



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2021 – 05:18 PM EDT

PDB ID : 3FLK  
Title : Crystal Structure of Tartrate Dehydrogenase from *Pseudomonas putida* in complex with NADH, oxalate and metal ion  
Authors : Malik, R.; Viola, R.E.  
Deposited on : 2008-12-18  
Resolution : 2.00 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
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) : 2.23.2

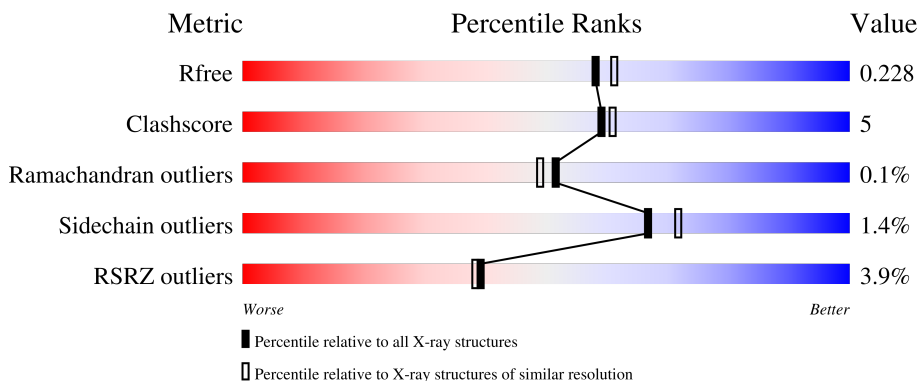
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	364	 4% 92% 6%
1	B	364	 3% 88% 10%
1	C	364	 5% 90% 8%
1	D	364	 3% 91% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	DTT	B	407	X	-	-	-
7	DTT	C	409	X	-	-	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12469 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 Tartrate dehydrogenase/decarboxylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	359	2809	1789	483	523	4	10	0	0	0
1	B	359	2813	1792	484	523	4	10	0	0	0
1	C	359	2813	1792	484	523	4	10	0	0	0
1	D	359	2813	1792	484	523	4	10	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	GLY	ASP	engineered mutation	UNP Q51945
A	?	-	VAL	deletion	UNP Q51945
B	79	GLY	ASP	engineered mutation	UNP Q51945
B	?	-	VAL	deletion	UNP Q51945
C	79	GLY	ASP	engineered mutation	UNP Q51945
C	?	-	VAL	deletion	UNP Q51945
D	79	GLY	ASP	engineered mutation	UNP Q51945
D	?	-	VAL	deletion	UNP Q51945

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

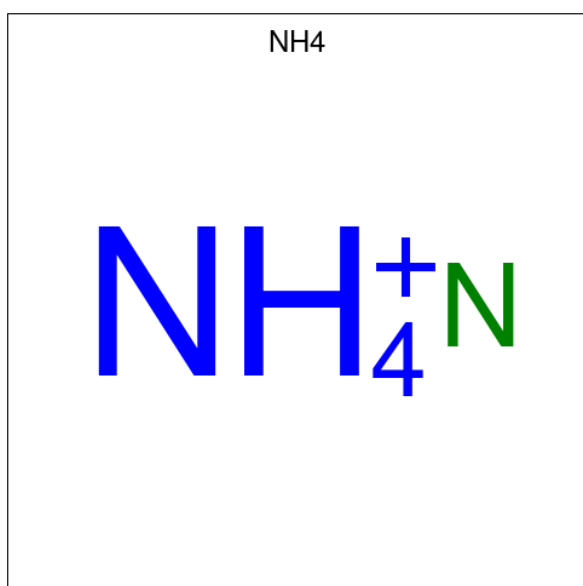
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		
2	C	2	Total	Mg	0	0
			2	2		

- Molecule 3 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C<sub>21</sub>H<sub>29</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



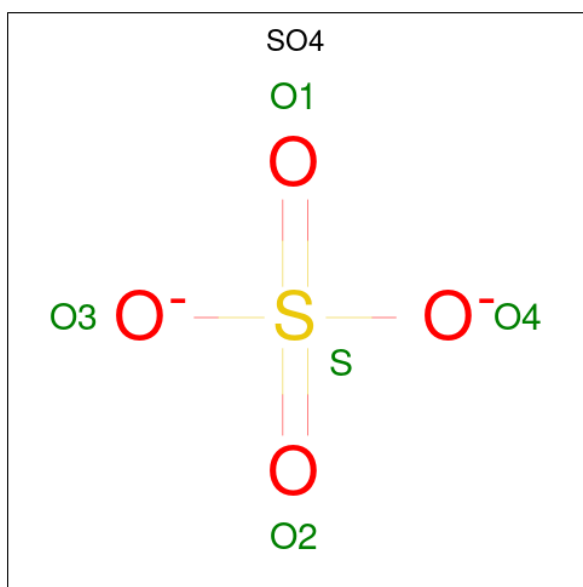
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 2 4	0	0
4	B	1	Total C O 6 2 4	0	0
4	C	1	Total C O 6 2 4	0	0
4	D	1	Total C O 6 2 4	0	0

- Molecule 5 is AMMONIUM ION (three-letter code: NH4) (formula: H<sub>4</sub>N).



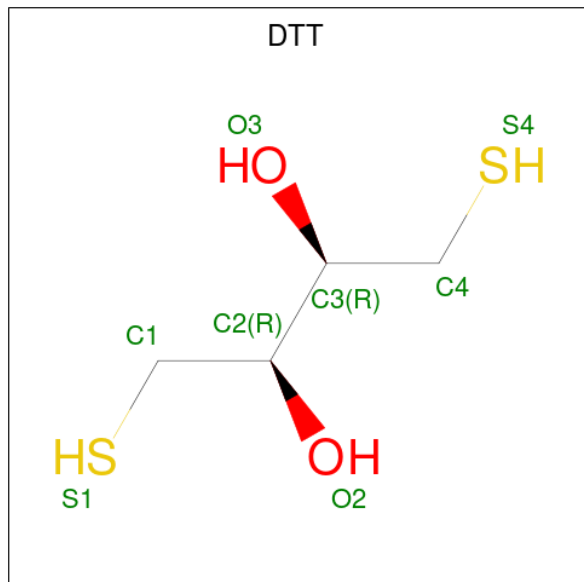
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total N 1 1	0	0
5	B	1	Total N 1 1	0	0
5	C	1	Total N 1 1	0	0
5	D	1	Total N 1 1	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 7 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula:  $C_4H_{10}O_2S_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	O	S	0	0
			8	4	2	2		
7	C	1	Total	C	O	S	0	0
			8	4	2	2		
7	D	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 8 is water.

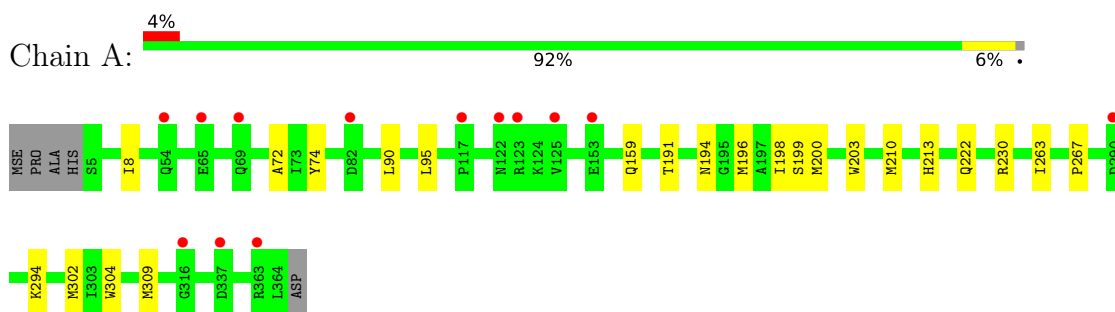
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	238	Total	O	0	0
			238	238		
8	B	217	Total	O	0	0
			217	217		
8	C	180	Total	O	0	0
			180	180		
8	D	284	Total	O	0	0
			284	284		



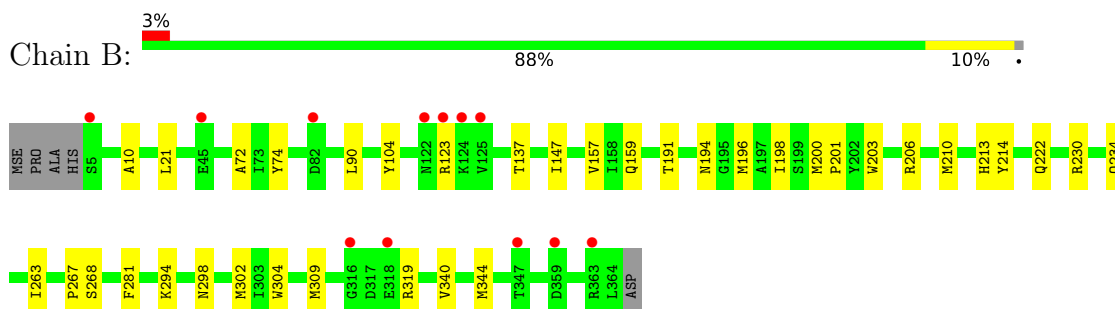
### 3 Residue-property plots [i](#)

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.

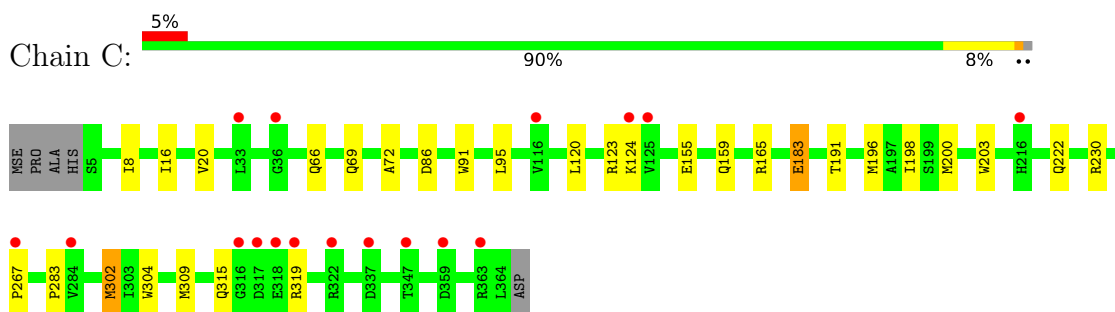
- Molecule 1: Tartrate dehydrogenase/decarboxylase



- Molecule 1: Tartrate dehydrogenase/decarboxylase

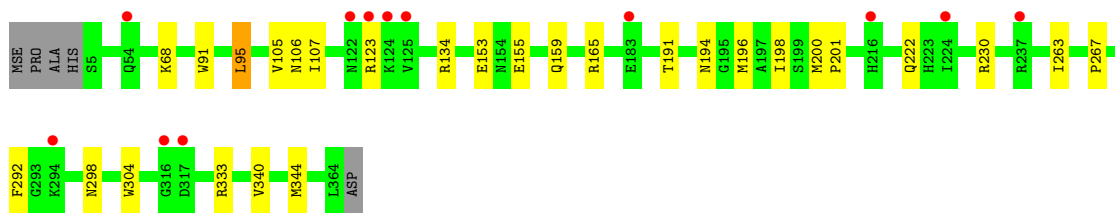


- Molecule 1: Tartrate dehydrogenase/decarboxylase



- Molecule 1: Tartrate dehydrogenase/decarboxylase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.28Å 117.28Å 291.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 35.63 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-2.00) 99.0 (35.63-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.95 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.208 , 0.227 0.209 , 0.228	Depositor DCC
$R_{free}$ test set	6868 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.8	Xtrriage
Anisotropy	0.152	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 47.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12469	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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: OXL, NAI, SO4, NH4, DTT, 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	0.34	0/2868	0.48	0/3877
1	B	0.33	0/2872	0.47	0/3881
1	C	0.33	0/2872	0.48	0/3881
1	D	0.35	0/2872	0.51	0/3881
All	All	0.34	0/11484	0.49	0/15520

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	2809	0	2735	26	0
1	B	2813	0	2746	38	0
1	C	2813	0	2746	29	0
1	D	2813	0	2746	25	0
2	A	2	0	0	0	0
2	C	2	0	0	0	0
3	A	44	0	27	0	0
3	B	44	0	27	0	0
3	C	44	0	27	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	44	0	27	0	0
4	A	6	0	0	0	0
4	B	6	0	0	0	0
4	C	6	0	0	0	0
4	D	6	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	20	0	0	0	0
6	B	15	0	0	0	0
6	C	15	0	0	0	0
6	D	20	0	0	0	0
7	B	8	0	10	1	0
7	C	8	0	10	0	0
7	D	8	0	10	1	0
8	A	238	0	0	1	0
8	B	217	0	0	1	0
8	C	180	0	0	2	0
8	D	284	0	0	3	0
All	All	12469	0	11111	107	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 5.

All (107) 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:72:ALA:HB3	1:A:309:MSE:HE3	1.21	1.16
1:A:8:ILE:HD12	1:A:309:MSE:HE2	1.38	1.04
1:C:72:ALA:HB3	1:C:309:MSE:HE3	1.38	1.01
1:C:8:ILE:HD12	1:C:309:MSE:HE2	1.51	0.92
1:C:8:ILE:HG23	1:C:309:MSE:HE1	1.53	0.91
1:A:72:ALA:CB	1:A:309:MSE:HE3	2.00	0.91
1:A:8:ILE:HG23	1:A:309:MSE:HE1	1.51	0.90
1:B:191:THR:HA	1:B:200:MSE:HE2	1.57	0.86
1:C:72:ALA:CB	1:C:309:MSE:HE3	2.05	0.86
1:B:340:VAL:HB	1:B:344:MSE:HE3	1.63	0.81
1:D:340:VAL:HB	1:D:344:MSE:HE3	1.62	0.79
1:C:191:THR:OG1	1:C:200:MSE:HE2	1.83	0.79
1:D:344:MSE:CE	8:D:712:HOH:O	2.30	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:191:THR:HA	1:D:200:MSE:HE2	1.65	0.78
1:A:8:ILE:HD12	1:A:309:MSE:CE	2.16	0.76
1:D:344:MSE:HE1	8:D:712:HOH:O	1.85	0.76
1:A:72:ALA:HB3	1:A:309:MSE:CE	2.12	0.73
1:A:191:THR:OG1	1:A:200:MSE:HE2	1.88	0.73
1:B:210:MSE:HE2	1:B:214:TYR:HE2	1.54	0.73
1:C:72:ALA:HB3	1:C:309:MSE:CE	2.17	0.70
1:B:298:ASN:ND2	1:B:344:MSE:HE2	2.06	0.69
1:D:298:ASN:ND2	1:D:344:MSE:HE2	2.08	0.69
1:C:183:GLU:H	1:C:183:GLU:CD	1.96	0.68
1:B:210:MSE:HE2	1:B:214:TYR:CE2	2.28	0.68
1:A:200:MSE:HE1	1:A:203:TRP:CD1	2.29	0.67
1:B:191:THR:CA	1:B:200:MSE:HE2	2.24	0.66
1:B:191:THR:OG1	1:B:200:MSE:HE2	1.98	0.63
1:C:159:GLN:HE22	1:D:198:ILE:H	1.46	0.63
1:A:210:MSE:HA	1:A:210:MSE:HE3	1.80	0.62
1:B:281:PHE:HB2	1:B:309:MSE:HE3	1.84	0.59
1:B:281:PHE:CD2	1:B:309:MSE:HE3	2.37	0.59
1:D:191:THR:CA	1:D:200:MSE:HE2	2.32	0.59
1:B:191:THR:HA	1:B:200:MSE:CE	2.32	0.58
1:B:200:MSE:HE1	1:B:203:TRP:CD1	2.39	0.58
1:A:191:THR:HA	1:A:200:MSE:HE2	1.85	0.58
1:B:210:MSE:SE	8:B:707:HOH:O	2.73	0.56
1:A:159:GLN:HE22	1:B:198:ILE:H	1.51	0.56
1:D:191:THR:OG1	1:D:200:MSE:HE2	2.05	0.56
1:C:20:VAL:CG2	1:C:302:MSE:HG3	2.36	0.55
1:C:200:MSE:HE1	1:C:203:TRP:CD1	2.42	0.54
1:B:10:ALA:HB1	1:B:21:LEU:HD21	1.90	0.54
1:C:198:ILE:H	1:D:159:GLN:HE22	1.54	0.54
1:C:8:ILE:HD12	1:C:309:MSE:CE	2.29	0.53
1:C:283:PRO:HD3	1:C:302:MSE:HE3	1.89	0.53
1:C:200:MSE:HE3	1:C:203:TRP:HB3	1.90	0.53
1:B:72:ALA:HB1	1:B:309:MSE:HE2	1.89	0.53
1:B:206:ARG:HH12	7:B:407:DTT:H41	1.74	0.53
8:C:562:HOH:O	1:D:153:GLU:HG3	2.10	0.52
1:C:267:PRO:HG3	1:C:304:TRP:CD2	2.45	0.52
1:A:194:ASN:HB2	1:B:90:LEU:HD22	1.91	0.52
1:C:20:VAL:HG23	1:C:302:MSE:HG3	1.92	0.51
1:D:267:PRO:HG3	1:D:304:TRP:CD2	2.46	0.50
1:B:196:MSE:HE2	1:B:200:MSE:HG2	1.92	0.50
1:D:222:GLN:HE22	1:D:230:ARG:HD2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:GLN:NE2	1:C:230:ARG:HD2	2.27	0.50
1:A:90:LEU:HD22	1:B:194:ASN:HB2	1.93	0.50
1:D:91:TRP:CD2	1:D:95:LEU:HD23	2.46	0.50
1:B:230:ARG:HD3	1:B:234:GLN:HE21	1.78	0.48
1:A:267:PRO:HG3	1:A:304:TRP:CD2	2.48	0.48
1:B:222:GLN:HE22	1:B:230:ARG:HD2	1.77	0.48
1:C:191:THR:HA	1:C:200:MSE:HE2	1.96	0.48
1:B:74:TYR:CE1	1:B:302:MSE:HE2	2.49	0.48
1:C:16:ILE:O	1:C:20:VAL:HG22	2.14	0.48
1:A:199:SER:H	1:B:159:GLN:NE2	2.11	0.48
1:B:222:GLN:NE2	1:B:230:ARG:HD2	2.30	0.47
1:D:91:TRP:CE2	1:D:95:LEU:HD23	2.50	0.47
1:C:222:GLN:HE22	1:C:230:ARG:HD2	1.79	0.47
1:A:198:ILE:H	1:B:159:GLN:NE2	2.13	0.47
1:C:155:GLU:HB3	1:D:165:ARG:HB2	1.97	0.47
1:A:191:THR:CB	1:A:200:MSE:HE2	2.44	0.46
1:A:191:THR:CA	1:A:200:MSE:HE2	2.46	0.46
1:A:196:MSE:HE2	1:A:200:MSE:HG2	1.97	0.46
1:B:298:ASN:HD21	1:B:344:MSE:HE2	1.80	0.46
1:B:267:PRO:HG3	1:B:304:TRP:CD2	2.50	0.46
1:B:191:THR:CB	1:B:200:MSE:HE2	2.46	0.45
1:C:86:ASP:HB3	1:D:194:ASN:HB3	1.99	0.45
1:C:191:THR:CB	1:C:200:MSE:HE2	2.46	0.45
1:B:281:PHE:CD2	1:B:309:MSE:CE	3.00	0.45
1:A:74:TYR:CE1	1:A:302:MSE:HE2	2.52	0.45
1:D:191:THR:HA	1:D:200:MSE:CE	2.42	0.44
1:A:210:MSE:HE2	1:A:213:HIS:HB2	1.99	0.44
1:A:222:GLN:NE2	1:A:230:ARG:HD2	2.31	0.44
1:D:292:PHE:CE2	7:D:408:DTT:H11	2.52	0.44
1:A:196:MSE:HE3	8:A:672:HOH:O	2.18	0.44
1:D:196:MSE:HE3	8:D:715:HOH:O	2.18	0.44
1:B:147:ILE:HG13	1:B:157:VAL:HG22	1.99	0.43
1:D:191:THR:CB	1:D:200:MSE:HE2	2.48	0.43
1:A:222:GLN:HE22	1:A:230:ARG:HD2	1.84	0.43
1:B:281:PHE:HD2	1:B:309:MSE:CE	2.31	0.43
1:A:200:MSE:HE3	1:A:203:TRP:HB3	1.99	0.43
1:B:210:MSE:CE	1:B:213:HIS:HB2	2.49	0.43
1:A:198:ILE:HB	1:B:159:GLN:HE21	1.84	0.43
1:C:196:MSE:HE2	1:C:200:MSE:HG2	2.00	0.43
1:C:91:TRP:CE2	1:C:95:LEU:HD23	2.55	0.42
1:C:196:MSE:HE3	8:C:679:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:MSE:O	1:D:201:PRO:HD3	2.20	0.42
1:D:222:GLN:NE2	1:D:230:ARG:HD2	2.34	0.41
1:B:267:PRO:HG3	1:B:304:TRP:CG	2.56	0.41
1:B:281:PHE:HD2	1:B:309:MSE:HE3	1.81	0.41
1:C:165:ARG:HB2	1:D:155:GLU:HB3	2.03	0.41
1:C:120:LEU:HB2	1:C:123:ARG:HG3	2.02	0.41
1:B:196:MSE:O	1:B:201:PRO:HD3	2.21	0.41
1:D:105:VAL:HG12	1:D:107:ILE:HG12	2.02	0.41
1:C:66:GLN:O	1:C:69:GLN:HG2	2.21	0.41
1:B:104:TYR:HA	1:B:137:THR:HG23	2.03	0.40
1:D:106:ASN:HB3	1:D:134:ARG:HB3	2.03	0.40
1:B:191:THR:OG1	1:B:200:MSE:CE	2.67	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	357/364 (98%)	349 (98%)	8 (2%)	0	100	100
1	B	357/364 (98%)	347 (97%)	10 (3%)	0	100	100
1	C	357/364 (98%)	346 (97%)	10 (3%)	1 (0%)	41	37
1	D	357/364 (98%)	348 (98%)	9 (2%)	0	100	100
All	All	1428/1456 (98%)	1390 (97%)	37 (3%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	315	GLN



### 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	294/288 (102%)	291 (99%)	3 (1%)	76	81
1	B	295/288 (102%)	290 (98%)	5 (2%)	60	65
1	C	295/288 (102%)	291 (99%)	4 (1%)	67	72
1	D	295/288 (102%)	290 (98%)	5 (2%)	60	65
All	All	1179/1152 (102%)	1162 (99%)	17 (1%)	67	72

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	LEU
1	A	263	ILE
1	A	294	LYS
1	B	123	ARG
1	B	263	ILE
1	B	268	SER
1	B	294	LYS
1	B	319	ARG
1	C	124	LYS
1	C	183	GLU
1	C	302	MSE
1	C	319	ARG
1	D	68	LYS
1	D	95	LEU
1	D	123	ARG
1	D	263	ILE
1	D	333	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	159	GLN
1	A	186	HIS

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Mol	Chain	Res	Type
1	A	222	GLN
1	B	159	GLN
1	B	222	GLN
1	B	234	GLN
1	C	69	GLN
1	C	159	GLN
1	C	222	GLN
1	D	159	GLN
1	D	222	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 4 are monoatomic and 4 are modelled with single atom - leaving 25 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	$\# Z  > 2$
6	SO4	C	407	-	4,4,4	0.14	0	6,6,6	0.04	0
4	OXL	B	402	2	0,5,5	-	-	0,6,6	-	-
6	SO4	B	405	-	4,4,4	0.14	0	6,6,6	0.06	0
4	OXL	C	403	2	0,5,5	-	-	0,6,6	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	SO4	B	404	-	4,4,4	0.15	0	6,6,6	0.06	0
6	SO4	B	406	-	4,4,4	0.13	0	6,6,6	0.05	0
7	DTT	C	409	-	7,7,7	0.59	0	4,8,8	0.26	0
6	SO4	A	409	-	4,4,4	0.14	0	6,6,6	0.05	0
7	DTT	B	407	-	7,7,7	0.60	0	4,8,8	0.37	0
6	SO4	A	407	-	4,4,4	0.14	0	6,6,6	0.05	0
6	SO4	D	407	-	4,4,4	0.14	0	6,6,6	0.06	0
6	SO4	D	404	-	4,4,4	0.14	0	6,6,6	0.08	0
4	OXL	A	403	2	0,5,5	-	-	0,6,6	-	-
3	NAI	C	402	-	42,48,48	1.87	6 (14%)	47,73,73	1.18	2 (4%)
7	DTT	D	408	-	7,7,7	0.55	0	4,8,8	0.54	0
6	SO4	C	406	-	4,4,4	0.14	0	6,6,6	0.05	0
3	NAI	B	401	-	42,48,48	1.87	6 (14%)	47,73,73	1.16	1 (2%)
6	SO4	C	408	-	4,4,4	0.14	0	6,6,6	0.05	0
6	SO4	A	408	-	4,4,4	0.14	0	6,6,6	0.07	0
6	SO4	D	405	-	4,4,4	0.15	0	6,6,6	0.04	0
3	NAI	D	401	-	42,48,48	1.86	6 (14%)	47,73,73	1.18	2 (4%)
6	SO4	A	406	-	4,4,4	0.14	0	6,6,6	0.09	0
6	SO4	D	406	-	4,4,4	0.13	0	6,6,6	0.05	0
4	OXL	D	402	2	0,5,5	-	-	0,6,6	-	-
3	NAI	A	402	-	42,48,48	1.88	6 (14%)	47,73,73	1.18	2 (4%)

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	NAI	C	402	-	-	6/25/72/72	0/5/5/5
7	DTT	D	408	-	-	1/8/8/8	-
3	NAI	D	401	-	-	3/25/72/72	0/5/5/5
4	OXL	B	402	2	-	0/0/4/4	-
7	DTT	B	407	-	1/1/2/2	2/8/8/8	-
3	NAI	B	401	-	-	6/25/72/72	0/5/5/5
4	OXL	C	403	2	-	0/0/4/4	-
4	OXL	D	402	2	-	0/0/4/4	-
7	DTT	C	409	-	1/1/2/2	3/8/8/8	-
3	NAI	A	402	-	-	4/25/72/72	0/5/5/5
4	OXL	A	403	2	-	0/0/4/4	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	NAI	O7N-C7N	7.20	1.41	1.24
3	C	402	NAI	O7N-C7N	7.17	1.41	1.24
3	B	401	NAI	O7N-C7N	7.11	1.41	1.24
3	D	401	NAI	O7N-C7N	7.04	1.41	1.24
3	D	401	NAI	C4N-C3N	-5.08	1.39	1.49
3	A	402	NAI	C4N-C3N	-5.07	1.40	1.49
3	B	401	NAI	C4N-C3N	-5.03	1.40	1.49
3	C	402	NAI	C4N-C3N	-5.01	1.40	1.49
3	D	401	NAI	C2A-N3A	4.15	1.38	1.32
3	B	401	NAI	C2A-N3A	4.12	1.38	1.32
3	C	402	NAI	C2A-N3A	4.12	1.38	1.32
3	A	402	NAI	C2A-N3A	4.08	1.38	1.32
3	A	402	NAI	C6N-C5N	3.69	1.39	1.33
3	B	401	NAI	C6N-C5N	3.67	1.39	1.33
3	C	402	NAI	C6N-C5N	3.55	1.39	1.33
3	D	401	NAI	C6N-C5N	3.55	1.39	1.33
3	C	402	NAI	C4N-C5N	-3.46	1.39	1.48
3	A	402	NAI	C4N-C5N	-3.43	1.39	1.48
3	D	401	NAI	C4N-C5N	-3.42	1.40	1.48
3	B	401	NAI	C4N-C5N	-3.36	1.40	1.48
3	B	401	NAI	C2A-N1A	2.60	1.38	1.33
3	C	402	NAI	C2A-N1A	2.59	1.38	1.33
3	D	401	NAI	C2A-N1A	2.56	1.38	1.33
3	A	402	NAI	C2A-N1A	2.37	1.38	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	NAI	N3A-C2A-N1A	-5.83	119.56	128.68
3	D	401	NAI	N3A-C2A-N1A	-5.81	119.61	128.68
3	C	402	NAI	N3A-C2A-N1A	-5.77	119.66	128.68
3	B	401	NAI	N3A-C2A-N1A	-5.61	119.91	128.68
3	A	402	NAI	C1D-N1N-C2N	-2.37	117.16	121.11
3	D	401	NAI	C1D-N1N-C2N	-2.17	117.49	121.11
3	C	402	NAI	C1D-N1N-C2N	-2.02	117.75	121.11

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	B	407	DTT	C3
7	C	409	DTT	C3

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	NAI	C5D-O5D-PN-O1N
3	C	402	NAI	C5D-O5D-PN-O1N
7	B	407	DTT	S1-C1-C2-O2
7	B	407	DTT	S1-C1-C2-C3
7	C	409	DTT	C1-C2-C3-C4
7	C	409	DTT	C2-C3-C4-S4
7	C	409	DTT	O3-C3-C4-S4
3	A	402	NAI	PN-O3-PA-O5B
3	B	401	NAI	C5D-O5D-PN-O3
3	C	402	NAI	C5D-O5D-PN-O3
7	D	408	DTT	O3-C3-C4-S4
3	B	401	NAI	O4D-C1D-N1N-C2N
3	C	402	NAI	O4D-C1D-N1N-C2N
3	A	402	NAI	O4D-C1D-N1N-C2N
3	D	401	NAI	O4D-C1D-N1N-C2N
3	B	401	NAI	C2D-C1D-N1N-C2N
3	C	402	NAI	C2D-C1D-N1N-C2N
3	A	402	NAI	C2D-C1D-N1N-C2N
3	D	401	NAI	C2D-C1D-N1N-C2N
3	D	401	NAI	C5D-O5D-PN-O3
3	A	402	NAI	C5B-O5B-PA-O1A
3	B	401	NAI	C5B-O5B-PA-O1A
3	B	401	NAI	C5D-O5D-PN-O2N
3	C	402	NAI	C5B-O5B-PA-O1A
3	C	402	NAI	C5D-O5D-PN-O2N

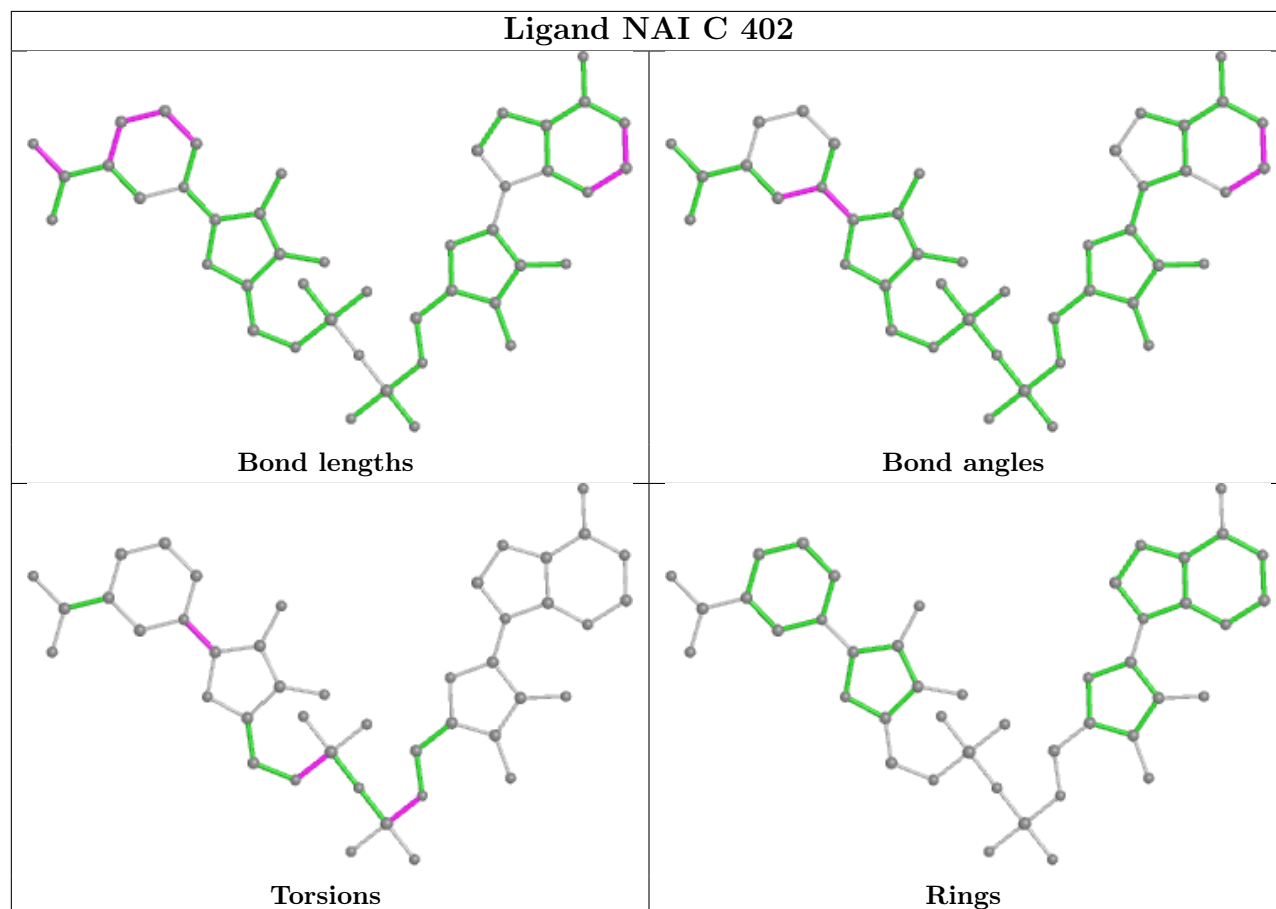
There are no ring outliers.

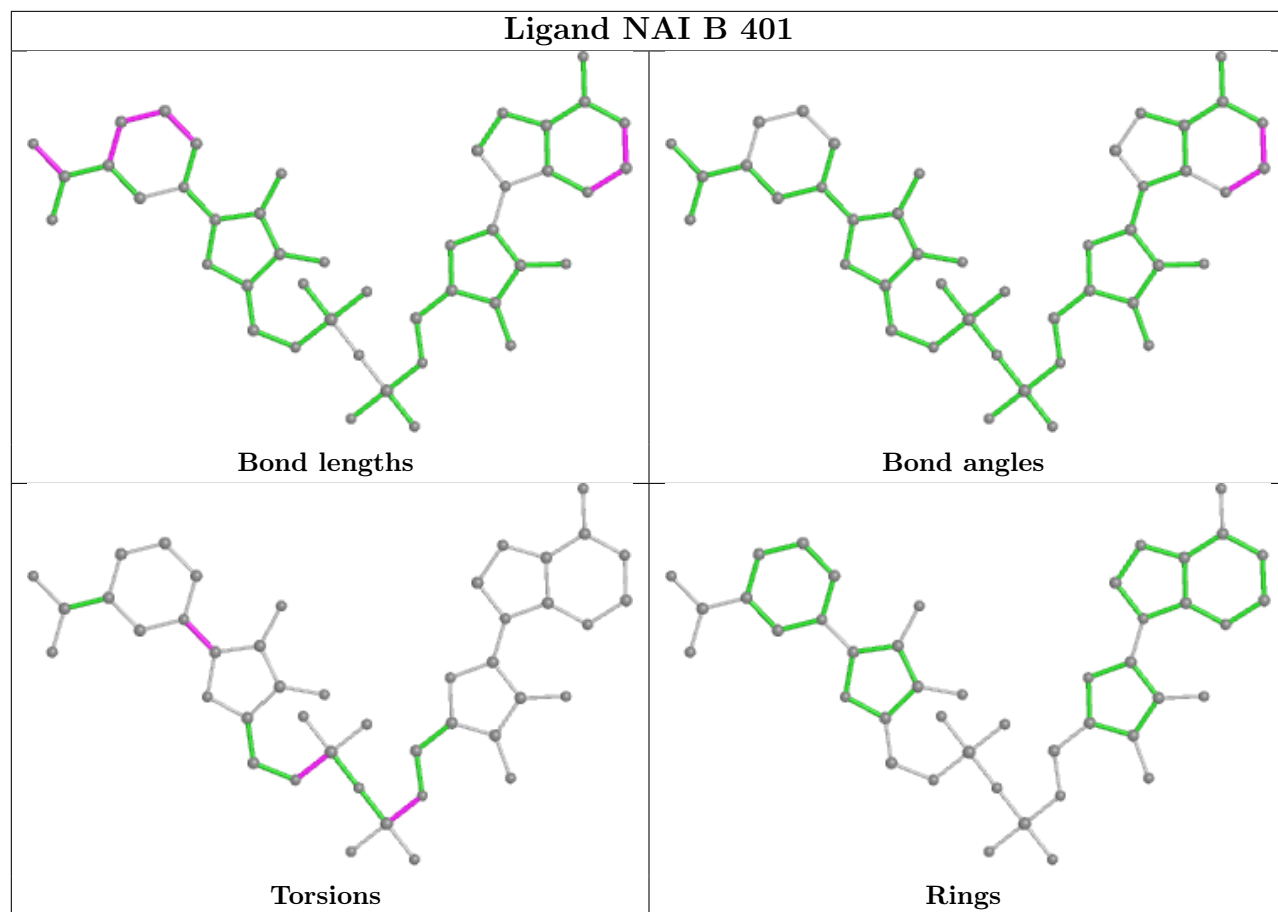
2 monomers are involved in 2 short contacts:

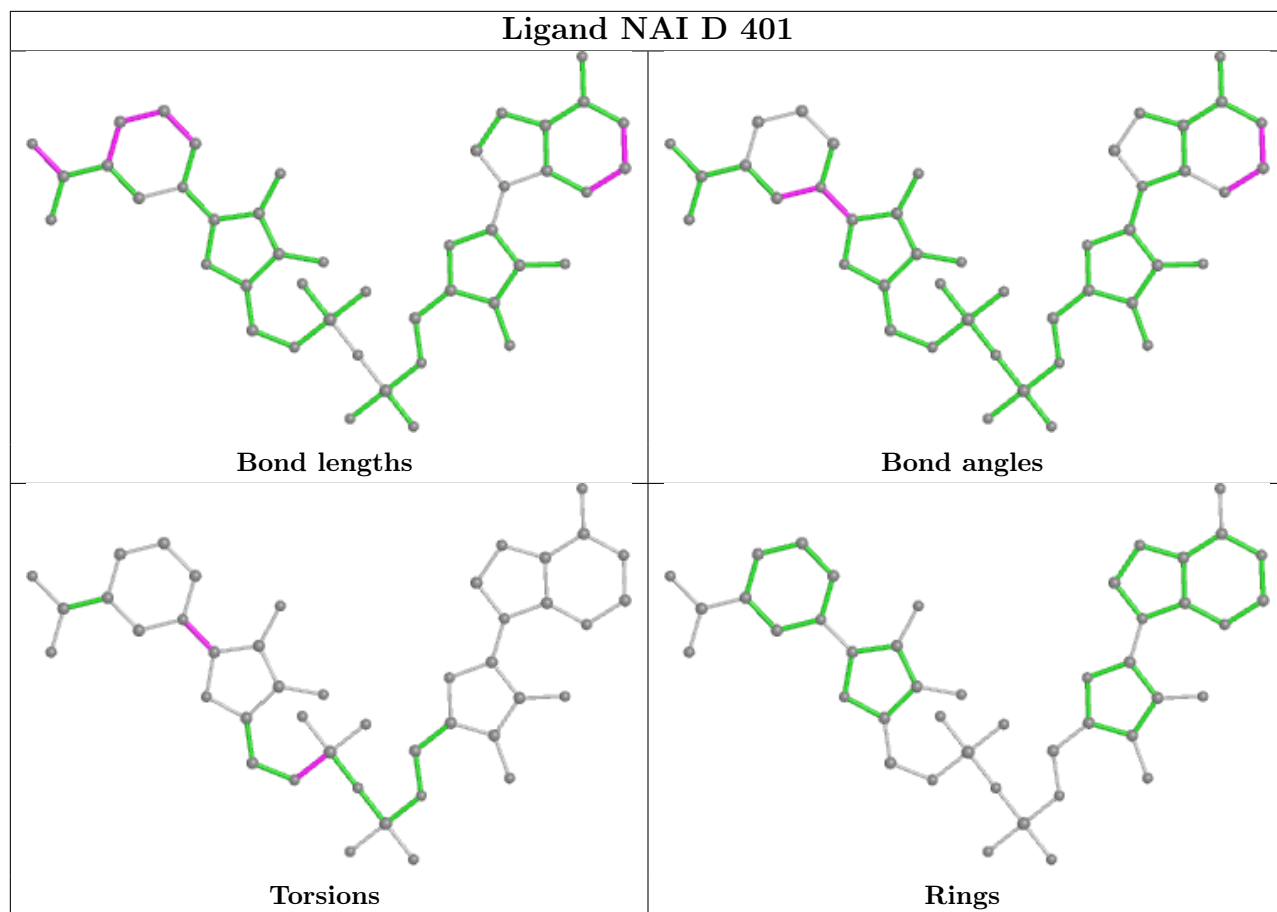
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	407	DTT	1	0
7	D	408	DTT	1	0

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

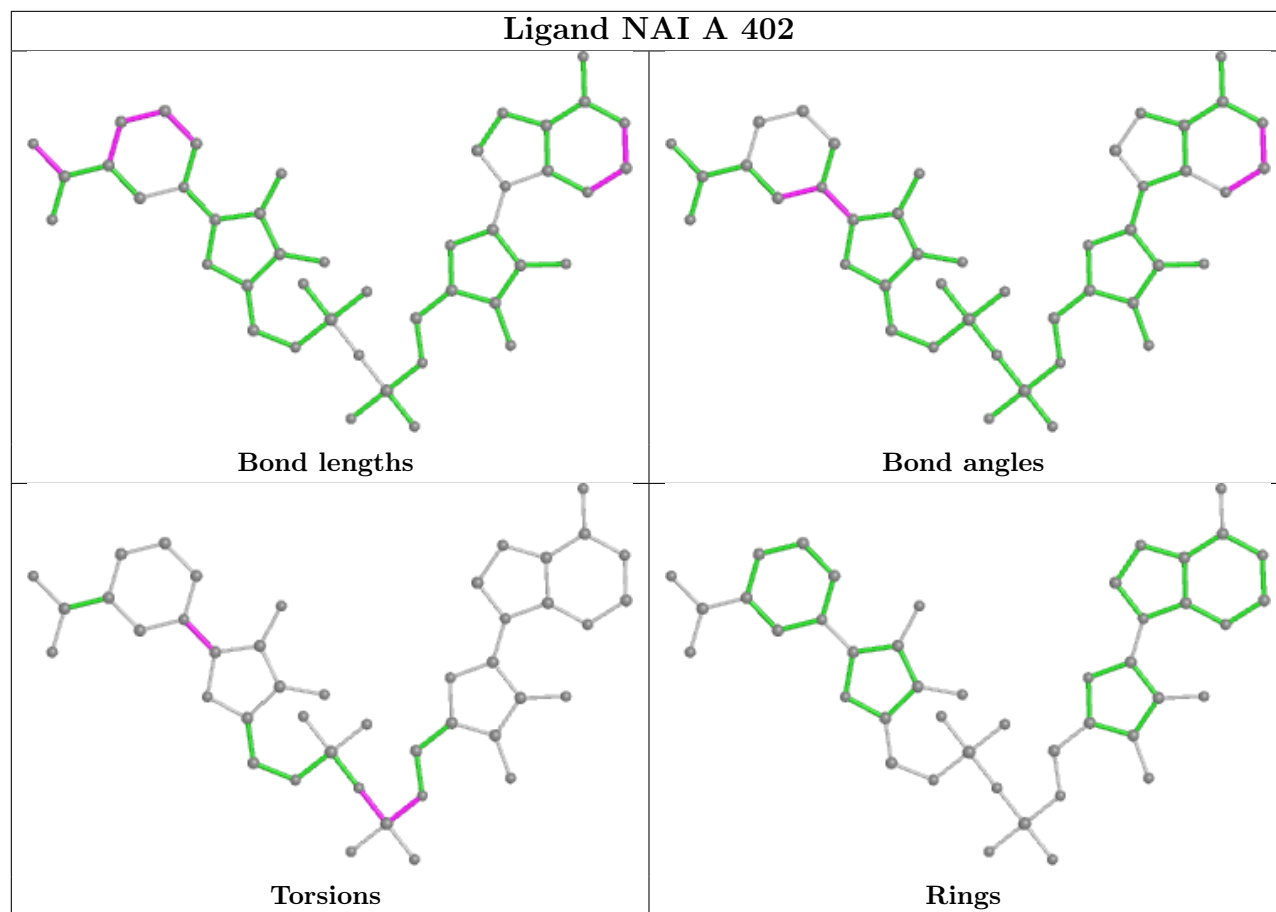
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 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	349/364 (95%)	0.17	13 (3%) 41 41	10, 18, 28, 36	0
1	B	349/364 (95%)	0.25	12 (3%) 45 44	10, 20, 31, 37	0
1	C	349/364 (95%)	0.40	17 (4%) 29 28	12, 22, 35, 45	0
1	D	349/364 (95%)	0.11	12 (3%) 45 44	8, 16, 29, 35	0
All	All	1396/1456 (95%)	0.23	54 (3%) 39 38	8, 19, 32, 45	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	316	GLY	5.2
1	D	316	GLY	5.1
1	D	124	LYS	4.5
1	C	316	GLY	4.2
1	B	122	ASN	4.1
1	A	122	ASN	3.9
1	C	125	VAL	3.7
1	B	82	ASP	3.5
1	B	125	VAL	3.2
1	D	125	VAL	3.2
1	C	359	ASP	3.1
1	D	54	GLN	3.1
1	B	5	SER	3.0
1	C	318	GLU	3.0
1	C	33	LEU	3.0
1	C	347	THR	3.0
1	D	216	HIS	2.9
1	A	65	GLU	2.8
1	B	363	ARG	2.8
1	A	290	ASP	2.8
1	A	125	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	124	LYS	2.8
1	C	116	VAL	2.7
1	B	316	GLY	2.7
1	C	124	LYS	2.7
1	A	82	ASP	2.7
1	C	317	ASP	2.7
1	D	122	ASN	2.7
1	C	363	ARG	2.5
1	B	45	GLU	2.5
1	D	183	GLU	2.5
1	C	216	HIS	2.5
1	A	123	ARG	2.4
1	B	123	ARG	2.4
1	C	267	PRO	2.3
1	C	319	ARG	2.3
1	B	359	ASP	2.3
1	A	54	GLN	2.3
1	A	363	ARG	2.3
1	C	284	VAL	2.2
1	D	224	ILE	2.2
1	A	153	GLU	2.2
1	D	317	ASP	2.2
1	D	294	LYS	2.2
1	D	123	ARG	2.2
1	D	237	ARG	2.1
1	A	69	GLN	2.1
1	B	318	GLU	2.1
1	A	117	PRO	2.1
1	A	337	ASP	2.0
1	B	347	THR	2.0
1	C	322	ARG	2.0
1	C	36	GLY	2.0
1	C	337	ASP	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.

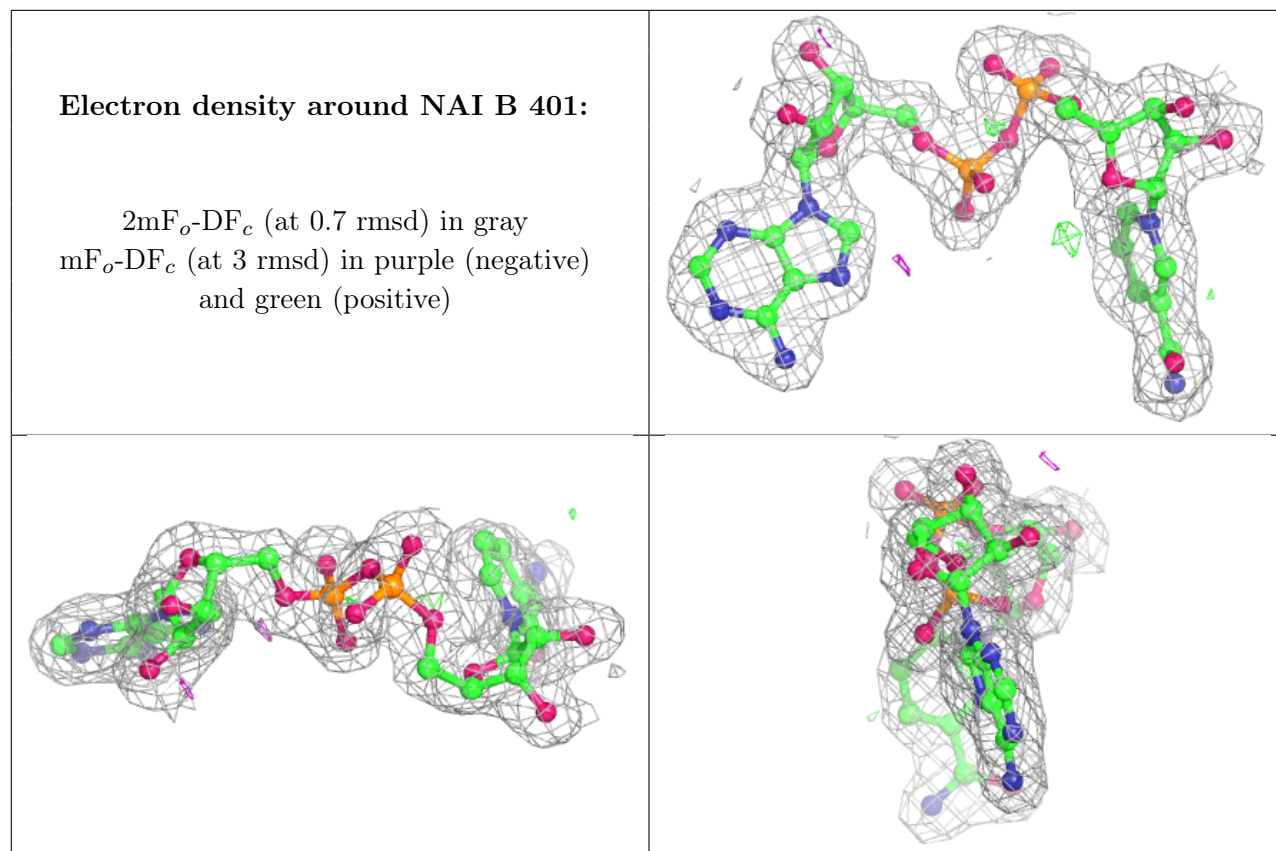
## 6.4 Ligands [i](#)

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
7	DTT	B	407	8/8	0.72	0.28	81,81,81,81	0
7	DTT	C	409	8/8	0.73	0.29	56,57,58,58	0
4	OXL	B	402	6/6	0.81	0.21	23,24,25,25	0
6	SO4	A	408	5/5	0.82	0.23	61,62,62,62	0
6	SO4	B	406	5/5	0.82	0.17	79,79,79,79	0
6	SO4	C	408	5/5	0.85	0.25	64,65,65,65	0
6	SO4	D	407	5/5	0.85	0.37	71,71,71,71	0
6	SO4	C	407	5/5	0.86	0.29	65,65,65,65	0
2	MG	C	401	1/1	0.86	0.19	20,20,20,20	0
6	SO4	D	405	5/5	0.86	0.20	79,79,79,79	0
6	SO4	D	406	5/5	0.87	0.25	48,48,49,49	0
6	SO4	C	406	5/5	0.88	0.24	62,62,62,62	0
4	OXL	C	403	6/6	0.88	0.20	24,24,25,26	0
6	SO4	B	405	5/5	0.88	0.23	62,62,63,63	0
4	OXL	D	402	6/6	0.88	0.18	19,20,20,21	0
6	SO4	D	404	5/5	0.89	0.30	50,51,51,51	0
4	OXL	A	403	6/6	0.89	0.19	22,23,24,24	0
6	SO4	A	407	5/5	0.89	0.18	73,73,73,73	0
2	MG	C	405	1/1	0.91	0.15	16,16,16,16	0
2	MG	A	405	1/1	0.91	0.15	17,17,17,17	0
6	SO4	A	409	5/5	0.92	0.27	66,66,66,66	0
6	SO4	A	406	5/5	0.93	0.25	43,43,43,44	0
6	SO4	B	404	5/5	0.95	0.14	41,41,42,42	0
2	MG	A	401	1/1	0.95	0.18	16,16,16,16	0
7	DTT	D	408	8/8	0.95	0.10	23,24,24,24	0
5	NH4	A	404	1/1	0.97	0.23	13,13,13,13	0
3	NAI	B	401	44/44	0.97	0.10	15,16,17,18	0
3	NAI	C	402	44/44	0.97	0.12	16,19,20,20	0
3	NAI	A	402	44/44	0.98	0.12	10,12,13,14	0
5	NH4	B	403	1/1	0.98	0.36	17,17,17,17	0
5	NH4	C	404	1/1	0.98	0.11	14,14,14,14	0
3	NAI	D	401	44/44	0.98	0.11	9,11,12,12	0
5	NH4	D	403	1/1	0.99	0.26	8,8,8,8	0

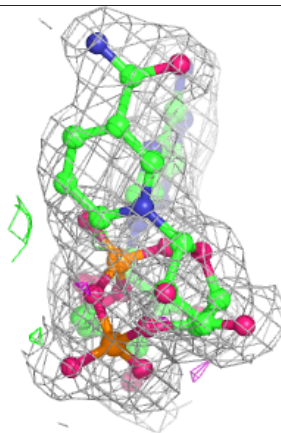
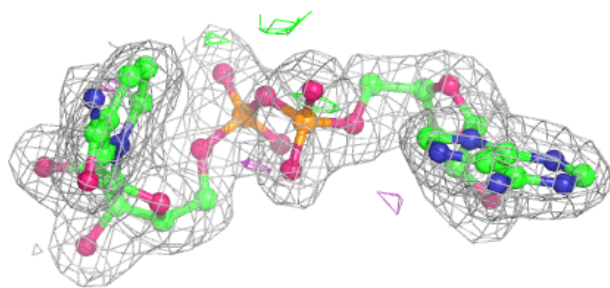
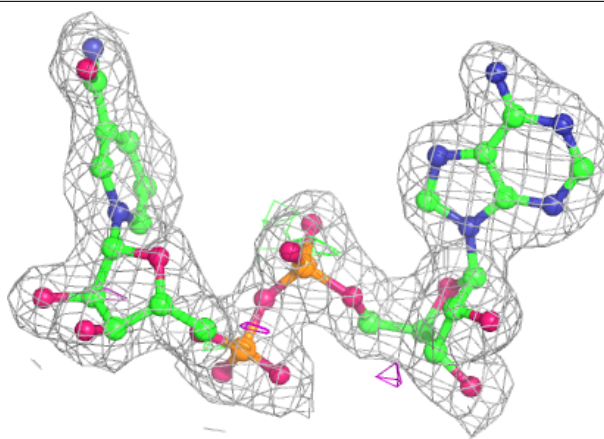
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

orientation to approximate a three-dimensional view.



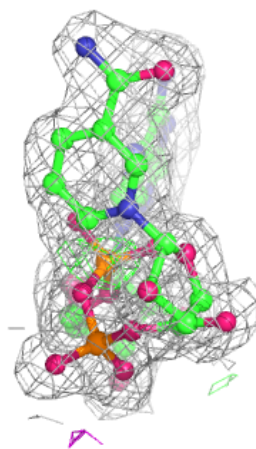
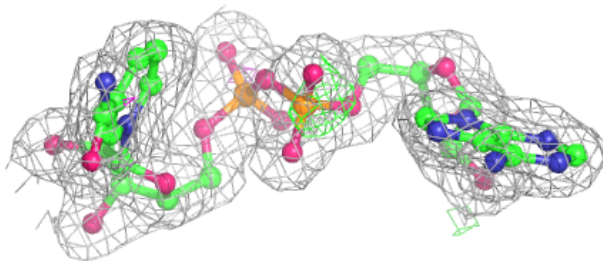
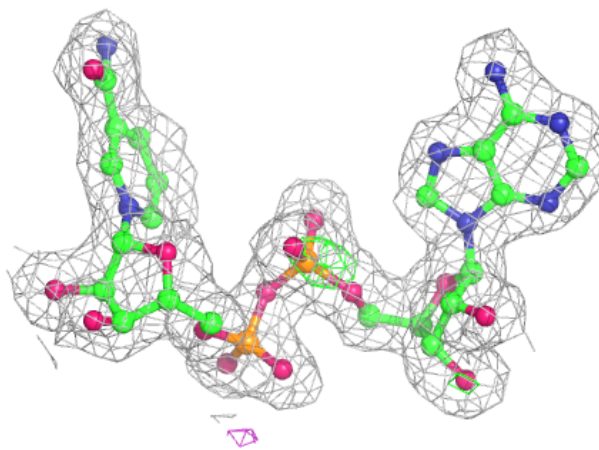
**Electron density around NAI C 402:**

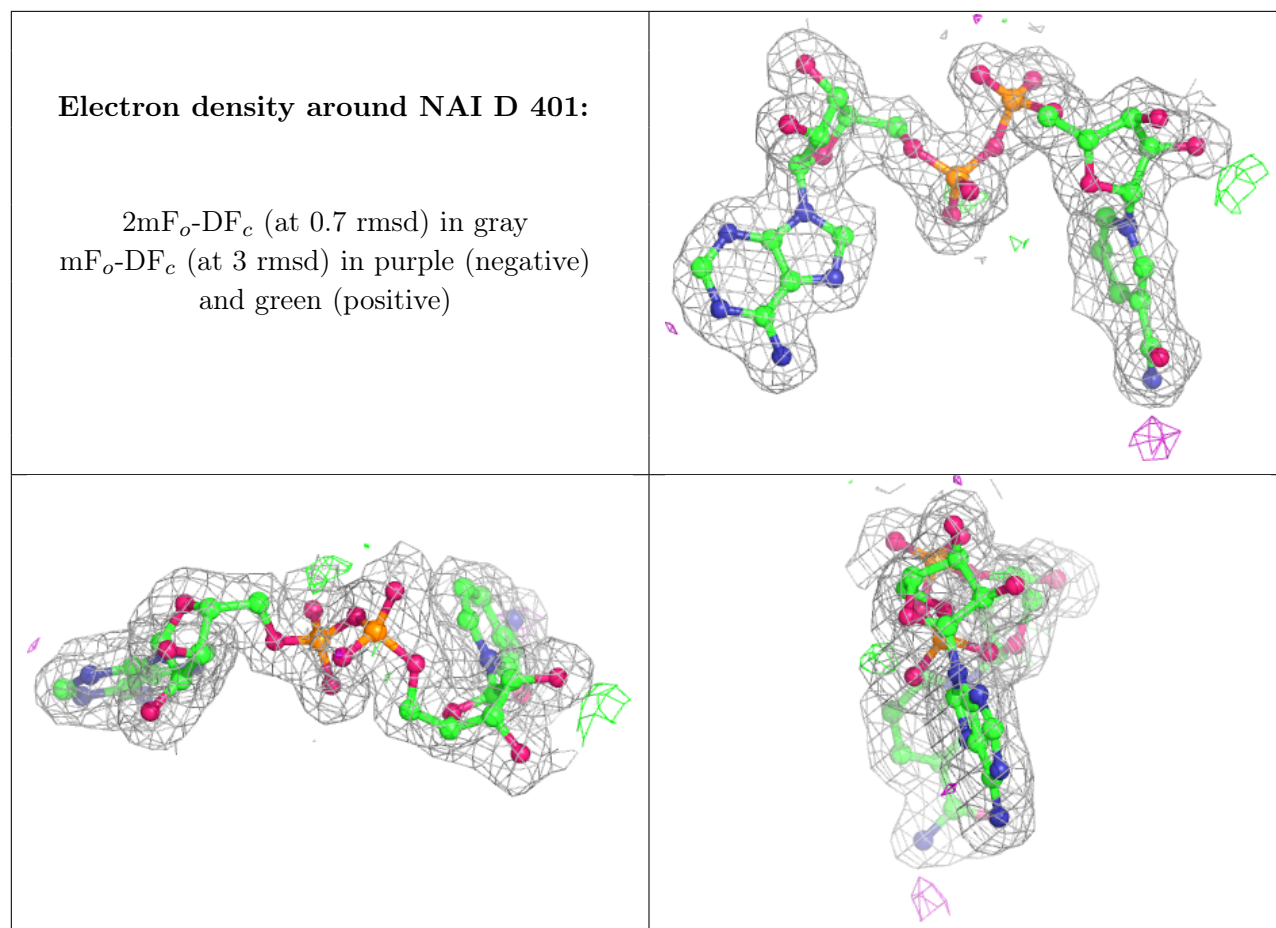
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around NAI A 402:**

$2mF_o-DF_c$  (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.