NAP	C3N-C7N-N7N	2.18	120.42	117.74
2	D	101	NAP	O4B-C1B-C2B	-2.15	102.93	106.61
2	C	101	NAP	O4B-C1B-C2B	-2.15	102.95	106.61
2	A	101	NAP	O4B-C1B-C2B	-2.11	103.02	106.61
2	B	101	NAP	C1B-N9A-C4A	-2.09	122.98	126.64
2	A	101	NAP	C4A-C5A-N7A	-2.03	107.19	109.34

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	101	NAP	C5D-O5D-PN-O3
2	A	101	NAP	C5D-O5D-PN-O1N

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Mol	Chain	Res	Type	Atoms
2	B	101	NAP	C5D-O5D-PN-O3
2	B	101	NAP	C5D-O5D-PN-O1N
2	C	101	NAP	C5D-O5D-PN-O3
2	C	101	NAP	C5D-O5D-PN-O1N
2	D	101	NAP	C5D-O5D-PN-O3
2	D	101	NAP	C5D-O5D-PN-O1N
4	B	108	GOL	C1-C2-C3-O3
4	B	108	GOL	O2-C2-C3-O3
4	C	109	GOL	O1-C1-C2-C3
4	C	109	GOL	C1-C2-C3-O3
4	C	109	GOL	O2-C2-C3-O3
4	C	109	GOL	O1-C1-C2-O2
2	A	101	NAP	PN-O3-PA-O1A
2	B	101	NAP	PN-O3-PA-O1A
4	B	108	GOL	O1-C1-C2-O2
2	A	101	NAP	C4D-C5D-O5D-PN
2	C	101	NAP	C4D-C5D-O5D-PN
2	D	101	NAP	C4D-C5D-O5D-PN
2	B	101	NAP	C4D-C5D-O5D-PN
4	A	108	GOL	O1-C1-C2-O2
2	A	101	NAP	C5D-O5D-PN-O2N
2	B	101	NAP	C5D-O5D-PN-O2N
2	C	101	NAP	C5B-O5B-PA-O1A
2	C	101	NAP	C5D-O5D-PN-O2N
2	D	101	NAP	C5D-O5D-PN-O2N
4	D	107	GOL	O2-C2-C3-O3
2	C	101	NAP	PN-O3-PA-O2A
2	D	101	NAP	PN-O3-PA-O2A
2	A	101	NAP	PN-O3-PA-O2A
2	C	101	NAP	PN-O3-PA-O1A
2	D	101	NAP	PN-O3-PA-O1A
4	A	108	GOL	O2-C2-C3-O3
2	B	101	NAP	PN-O3-PA-O2A

There are no ring outliers.

7 monomers are involved in 28 short contacts:

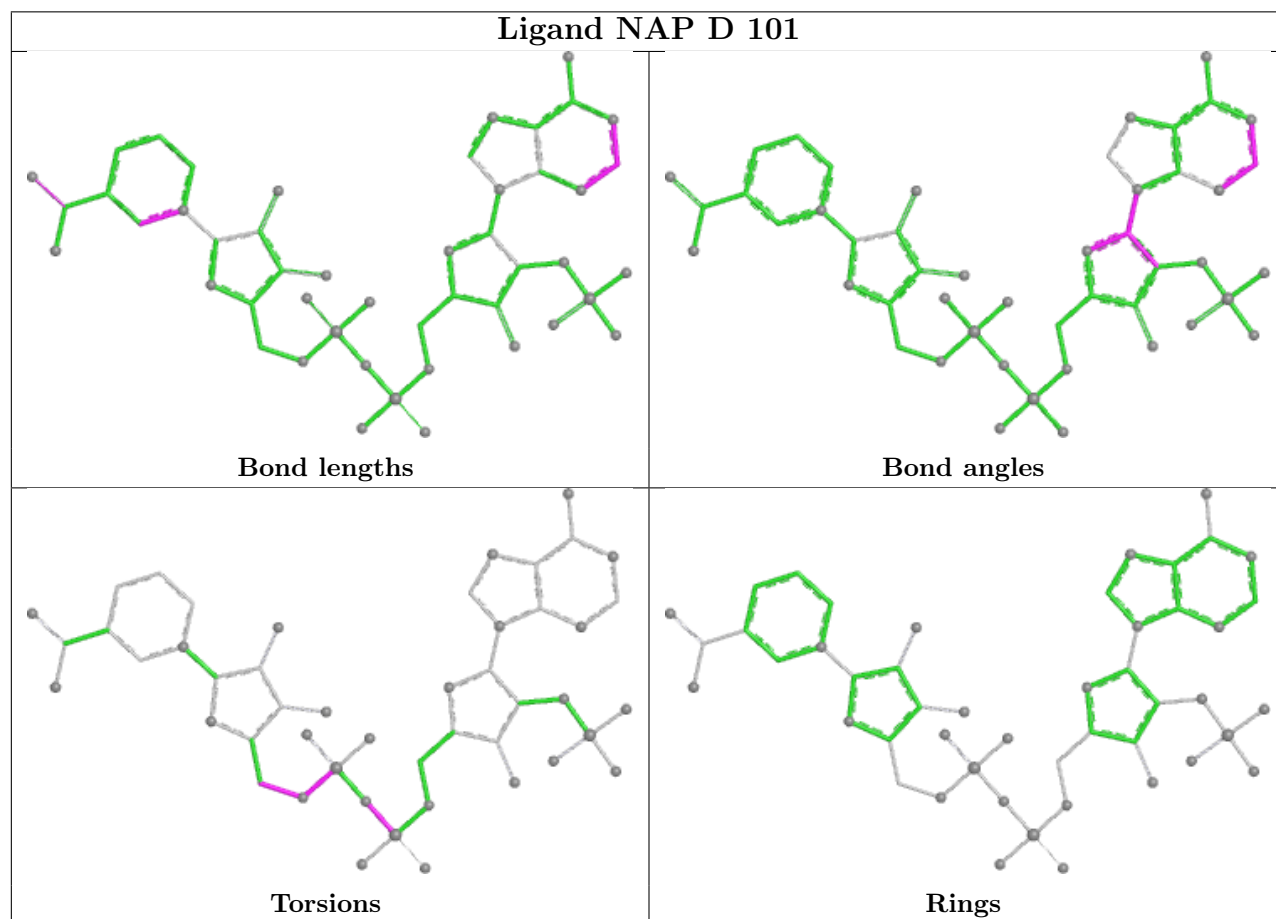
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	101	NAP	7	0
2	A	101	NAP	6	0
3	D	106	SO4	1	0
3	A	106	SO4	1	0

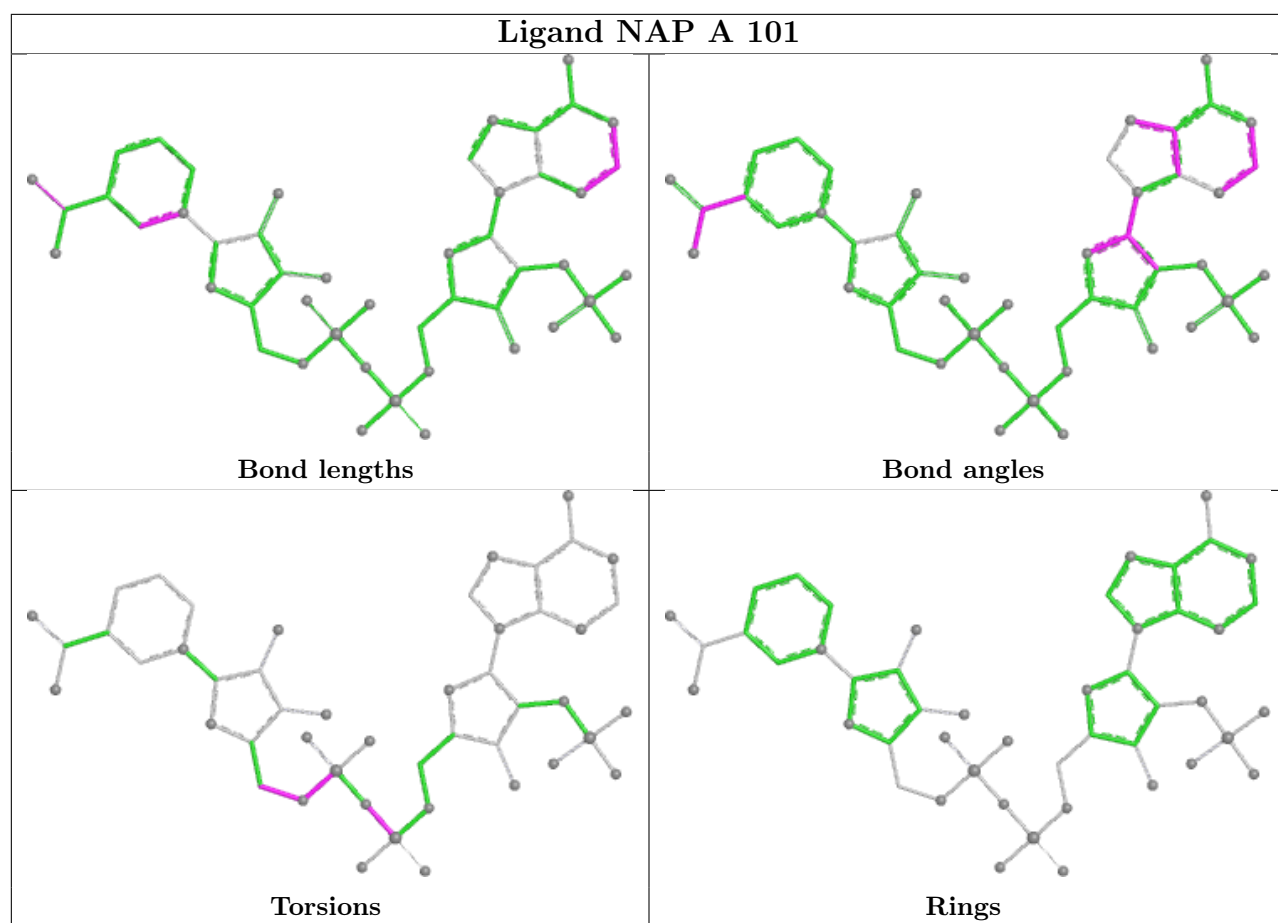
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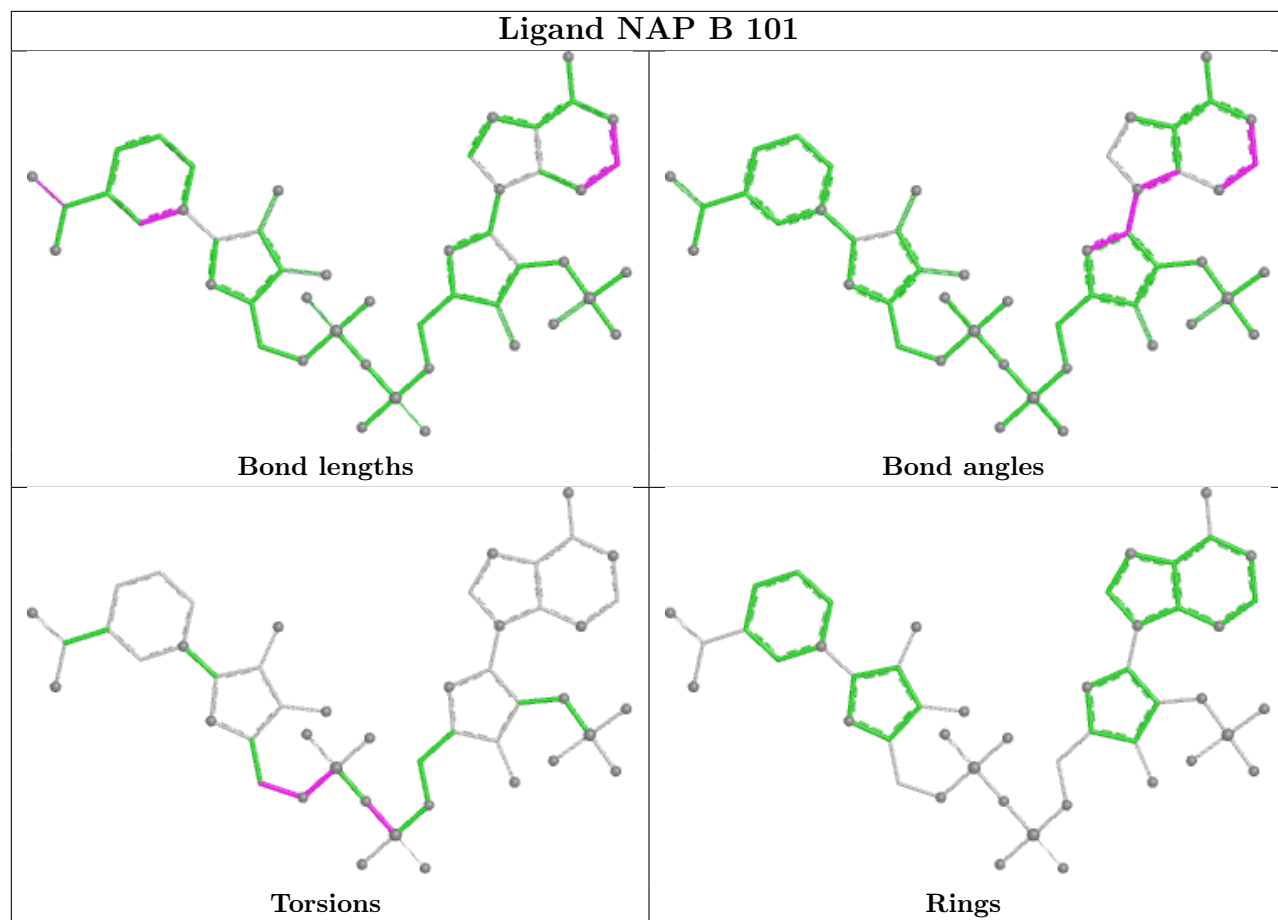
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	101	NAP	7	0
3	C	102	SO4	1	0
2	C	101	NAP	5	0

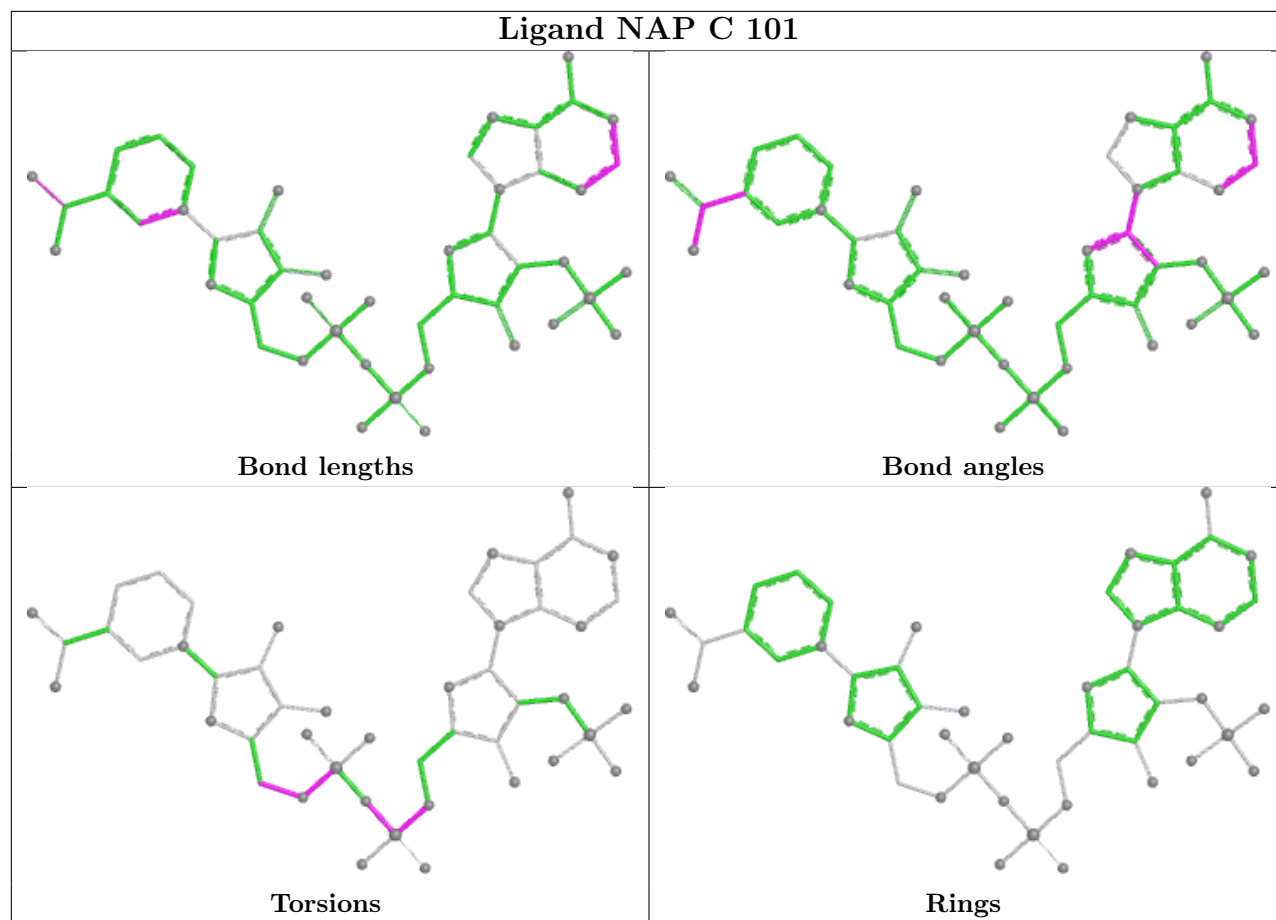
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	498/517 (96%)	0.40	23 (4%)	38 39	14, 34, 45, 52	36 (7%)
1	B	498/517 (96%)	0.44	14 (2%)	55 57	17, 36, 47, 58	36 (7%)
1	C	498/517 (96%)	0.22	15 (3%)	52 55	14, 31, 40, 51	33 (6%)
1	D	498/517 (96%)	0.34	13 (2%)	57 59	16, 34, 45, 56	36 (7%)
All	All	1992/2068 (96%)	0.35	65 (3%)	49 51	14, 34, 45, 58	141 (7%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	405	VAL	5.3
1	C	780	PRO	5.2
1	B	405	VAL	4.8
1	B	657[A]	HIS	4.7
1	D	657[A]	HIS	4.6
1	A	657[A]	HIS	4.2
1	C	405	VAL	4.2
1	C	571	ILE	4.0
1	C	657[A]	HIS	3.9
1	B	571	ILE	3.8
1	C	777	ASN	3.8
1	A	405	VAL	3.7
1	A	655	GLY	3.6
1	C	819	ASP	3.5
1	A	571	ILE	3.4
1	B	620[A]	LYS	3.4
1	D	571	ILE	3.4
1	B	569	ILE	3.2
1	D	620[A]	LYS	3.2
1	A	652	THR	3.0
1	C	569	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	829[A]	ALA	2.9
1	D	569	ILE	2.9
1	B	742	ARG	2.8
1	B	819	ASP	2.8
1	A	569	ILE	2.8
1	D	742	ARG	2.7
1	A	820	VAL	2.7
1	A	819	ASP	2.7
1	A	772	LEU	2.7
1	A	756[A]	ARG	2.6
1	D	550	ALA	2.6
1	A	773	VAL	2.6
1	A	434	GLU	2.6
1	B	818	GLY	2.6
1	C	756	ARG	2.5
1	A	794	VAL	2.5
1	C	820	VAL	2.5
1	A	742	ARG	2.5
1	A	890	ASN	2.5
1	C	818	GLY	2.4
1	D	819	ASP	2.4
1	A	818	GLY	2.4
1	B	408	TYR	2.3
1	B	520	LYS	2.3
1	C	757	LYS	2.3
1	A	509	LEU	2.3
1	D	745	ASN	2.2
1	B	814	ARG	2.2
1	C	843	ILE	2.2
1	C	760	GLU	2.2
1	B	494	ASP	2.1
1	D	415	LYS	2.1
1	A	731	VAL	2.1
1	A	620[A]	LYS	2.1
1	D	793	ASP	2.1
1	C	652	THR	2.1
1	A	841[A]	ARG	2.1
1	D	773	VAL	2.0
1	A	632	LEU	2.0
1	B	632	LEU	2.0
1	A	478	GLY	2.0
1	D	851	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	620[A]	LYS	2.0
1	A	764	ARG	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, 95<sup>th</sup> 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.

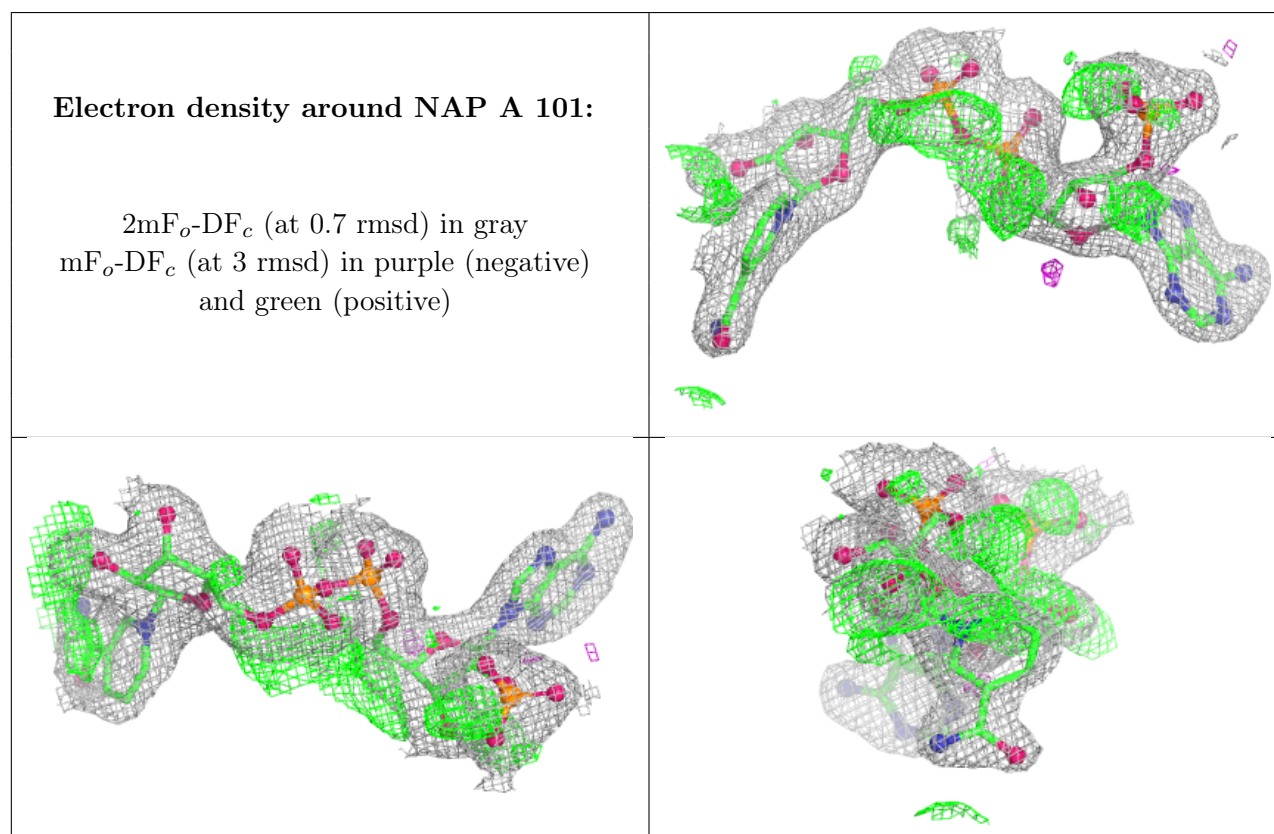
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	A	105	5/5	0.73	0.29	62,63,64,64	5
3	SO4	D	105	5/5	0.74	0.22	57,57,57,57	5
3	SO4	D	104	5/5	0.76	0.20	57,58,58,58	5
3	SO4	A	107	5/5	0.78	0.19	44,50,51,51	5
3	SO4	C	104	5/5	0.80	0.17	55,55,56,56	5
3	SO4	B	107	5/5	0.82	0.18	48,53,55,56	5
3	SO4	B	105	5/5	0.82	0.21	56,57,57,57	5
3	SO4	D	106	5/5	0.83	0.18	51,56,56,57	5
3	SO4	B	104	5/5	0.85	0.17	55,56,56,57	5
3	SO4	C	107	5/5	0.86	0.17	48,52,54,54	5
3	SO4	A	106	5/5	0.87	0.21	57,57,57,57	5
3	SO4	A	104	5/5	0.88	0.13	53,54,55,55	5
4	GOL	A	108	6/6	0.88	0.24	70,71,71,72	0
4	GOL	D	107	6/6	0.88	0.24	79,80,80,81	0
3	SO4	D	102	5/5	0.89	0.13	46,46,47,47	5
4	GOL	B	108	6/6	0.89	0.24	75,75,76,76	0
3	SO4	B	106	5/5	0.89	0.19	51,52,52,52	5
3	SO4	C	105	5/5	0.90	0.17	58,59,59,60	5
4	GOL	C	109	6/6	0.90	0.23	79,79,80,81	0
3	SO4	C	106	5/5	0.90	0.15	54,55,55,56	5
3	SO4	A	102	5/5	0.91	0.14	52,52,53,53	5

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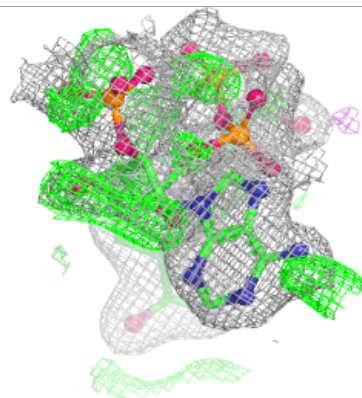
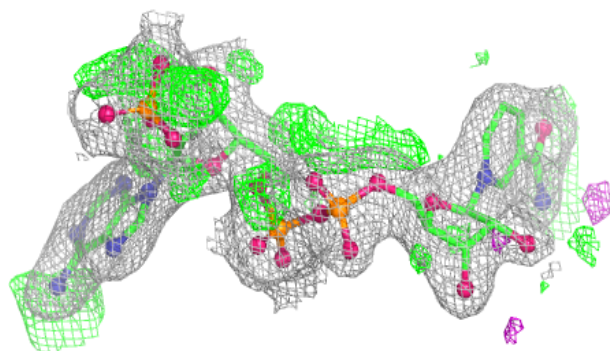
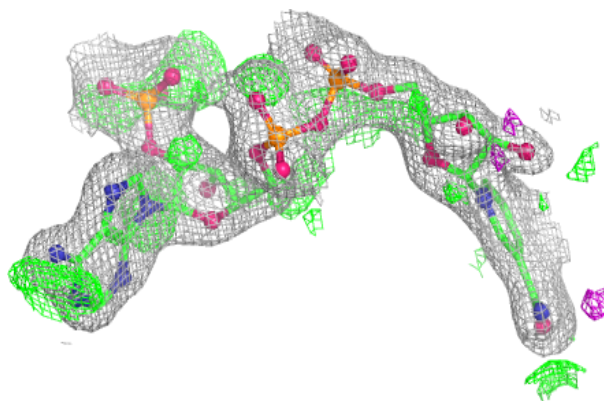
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	B	102	5/5	0.91	0.14	39,39,39,40	5
3	SO4	C	102	5/5	0.91	0.12	50,51,51,51	5
3	SO4	A	103	5/5	0.92	0.11	48,48,50,51	5
3	SO4	B	103	5/5	0.93	0.09	58,58,59,59	5
3	SO4	D	103	5/5	0.93	0.10	48,49,50,50	5
2	NAP	A	101	48/48	0.93	0.12	34,38,40,42	48
2	NAP	D	101	48/48	0.94	0.12	31,36,41,43	48
2	NAP	B	101	48/48	0.94	0.11	35,40,44,45	48
3	SO4	C	108	5/5	0.94	0.09	43,45,46,46	5
2	NAP	C	101	48/48	0.95	0.10	29,33,38,41	48
3	SO4	C	103	5/5	0.96	0.08	48,49,49,50	5

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.

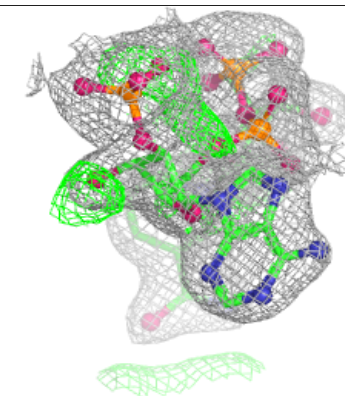
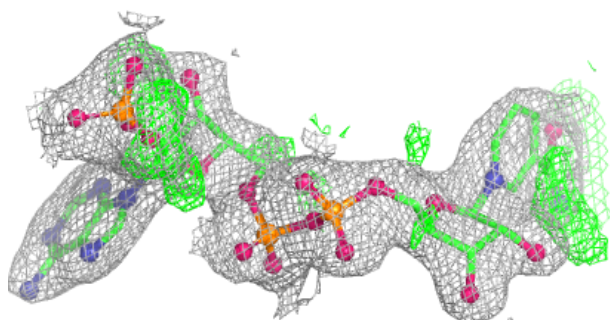
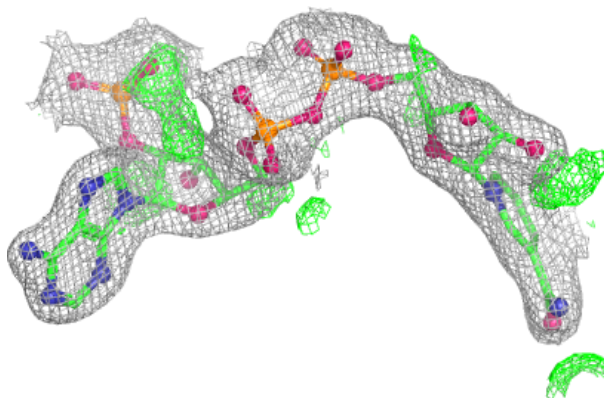


**Electron density around NAP D 101:**

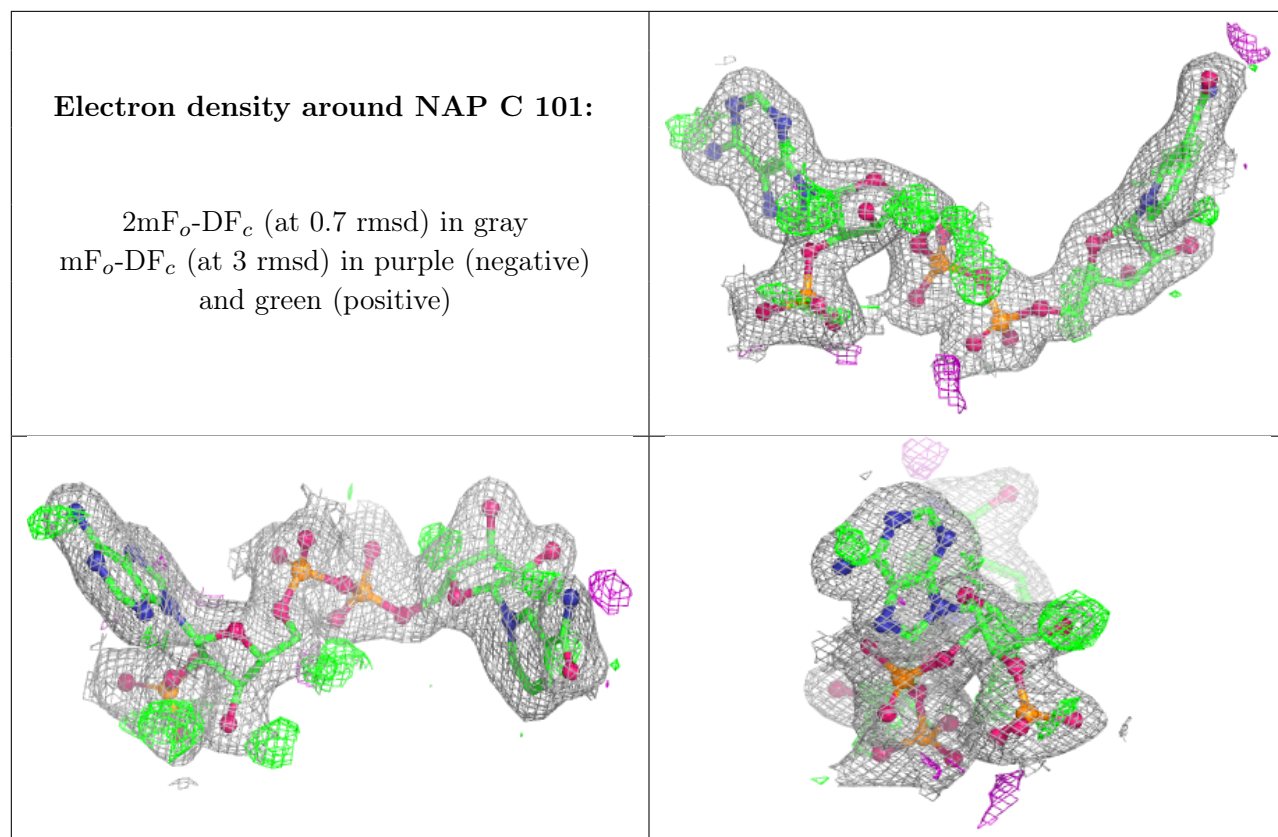
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around NAP B 101:**

$2mF_o-DF_c$  (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.