



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 11:59 PM EDT

PDB ID : 3WID  
Title : Structure of a glucose dehydrogenase T277F mutant in complex with NADP  
Authors : Sakuraba, H.; Kanoh, Y.; Yoneda, K.; Ohshima, T.  
Deposited on : 2013-09-10  
Resolution : 2.25 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)	:	1.20.1
EDS	:	2.36.2
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)	:	2.36.2

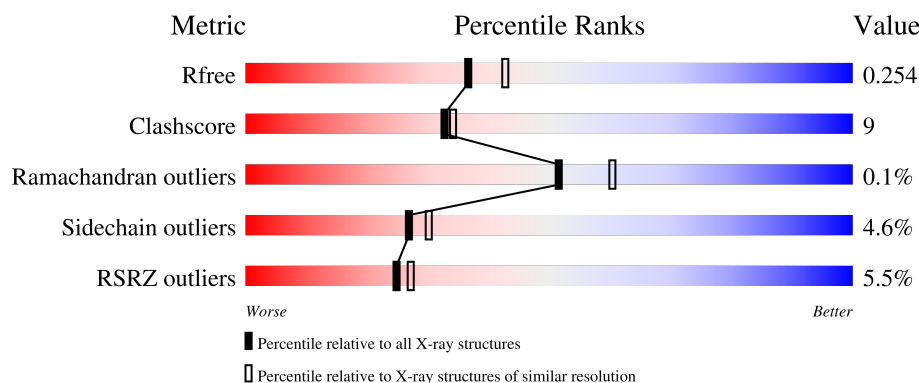
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	369	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>..</div> </div> </div>
1	B	369	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>..</div> </div> </div>
1	C	369	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>..</div> </div> </div>
1	D	369	<div> <div>11%</div> <div> <div></div> <div>78%</div> <div>18%</div> <div>..</div> </div> </div>

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
5	1PE	A	1004	-	-	X	-
5	1PE	B	4005	-	-	X	-
5	1PE	B	4006	-	-	X	-
5	1PE	C	1004	-	-	X	-
5	1PE	C	1005	-	-	X	-
5	1PE	D	4001	-	-	X	-
5	1PE	D	4005	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11962 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 Glucose 1-dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	360	Total	C	N	O	S	0	0	0
			2827	1804	473	537	13			
1	B	360	Total	C	N	O	S	0	0	0
			2827	1804	473	537	13			
1	C	358	Total	C	N	O	S	0	0	0
			2809	1793	470	533	13			
1	D	360	Total	C	N	O	S	0	0	0
			2827	1804	473	537	13			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	277	PHE	THR	engineered mutation	UNP Q979W2
A	362	LEU	-	expression tag	UNP Q979W2
A	363	GLU	-	expression tag	UNP Q979W2
A	364	HIS	-	expression tag	UNP Q979W2
A	365	HIS	-	expression tag	UNP Q979W2
A	366	HIS	-	expression tag	UNP Q979W2
A	367	HIS	-	expression tag	UNP Q979W2
A	368	HIS	-	expression tag	UNP Q979W2
A	369	HIS	-	expression tag	UNP Q979W2
B	277	PHE	THR	engineered mutation	UNP Q979W2
B	362	LEU	-	expression tag	UNP Q979W2
B	363	GLU	-	expression tag	UNP Q979W2
B	364	HIS	-	expression tag	UNP Q979W2
B	365	HIS	-	expression tag	UNP Q979W2
B	366	HIS	-	expression tag	UNP Q979W2
B	367	HIS	-	expression tag	UNP Q979W2
B	368	HIS	-	expression tag	UNP Q979W2
B	369	HIS	-	expression tag	UNP Q979W2
C	277	PHE	THR	engineered mutation	UNP Q979W2
C	362	LEU	-	expression tag	UNP Q979W2
C	363	GLU	-	expression tag	UNP Q979W2

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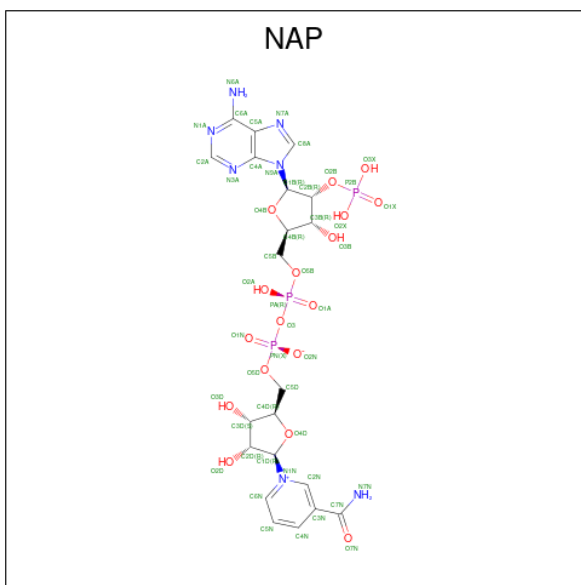
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Chain	Residue	Modelled	Actual	Comment	Reference
C	364	HIS	-	expression tag	UNP Q979W2
C	365	HIS	-	expression tag	UNP Q979W2
C	366	HIS	-	expression tag	UNP Q979W2
C	367	HIS	-	expression tag	UNP Q979W2
C	368	HIS	-	expression tag	UNP Q979W2
C	369	HIS	-	expression tag	UNP Q979W2
D	277	PHE	THR	engineered mutation	UNP Q979W2
D	362	LEU	-	expression tag	UNP Q979W2
D	363	GLU	-	expression tag	UNP Q979W2
D	364	HIS	-	expression tag	UNP Q979W2
D	365	HIS	-	expression tag	UNP Q979W2
D	366	HIS	-	expression tag	UNP Q979W2
D	367	HIS	-	expression tag	UNP Q979W2
D	368	HIS	-	expression tag	UNP Q979W2
D	369	HIS	-	expression tag	UNP Q979W2

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

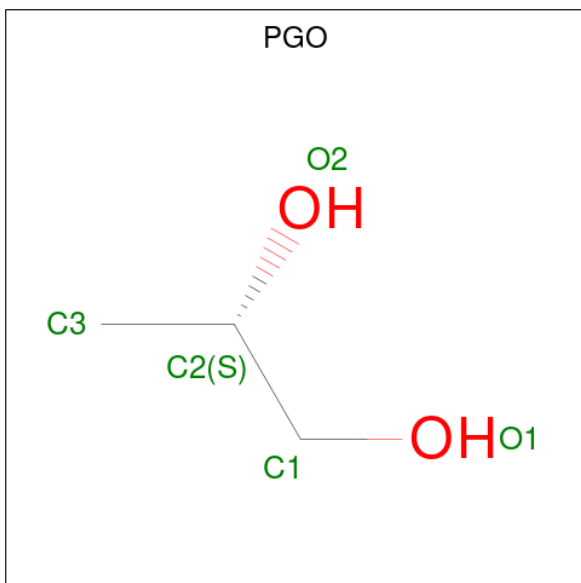
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

- Molecule 3 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>).



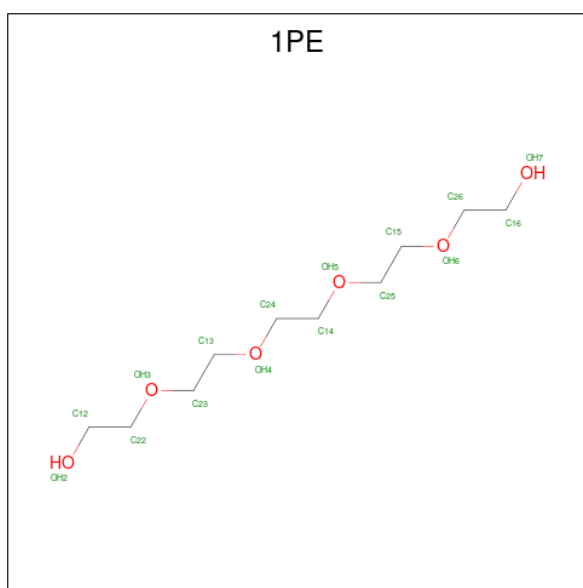
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	C	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	D	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 4 is S-1,2-PROPANEDIOL (three-letter code: PGO) (formula:  $C_3H_8O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			5	3	2		
4	B	1	Total	C	O	0	0
			5	3	2		
4	C	1	Total	C	O	0	0
			5	3	2		
4	D	1	Total	C	O	0	0
			5	3	2		

- Molecule 5 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			16	10	6		
5	B	1	Total	C	O	0	0
			16	10	6		
5	B	1	Total	C	O	0	0
			16	10	6		
5	B	1	Total	C	O	0	0
			16	10	6		
5	C	1	Total	C	O	0	0
			16	10	6		
5	C	1	Total	C	O	0	0
			16	10	6		
5	D	1	Total	C	O	0	0
			16	10	6		
5	D	1	Total	C	O	0	0
			16	10	6		

- Molecule 6 is water.

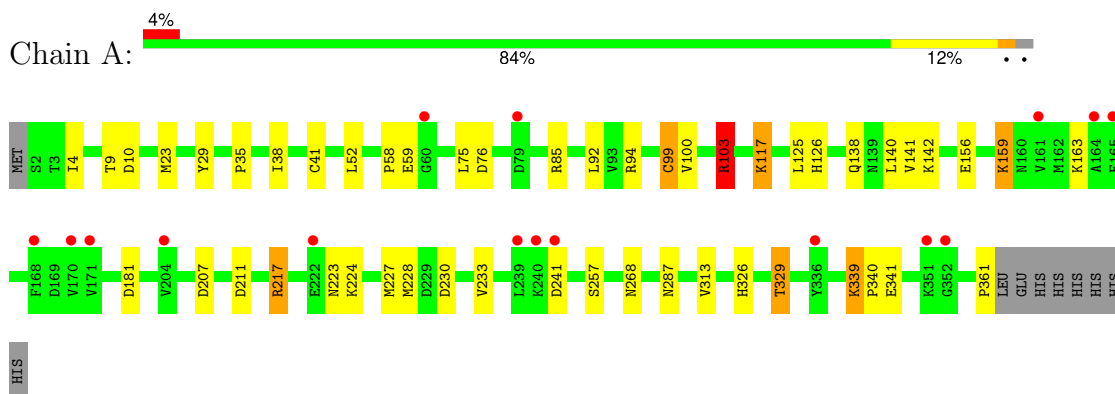
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	92	Total 92	O 92	0	0
6	B	109	Total 109	O 109	0	0
6	C	58	Total 58	O 58	0	0
6	D	69	Total 69	O 69	0	0



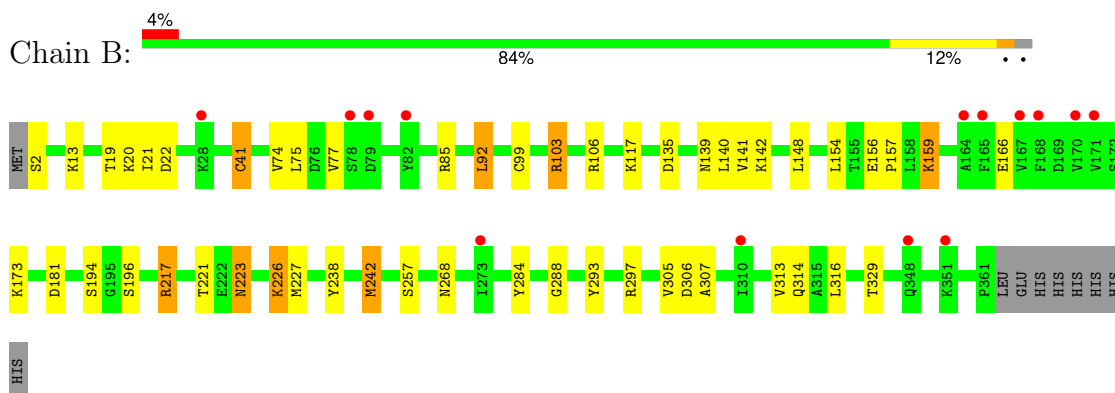
### 3 Residue-property plots [i](#)

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.

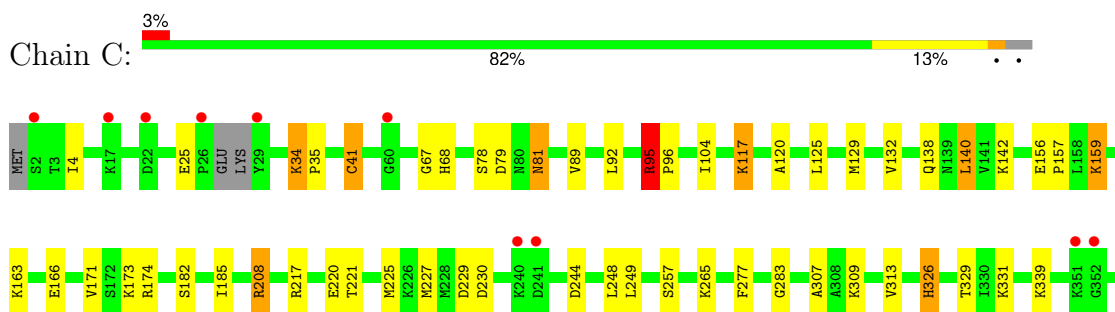
- Molecule 1: Glucose 1-dehydrogenase



- Molecule 1: Glucose 1-dehydrogenase



- Molecule 1: Glucose 1-dehydrogenase



[illegible]

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.17Å 90.35Å 120.37Å 90.00° 90.84° 90.00°	Depositor
Resolution (Å)	39.27 – 2.25 39.23 – 2.25	Depositor EDS
% Data completeness (in resolution range)	94.3 (39.27-2.25) 94.3 (39.23-2.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.60 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.197 , 0.251 0.205 , 0.254	Depositor DCC
$R_{free}$ test set	3827 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.1	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 57.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.012 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11962	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1PE, NAP, ZN, PGO

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	0.86	0/2887	0.90	4/3904 (0.1%)
1	B	0.94	0/2887	0.90	3/3904 (0.1%)
1	C	0.79	2/2868 (0.1%)	0.88	5/3878 (0.1%)
1	D	0.78	0/2887	0.84	2/3904 (0.1%)
All	All	0.84	2/11529 (0.0%)	0.88	14/15590 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	166	GLU	CD-OE1	-5.62	1.19	1.25
1	C	96	PRO	N-CD	5.39	1.55	1.47

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	208	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	C	208	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	B	103	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	A	207	ASP	CB-CG-OD1	5.68	123.42	118.30
1	D	174	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	C	326	HIS	C-N-CD	5.51	139.98	128.40
1	B	103	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	A	211	ASP	CB-CG-OD2	5.40	123.16	118.30
1	D	306	ASP	CB-CG-OD1	5.26	123.04	118.30
1	A	103	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	C	95	ARG	C-N-CD	5.16	139.22	128.40
1	B	135	ASP	CB-CG-OD1	5.15	122.93	118.30
1	C	95	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	217	ARG	NE-CZ-NH2	5.05	122.83	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	2827	0	2808	36	0
1	B	2827	0	2808	49	0
1	C	2809	0	2788	42	0
1	D	2827	0	2808	66	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	48	0	25	1	0
3	B	48	0	25	2	0
3	C	48	0	25	1	0
3	D	48	0	25	0	0
4	A	5	0	8	3	0
4	B	5	0	8	0	0
4	C	5	0	8	0	0
4	D	5	0	8	3	0
5	A	16	0	22	9	0
5	B	48	0	66	24	0
5	C	32	0	44	19	0
5	D	32	0	44	19	0
6	A	92	0	0	3	0
6	B	109	0	0	6	0
6	C	58	0	0	8	0
6	D	69	0	0	4	0
All	All	11962	0	11520	202	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 9.

All (202) 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:B:106:ARG:HH11	5:B:4005:1PE:H241	1.18	1.03
1:B:106:ARG:HD3	5:B:4005:1PE:H241	1.49	0.95
1:A:100:VAL:HA	1:A:103:ARG:HD3	1.49	0.91
1:B:173:LYS:HE2	5:B:4001:1PE:H221	1.52	0.88
5:B:4005:1PE:H152	5:B:4005:1PE:H242	1.57	0.85
1:B:106:ARG:HH11	5:B:4005:1PE:C24	1.92	0.83
1:D:41:CYS:SG	6:D:4169:HOH:O	2.22	0.81
5:B:4005:1PE:H231	6:B:4200:HOH:O	1.83	0.78
1:B:41:CYS:SG	6:B:4209:HOH:O	2.40	0.76
1:B:166:GLU:OE2	5:B:4005:1PE:H261	1.86	0.75
1:B:106:ARG:HG3	5:B:4005:1PE:H131	1.67	0.75
1:D:309:LYS:HZ1	5:D:4005:1PE:H151	1.51	0.75
1:D:173:LYS:HE3	5:D:4001:1PE:H221	1.69	0.74
1:C:41:CYS:SG	6:C:1158:HOH:O	2.23	0.74
1:B:173:LYS:CE	5:B:4001:1PE:H221	2.19	0.72
1:A:141:VAL:HA	5:A:1004:1PE:H242	1.71	0.71
5:C:1005:1PE:H232	6:C:1155:HOH:O	1.89	0.71
1:C:142:LYS:O	5:C:1004:1PE:H221	1.91	0.71
1:B:221:THR:OG1	1:B:223:ASN:ND2	2.25	0.70
1:C:182:SER:HA	5:C:1005:1PE:H162	1.75	0.69
1:D:159:LYS:HG2	1:D:160:ASN:N	2.07	0.69
1:C:68:HIS:NE2	6:C:1158:HOH:O	2.26	0.68
5:D:4001:1PE:H232	6:D:4132:HOH:O	1.93	0.68
1:B:313:VAL:HA	5:B:4006:1PE:H121	1.77	0.66
5:B:4005:1PE:H242	5:B:4005:1PE:C15	2.24	0.65
1:D:158:LEU:HD13	1:D:315:ALA:HA	1.79	0.65
1:C:173:LYS:NZ	5:C:1005:1PE:H221	2.14	0.63
1:D:227:MET:HE1	1:D:354:ILE:HD11	1.80	0.63
1:D:128:PHE:CE1	4:D:4004:PGO:C3	2.82	0.63
1:A:142:LYS:H	5:A:1004:1PE:C13	2.11	0.63
1:A:230:ASP:OD2	1:A:329:THR:HG21	1.98	0.63
1:A:224:LYS:HA	1:A:227:MET:HE3	1.79	0.63
5:C:1005:1PE:H251	1:D:106:ARG:HG3	1.80	0.63
1:C:227:MET:HG2	1:C:329:THR:HG23	1.80	0.62
1:A:41:CYS:HA	6:A:1168:HOH:O	1.99	0.62
1:B:141:VAL:HA	5:B:4006:1PE:H241	1.81	0.61
1:D:4:ILE:O	1:D:20:LYS:HA	1.99	0.61
1:D:18:TYR:HE2	1:D:341:GLU:OE2	1.84	0.61
1:D:224:LYS:HA	1:D:227:MET:HE2	1.83	0.60
1:D:142:LYS:H	5:D:4005:1PE:H242	1.67	0.60
1:C:4:ILE:HG21	1:C:132:VAL:HG12	1.84	0.59
1:A:100:VAL:CA	1:A:103:ARG:HD3	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:SER:HA	5:C:1005:1PE:C16	2.31	0.59
1:B:106:ARG:HG3	5:B:4005:1PE:C13	2.31	0.59
1:D:95:ARG:HG2	6:D:4150:HOH:O	2.02	0.59
1:B:329:THR:HG22	6:B:4183:HOH:O	2.01	0.59
1:D:173:LYS:CE	5:D:4001:1PE:H221	2.34	0.58
5:C:1005:1PE:C15	5:C:1005:1PE:H241	2.32	0.58
1:A:142:LYS:H	5:A:1004:1PE:H131	1.68	0.58
1:A:75:LEU:O	1:A:85:ARG:HG3	2.04	0.57
1:D:151:ILE:HD12	1:D:330:ILE:HG22	1.84	0.57
1:D:188:LYS:NZ	1:D:244:ASP:O	2.24	0.57
1:D:336:TYR:CE2	1:D:338:ALA:HB2	2.40	0.57
1:C:81:ASN:OD1	1:C:81:ASN:N	2.35	0.57
1:C:142:LYS:H	5:C:1004:1PE:H242	1.69	0.56
1:D:4:ILE:HD13	1:D:132:VAL:HG12	1.88	0.56
1:D:141:VAL:HA	5:D:4005:1PE:H242	1.88	0.56
1:A:181:ASP:OD2	5:B:4006:1PE:H162	2.05	0.56
1:A:326:HIS:HB3	1:A:329:THR:CG2	2.36	0.56
5:C:1005:1PE:C25	1:D:106:ARG:HG3	2.36	0.56
1:D:140:LEU:O	5:D:4005:1PE:OH5	2.24	0.56
1:D:159:LYS:HG3	1:D:307:ALA:HB3	1.87	0.56
1:C:313:VAL:HA	5:C:1004:1PE:H121	1.88	0.55
1:D:158:LEU:HB3	1:D:315:ALA:HB1	1.88	0.55
1:A:4:ILE:HD11	1:A:23:MET:HG3	1.89	0.55
1:D:309:LYS:NZ	5:D:4005:1PE:H151	2.21	0.55
1:C:244:ASP:HB3	1:C:265:LYS:HD2	1.88	0.55
1:A:35:PRO:HB2	1:A:38:ILE:HD11	1.89	0.55
1:B:141:VAL:HA	5:B:4006:1PE:C24	2.36	0.55
1:D:19:THR:OG1	1:D:20:LYS:N	2.40	0.54
1:A:125:LEU:HD21	4:A:1003:PGO:H31	1.90	0.54
1:C:173:LYS:HZ2	5:C:1005:1PE:H221	1.72	0.54
1:A:125:LEU:CD2	4:A:1003:PGO:H31	2.38	0.54
1:D:313:VAL:HA	5:D:4005:1PE:H121	1.88	0.54
1:A:126:HIS:O	4:A:1003:PGO:O2	2.24	0.54
1:B:99:CYS:O	1:B:103:ARG:HD3	2.08	0.54
1:D:176:ILE:HG23	5:D:4001:1PE:H262	1.90	0.53
1:D:227:MET:CE	1:D:354:ILE:HD11	2.39	0.53
1:B:238:TYR:HB2	1:B:242:MET:HG3	1.91	0.53
1:D:18:TYR:CE2	1:D:340:PRO:HB2	2.43	0.53
1:C:309:LYS:HZ3	5:C:1004:1PE:H151	1.73	0.53
1:D:227:MET:CE	1:D:354:ILE:CD1	2.87	0.52
1:D:309:LYS:HZ1	5:D:4005:1PE:C15	2.20	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:ARG:NH1	1:D:133:ILE:HA	2.23	0.52
1:A:41:CYS:SG	6:A:1192:HOH:O	2.44	0.52
1:D:18:TYR:CE2	1:D:341:GLU:OE2	2.62	0.52
1:D:5:ASN:HB2	1:D:131:ASP:OD2	2.10	0.51
5:C:1005:1PE:H241	5:C:1005:1PE:H151	1.91	0.51
1:D:13:LYS:O	1:D:50:GLY:HA3	2.10	0.51
1:D:128:PHE:CE1	4:D:4004:PGO:H32	2.46	0.51
1:D:141:VAL:HA	5:D:4005:1PE:C24	2.41	0.51
1:D:313:VAL:HG13	5:D:4005:1PE:H121	1.92	0.51
1:A:9:THR:OG1	1:A:10:ASP:N	2.44	0.51
1:B:227:MET:HB3	6:B:4183:HOH:O	2.10	0.51
1:C:309:LYS:HZ3	5:C:1004:1PE:C15	2.24	0.51
1:A:141:VAL:HA	5:A:1004:1PE:C24	2.39	0.50
1:B:75:LEU:O	1:B:85:ARG:HG3	2.11	0.50
1:B:142:LYS:O	5:B:4006:1PE:H221	2.11	0.50
1:A:241:ASP:N	1:A:241:ASP:OD1	2.41	0.50
1:D:16:VAL:HG13	1:D:48:VAL:HG22	1.94	0.50
1:A:313:VAL:HG22	5:A:1004:1PE:H232	1.94	0.50
1:D:182:SER:HA	5:D:4001:1PE:H162	1.93	0.50
1:C:95:ARG:HG2	6:C:1150:HOH:O	2.11	0.50
1:B:92:LEU:HD22	1:B:139:ASN:HA	1.94	0.49
1:A:339:LYS:HD3	1:A:340:PRO:HD2	1.94	0.49
1:A:230:ASP:OD2	1:A:329:THR:CG2	2.60	0.49
1:B:154:LEU:C	1:B:157:PRO:HD2	2.33	0.49
1:D:159:LYS:HE3	1:D:312:TYR:OH	2.13	0.49
1:B:226:LYS:HA	1:B:226:LYS:HE2	1.94	0.49
1:A:217:ARG:HG2	1:A:217:ARG:HH21	1.77	0.49
1:B:314:GLN:CD	6:B:4169:HOH:O	2.51	0.49
1:C:67:GLY:HA3	1:C:129:MET:HG3	1.94	0.49
1:D:178:GLN:HB2	5:D:4001:1PE:H261	1.95	0.49
5:A:1004:1PE:OH6	5:A:1004:1PE:C14	2.61	0.48
1:B:268:ASN:ND2	1:B:297:ARG:HG2	2.28	0.48
1:B:217:ARG:HG2	1:B:217:ARG:O	2.14	0.48
1:C:230:ASP:OD2	1:C:329:THR:OG1	2.22	0.48
1:B:142:LYS:H	5:B:4006:1PE:H242	1.78	0.48
1:B:140:LEU:O	5:B:4006:1PE:OH5	2.32	0.48
1:C:309:LYS:NZ	5:C:1004:1PE:H152	2.28	0.48
1:C:35:PRO:HG2	1:C:360:TRP:CD1	2.49	0.47
1:D:156:GLU:O	1:D:159:LYS:HD3	2.14	0.47
1:B:306:ASP:H	3:B:4003:NAP:H72N	1.62	0.47
1:B:159:LYS:HD3	1:B:307:ALA:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:LYS:HE2	5:B:4001:1PE:C22	2.35	0.47
5:A:1004:1PE:H162	1:B:181:ASP:OD2	2.14	0.47
1:C:104:ILE:HD12	5:D:4001:1PE:H161	1.97	0.47
5:C:1005:1PE:C23	6:C:1155:HOH:O	2.57	0.47
1:C:138:GLN:O	1:C:309:LYS:NZ	2.47	0.46
1:C:163:LYS:HB2	1:C:307:ALA:CB	2.45	0.46
1:A:140:LEU:O	5:A:1004:1PE:H242	2.16	0.46
1:D:128:PHE:HE1	4:D:4004:PGO:H32	1.79	0.46
1:B:75:LEU:O	1:B:85:ARG:CG	2.64	0.46
1:B:142:LYS:H	5:B:4006:1PE:C24	2.28	0.46
1:B:227:MET:HE2	6:B:4183:HOH:O	2.15	0.46
1:B:154:LEU:O	1:B:157:PRO:HD2	2.16	0.46
1:D:130:ARG:HH12	1:D:133:ILE:HA	1.82	0.45
1:D:138:GLN:O	1:D:309:LYS:NZ	2.48	0.45
1:B:106:ARG:NH1	5:B:4005:1PE:H241	2.03	0.45
1:C:277:PHE:CD1	1:C:277:PHE:N	2.84	0.45
1:D:342:GLU:HG2	1:D:344:ASN:OD1	2.17	0.45
1:D:336:TYR:HE2	1:D:338:ALA:HB2	1.80	0.45
1:C:34:LYS:NZ	6:C:1142:HOH:O	2.50	0.45
1:C:185:ILE:CD1	5:D:4005:1PE:H142	2.46	0.44
1:D:7:ILE:HG23	1:D:129:MET:HB3	1.99	0.44
1:C:230:ASP:O	1:C:326:HIS:NE2	2.50	0.44
1:B:316:LEU:HB2	5:B:4006:1PE:H122	2.00	0.44
1:D:5:ASN:HB3	1:D:18:TYR:CE1	2.53	0.43
1:D:206:LYS:NZ	6:D:4165:HOH:O	2.50	0.43
1:D:83:ILE:HG22	1:D:142:LYS:HD2	2.00	0.43
1:A:138:GLN:HB2	6:A:1138:HOH:O	2.18	0.43
1:C:244:ASP:CB	1:C:265:LYS:HD2	2.48	0.43
1:C:173:LYS:HZ1	5:C:1005:1PE:H221	1.84	0.43
1:C:138:GLN:HA	5:C:1004:1PE:H152	2.00	0.43
1:A:156:GLU:O	1:A:159:LYS:HE3	2.19	0.42
1:B:293:TYR:CE2	1:B:297:ARG:CZ	3.02	0.42
1:C:4:ILE:HD13	1:C:132:VAL:HG12	2.01	0.42
1:D:65:VAL:HG21	1:D:130:ARG:HD3	2.01	0.42
1:D:142:LYS:O	5:D:4005:1PE:H221	2.19	0.42
1:D:357:VAL:HG12	1:D:358:ILE:N	2.34	0.42
1:A:58:PRO:HG2	1:A:126:HIS:CE1	2.54	0.42
1:A:223:ASN:C	1:A:227:MET:HE2	2.39	0.42
1:A:340:PRO:HG3	1:A:361:PRO:HD3	2.01	0.42
3:C:1002:NAP:H4N	6:C:1129:HOH:O	2.18	0.42
1:D:227:MET:HE1	1:D:354:ILE:CD1	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:LEU:HD13	1:D:315:ALA:CA	2.47	0.42
1:D:339:LYS:O	1:D:340:PRO:C	2.57	0.42
3:A:1002:NAP:H2D	3:A:1002:NAP:H6N	1.83	0.42
1:D:89:VAL:HG21	1:D:140:LEU:HG	2.01	0.42
1:C:185:ILE:HD11	5:D:4005:1PE:H131	2.01	0.42
1:B:74:VAL:HG13	1:B:77:VAL:HG13	2.01	0.42
1:C:309:LYS:NZ	5:C:1004:1PE:C15	2.83	0.42
1:C:89:VAL:HG21	1:C:140:LEU:HG	2.01	0.41
1:D:228:MET:SD	1:D:235:PHE:HB2	2.59	0.41
1:D:121:GLY:C	1:D:122:ILE:HG13	2.41	0.41
1:A:142:LYS:N	5:A:1004:1PE:H131	2.35	0.41
1:B:156:GLU:O	1:B:159:LYS:HG3	2.20	0.41
1:B:74:VAL:CG1	1:B:77:VAL:HG13	2.51	0.41
1:A:228:MET:HB3	1:A:233:VAL:O	2.21	0.41
1:C:208:ARG:NH1	6:C:1135:HOH:O	2.47	0.41
1:D:163:LYS:HB2	1:D:307:ALA:HB2	2.03	0.41
1:C:171:VAL:O	1:C:174:ARG:HG2	2.20	0.41
1:A:99:CYS:O	1:A:103:ARG:CD	2.69	0.41
1:B:2:SER:N	1:B:22:ASP:OD1	2.54	0.41
1:B:288:GLY:HA3	1:D:278:ASN:O	2.21	0.41
1:C:156:GLU:N	1:C:157:PRO:HD2	2.36	0.41
1:D:77:VAL:O	1:D:77:VAL:HG13	2.21	0.41
1:B:19:THR:OG1	1:B:20:LYS:N	2.54	0.41
1:B:257:SER:HB2	1:B:284:TYR:CD1	2.56	0.41
1:B:305:VAL:HA	3:B:4003:NAP:H72N	1.86	0.41
1:C:120:ALA:HA	1:C:125:LEU:HB3	2.03	0.40
1:C:156:GLU:O	1:C:159:LYS:HG3	2.22	0.40
1:A:287:ASN:HA	1:C:283:GLY:HA2	2.03	0.40
1:B:21:ILE:HD13	1:B:21:ILE:HG21	1.86	0.40
1:B:106:ARG:HD3	5:B:4005:1PE:C24	2.34	0.40
1:B:166:GLU:OE2	5:B:4005:1PE:C26	2.63	0.40
1:D:255:ASP:OD2	1:D:258:THR:OG1	2.21	0.40
1:D:95:ARG:HD2	1:D:95:ARG:N	2.36	0.40
1:C:117:LYS:C	1:C:117:LYS:HD2	2.42	0.40
1:A:29:TYR:OH	1:A:76:ASP:OD2	2.25	0.40
1:A:94:ARG:HD3	1:A:117:LYS:HG3	2.04	0.40
1:C:220:GLU:OE2	1:C:221:THR:N	2.53	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	358/369 (97%)	347 (97%)	10 (3%)	1 (0%)	41	46
1	B	358/369 (97%)	351 (98%)	7 (2%)	0	100	100
1	C	354/369 (96%)	336 (95%)	18 (5%)	0	100	100
1	D	358/369 (97%)	339 (95%)	19 (5%)	0	100	100
All	All	1428/1476 (97%)	1373 (96%)	54 (4%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	CYS

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	313/322 (97%)	301 (96%)	12 (4%)	33	39
1	B	313/322 (97%)	301 (96%)	12 (4%)	33	39
1	C	311/322 (97%)	292 (94%)	19 (6%)	18	18
1	D	313/322 (97%)	299 (96%)	14 (4%)	27	31
All	All	1250/1288 (97%)	1193 (95%)	57 (5%)	27	30

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LEU
1	A	59	GLU
1	A	92	LEU
1	A	103	ARG
1	A	117	LYS
1	A	159	LYS
1	A	163	LYS
1	A	257	SER
1	A	268	ASN
1	A	329	THR
1	A	339	LYS
1	A	341	GLU
1	B	13	LYS
1	B	41	CYS
1	B	92	LEU
1	B	117	LYS
1	B	148	LEU
1	B	159	LYS
1	B	194	SER
1	B	196	SER
1	B	217	ARG
1	B	223	ASN
1	B	226	LYS
1	B	242	MET
1	C	25	GLU
1	C	34	LYS
1	C	41	CYS
1	C	78	SER
1	C	79	ASP
1	C	81	ASN
1	C	92	LEU
1	C	95	ARG
1	C	117	LYS
1	C	140	LEU
1	C	159	LYS
1	C	217	ARG
1	C	225	MET
1	C	229	ASP
1	C	248	LEU
1	C	249	LEU
1	C	257	SER
1	C	331	LYS
1	C	339	LYS

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Mol	Chain	Res	Type
1	D	7	ILE
1	D	19	THR
1	D	41	CYS
1	D	92	LEU
1	D	95	ARG
1	D	117	LYS
1	D	125	LEU
1	D	140	LEU
1	D	158	LEU
1	D	159	LYS
1	D	194	SER
1	D	257	SER
1	D	339	LYS
1	D	349	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	GLN
1	A	268	ASN
1	A	269	ASN
1	B	81	ASN
1	B	223	ASN
1	B	268	ASN
1	B	269	ASN
1	B	321	ASN
1	B	348	GLN
1	C	144	ASN
1	C	267	ASN
1	C	269	ASN
1	C	321	ASN
1	C	326	HIS
1	C	348	GLN
1	D	62	ASN
1	D	118	HIS
1	D	138	GLN
1	D	144	ASN
1	D	321	ASN
1	D	324	HIS
1	D	348	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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$
5	1PE	B	4001	-	15,15,15	1.09	1 (6%)	14,14,14	0.99	0
5	1PE	D	4001	-	15,15,15	0.87	0	14,14,14	0.59	0
5	1PE	C	1005	-	15,15,15	1.08	0	14,14,14	1.21	2 (14%)
5	1PE	B	4006	-	15,15,15	1.08	1 (6%)	14,14,14	0.98	0
3	NAP	D	4003	-	46,52,52	1.14	3 (6%)	61,80,80	1.28	6 (9%)
3	NAP	B	4003	-	46,52,52	1.21	5 (10%)	61,80,80	2.11	17 (27%)
4	PGO	B	4004	-	4,4,4	0.48	0	4,4,4	0.69	0
5	1PE	B	4005	-	15,15,15	1.07	0	14,14,14	1.07	0
3	NAP	A	1002	-	46,52,52	1.14	3 (6%)	61,80,80	1.35	6 (9%)
5	1PE	D	4005	-	15,15,15	0.72	0	14,14,14	0.89	1 (7%)
5	1PE	A	1004	-	15,15,15	0.90	0	14,14,14	1.16	1 (7%)
3	NAP	C	1002	-	46,52,52	1.06	2 (4%)	61,80,80	1.66	17 (27%)
4	PGO	D	4004	-	4,4,4	0.42	0	4,4,4	1.21	1 (25%)
4	PGO	A	1003	-	4,4,4	0.48	0	4,4,4	1.13	1 (25%)
5	1PE	C	1004	-	15,15,15	0.74	0	14,14,14	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PGO	C	1003	-	4,4,4	0.67	0	4,4,4	0.75	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
5	1PE	B	4001	-	-	6/13/13/13	-
5	1PE	D	4001	-	-	8/13/13/13	-
5	1PE	C	1005	-	-	7/13/13/13	-
5	1PE	B	4006	-	-	6/13/13/13	-
3	NAP	D	4003	-	-	8/31/67/67	0/5/5/5
3	NAP	B	4003	-	-	9/31/67/67	0/5/5/5
4	PGO	B	4004	-	-	0/2/2/2	-
5	1PE	B	4005	-	-	6/13/13/13	-
3	NAP	A	1002	-	-	10/31/67/67	0/5/5/5
5	1PE	D	4005	-	-	6/13/13/13	-
5	1PE	A	1004	-	-	4/13/13/13	-
3	NAP	C	1002	-	-	6/31/67/67	0/5/5/5
4	PGO	D	4004	-	-	2/2/2/2	-
4	PGO	A	1003	-	-	0/2/2/2	-
5	1PE	C	1004	-	-	9/13/13/13	-
4	PGO	C	1003	-	-	0/2/2/2	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	4003	NAP	PA-O3	3.68	1.63	1.59
3	B	4003	NAP	O7N-C7N	3.26	1.30	1.24
3	B	4003	NAP	PN-O3	2.84	1.62	1.59
3	A	1002	NAP	C4A-N3A	-2.64	1.32	1.35
3	B	4003	NAP	P2B-O2B	2.60	1.64	1.59
5	B	4006	1PE	OH3-C23	2.58	1.53	1.42
3	B	4003	NAP	O4B-C1B	2.36	1.44	1.40
3	D	4003	NAP	C2N-N1N	-2.34	1.32	1.35
3	C	1002	NAP	C4A-N3A	-2.20	1.32	1.35
3	A	1002	NAP	P2B-O3X	-2.13	1.46	1.54
3	A	1002	NAP	P2B-O2X	-2.11	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4003	NAP	C5A-N7A	-2.09	1.32	1.39
5	B	4001	1PE	OH6-C15	2.02	1.50	1.42
3	D	4003	NAP	O7N-C7N	-2.02	1.20	1.24
3	C	1002	NAP	P2B-O3X	-2.01	1.47	1.54

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	4003	NAP	O7N-C7N-C3N	5.73	126.60	119.60
3	B	4003	NAP	C3N-C7N-N7N	-5.19	111.34	117.74
3	B	4003	NAP	N3A-C2A-N1A	-5.10	121.75	128.67
3	B	4003	NAP	C1B-N9A-C4A	-4.99	117.88	126.64
3	B	4003	NAP	C4B-O4B-C1B	-4.90	105.44	109.92
3	C	1002	NAP	N3A-C2A-N1A	-4.42	122.67	128.67
3	A	1002	NAP	N3A-C2A-N1A	-4.36	122.75	128.67
3	B	4003	NAP	O3X-P2B-O2X	3.99	122.75	107.80
3	C	1002	NAP	O4B-C1B-N9A	3.67	113.61	108.75
3	D	4003	NAP	N3A-C2A-N1A	-3.63	123.75	128.67
3	D	4003	NAP	O4B-C1B-C2B	-3.63	100.42	106.61
3	B	4003	NAP	C5N-C6N-N1N	-3.57	115.52	120.38
3	C	1002	NAP	O2D-C2D-C3D	-3.26	101.35	111.82
3	C	1002	NAP	O2B-P2B-O1X	-2.96	98.78	109.33
3	D	4003	NAP	C4A-C5A-N7A	-2.93	106.24	109.34
3	B	4003	NAP	C2N-C3N-C4N	-2.92	114.86	118.26
3	B	4003	NAP	C6N-N1N-C2N	2.88	124.33	121.88
5	C	1005	1PE	OH5-C25-C15	2.80	123.13	110.35
3	C	1002	NAP	C1B-N9A-C4A	-2.79	121.73	126.64
3	C	1002	NAP	O4B-C1B-C2B	-2.79	101.85	106.61
3	A	1002	NAP	C3N-C7N-N7N	2.69	121.05	117.74
3	B	4003	NAP	O2N-PN-O1N	2.69	124.95	112.44
3	C	1002	NAP	C4A-C5A-N7A	-2.67	106.51	109.34
3	C	1002	NAP	C3N-C7N-N7N	2.44	120.74	117.74
3	C	1002	NAP	C5B-C4B-C3B	-2.42	106.50	115.21
3	C	1002	NAP	O3D-C3D-C2D	-2.41	104.09	111.82
3	B	4003	NAP	C2D-C3D-C4D	2.41	107.27	102.61
3	A	1002	NAP	C1B-N9A-C4A	-2.39	122.44	126.64
3	A	1002	NAP	C4A-C5A-N7A	-2.30	106.91	109.34
3	C	1002	NAP	O2N-PN-O1N	2.22	122.78	112.44
3	B	4003	NAP	P2B-O2B-C2B	-2.21	117.52	123.43
3	C	1002	NAP	C2N-C3N-C4N	-2.19	115.71	118.26
4	A	1003	PGO	C3-C2-C1	-2.17	101.86	110.80
3	B	4003	NAP	O4B-C1B-N9A	-2.16	105.88	108.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	4003	NAP	O3D-C3D-C2D	-2.15	104.91	111.82
3	D	4003	NAP	O2B-P2B-O1X	-2.14	101.72	109.33
3	D	4003	NAP	C3N-C7N-N7N	2.12	120.34	117.74
3	B	4003	NAP	O3D-C3D-C4D	-2.11	105.03	111.08
5	C	1005	1PE	OH7-C16-C26	2.11	124.22	111.82
3	B	4003	NAP	O5D-C5D-C4D	2.10	116.14	108.99
3	D	4003	NAP	O2X-P2B-O1X	2.10	119.01	110.83
3	B	4003	NAP	O3B-C3B-C4B	-2.09	105.07	111.08
3	C	1002	NAP	O7N-C7N-N7N	-2.09	119.60	122.62
4	D	4004	PGO	O1-C1-C2	-2.09	103.46	114.54
3	C	1002	NAP	C2D-C3D-C4D	2.07	106.61	102.61
3	A	1002	NAP	C3B-C2B-C1B	-2.07	98.85	102.81
3	C	1002	NAP	C4B-O4B-C1B	-2.06	108.04	109.92
3	C	1002	NAP	C6N-N1N-C1D	2.03	123.70	119.73
5	D	4005	1PE	C25-OH5-C14	-2.01	104.47	113.26
5	A	1004	1PE	C25-OH5-C14	-2.01	104.47	113.26
3	C	1002	NAP	O5D-C5D-C4D	2.00	115.81	108.99
3	A	1002	NAP	O3D-C3D-C2D	-2.00	105.40	111.82

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	NAP	C5B-O5B-PA-O2A
3	A	1002	NAP	C5B-O5B-PA-O3
3	A	1002	NAP	O4D-C1D-N1N-C2N
3	A	1002	NAP	O4D-C1D-N1N-C6N
3	A	1002	NAP	C2D-C1D-N1N-C2N
3	A	1002	NAP	C2D-C1D-N1N-C6N
3	B	4003	NAP	C5B-O5B-PA-O2A
3	B	4003	NAP	O4D-C1D-N1N-C2N
3	B	4003	NAP	O4D-C1D-N1N-C6N
3	B	4003	NAP	C2D-C1D-N1N-C2N
3	B	4003	NAP	C2D-C1D-N1N-C6N
3	C	1002	NAP	O4D-C1D-N1N-C2N
3	C	1002	NAP	O4D-C1D-N1N-C6N
3	C	1002	NAP	C2D-C1D-N1N-C2N
3	C	1002	NAP	C2D-C1D-N1N-C6N
3	D	4003	NAP	C5B-O5B-PA-O2A
3	D	4003	NAP	C5B-O5B-PA-O3
3	D	4003	NAP	O4D-C1D-N1N-C2N
3	D	4003	NAP	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
3	D	4003	NAP	C2D-C1D-N1N-C2N
3	D	4003	NAP	C2D-C1D-N1N-C6N
4	D	4004	PGO	O1-C1-C2-C3
5	C	1004	1PE	OH5-C14-C24-OH4
5	D	4001	1PE	OH4-C13-C23-OH3
5	D	4005	1PE	OH6-C15-C25-OH5
5	B	4006	1PE	OH5-C14-C24-OH4
5	C	1005	1PE	OH6-C15-C25-OH5
5	B	4001	1PE	OH4-C13-C23-OH3
5	A	1004	1PE	OH5-C14-C24-OH4
5	D	4001	1PE	C24-C14-OH5-C25
5	D	4005	1PE	OH7-C16-C26-OH6
5	D	4001	1PE	OH6-C15-C25-OH5
5	C	1005	1PE	OH5-C14-C24-OH4
5	C	1004	1PE	OH2-C12-C22-OH3
5	C	1005	1PE	C24-C14-OH5-C25
5	D	4005	1PE	OH5-C14-C24-OH4
5	B	4001	1PE	OH5-C14-C24-OH4
5	A	1004	1PE	OH6-C15-C25-OH5
5	B	4006	1PE	OH2-C12-C22-OH3
5	C	1004	1PE	OH7-C16-C26-OH6
5	C	1005	1PE	OH7-C16-C26-OH6
5	D	4005	1PE	OH2-C12-C22-OH3
4	D	4004	PGO	O1-C1-C2-O2
5	C	1004	1PE	OH6-C15-C25-OH5
5	D	4001	1PE	C23-C13-OH4-C24
5	B	4005	1PE	C16-C26-OH6-C15
5	C	1004	1PE	C12-C22-OH3-C23
5	B	4001	1PE	OH2-C12-C22-OH3
5	D	4001	1PE	C16-C26-OH6-C15
5	B	4005	1PE	OH6-C15-C25-OH5
5	D	4005	1PE	C12-C22-OH3-C23
5	A	1004	1PE	OH2-C12-C22-OH3
5	B	4006	1PE	C23-C13-OH4-C24
5	B	4005	1PE	C14-C24-OH4-C13
5	D	4001	1PE	C13-C23-OH3-C22
5	D	4001	1PE	OH2-C12-C22-OH3
3	A	1002	NAP	C5B-O5B-PA-O1A
3	B	4003	NAP	C5B-O5B-PA-O1A
3	B	4003	NAP	C5B-O5B-PA-O3
3	D	4003	NAP	C5B-O5B-PA-O1A
5	B	4001	1PE	C23-C13-OH4-C24

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Mol	Chain	Res	Type	Atoms
5	A	1004	1PE	C24-C14-OH5-C25
5	B	4006	1PE	C24-C14-OH5-C25
3	A	1002	NAP	PA-O3-PN-O2N
5	B	4005	1PE	C23-C13-OH4-C24
3	B	4003	NAP	C2B-O2B-P2B-O3X
5	B	4005	1PE	OH5-C14-C24-OH4
5	B	4001	1PE	C16-C26-OH6-C15
5	D	4001	1PE	OH5-C14-C24-OH4
3	A	1002	NAP	O4B-C4B-C5B-O5B
5	C	1005	1PE	C23-C13-OH4-C24
5	D	4005	1PE	C16-C26-OH6-C15
5	C	1004	1PE	C23-C13-OH4-C24
5	C	1004	1PE	C25-C15-OH6-C26
5	C	1005	1PE	C12-C22-OH3-C23
5	C	1005	1PE	OH4-C13-C23-OH3
5	B	4006	1PE	C12-C22-OH3-C23
3	D	4003	NAP	PA-O3-PN-O2N
5	B	4001	1PE	OH6-C15-C25-OH5
3	A	1002	NAP	C3B-C4B-C5B-O5B
5	B	4006	1PE	C15-C25-OH5-C14
5	C	1004	1PE	C14-C24-OH4-C13
3	C	1002	NAP	C2B-O2B-P2B-O1X
5	B	4005	1PE	C24-C14-OH5-C25
3	B	4003	NAP	PA-O3-PN-O1N
5	C	1004	1PE	C15-C25-OH5-C14
3	C	1002	NAP	O4B-C4B-C5B-O5B

There are no ring outliers.

13 monomers are involved in 81 short contacts:

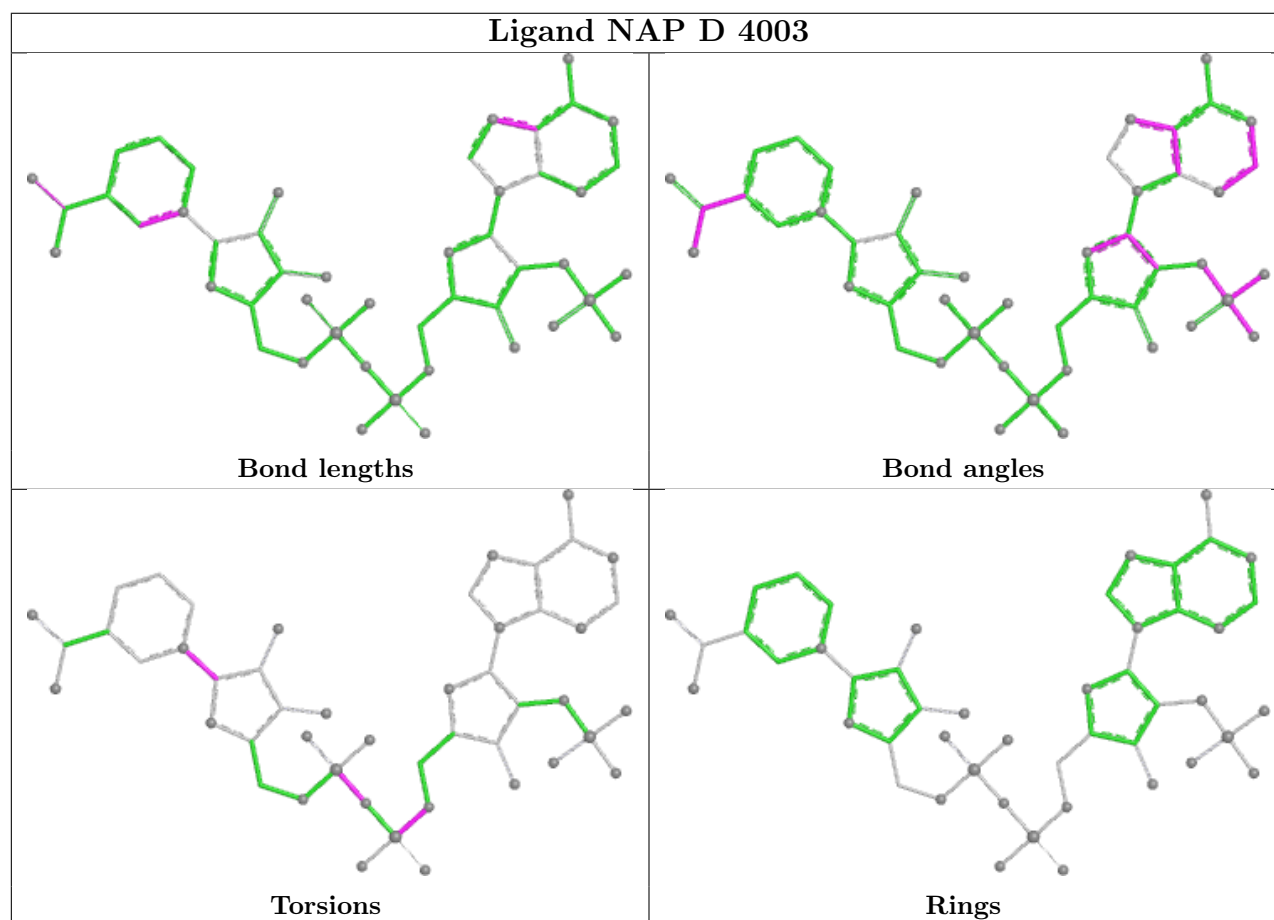
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	4001	1PE	3	0
5	D	4001	1PE	7	0
5	C	1005	1PE	11	0
5	B	4006	1PE	9	0
3	B	4003	NAP	2	0
5	B	4005	1PE	12	0
3	A	1002	NAP	1	0
5	D	4005	1PE	12	0
5	A	1004	1PE	9	0
3	C	1002	NAP	1	0
4	D	4004	PGO	3	0

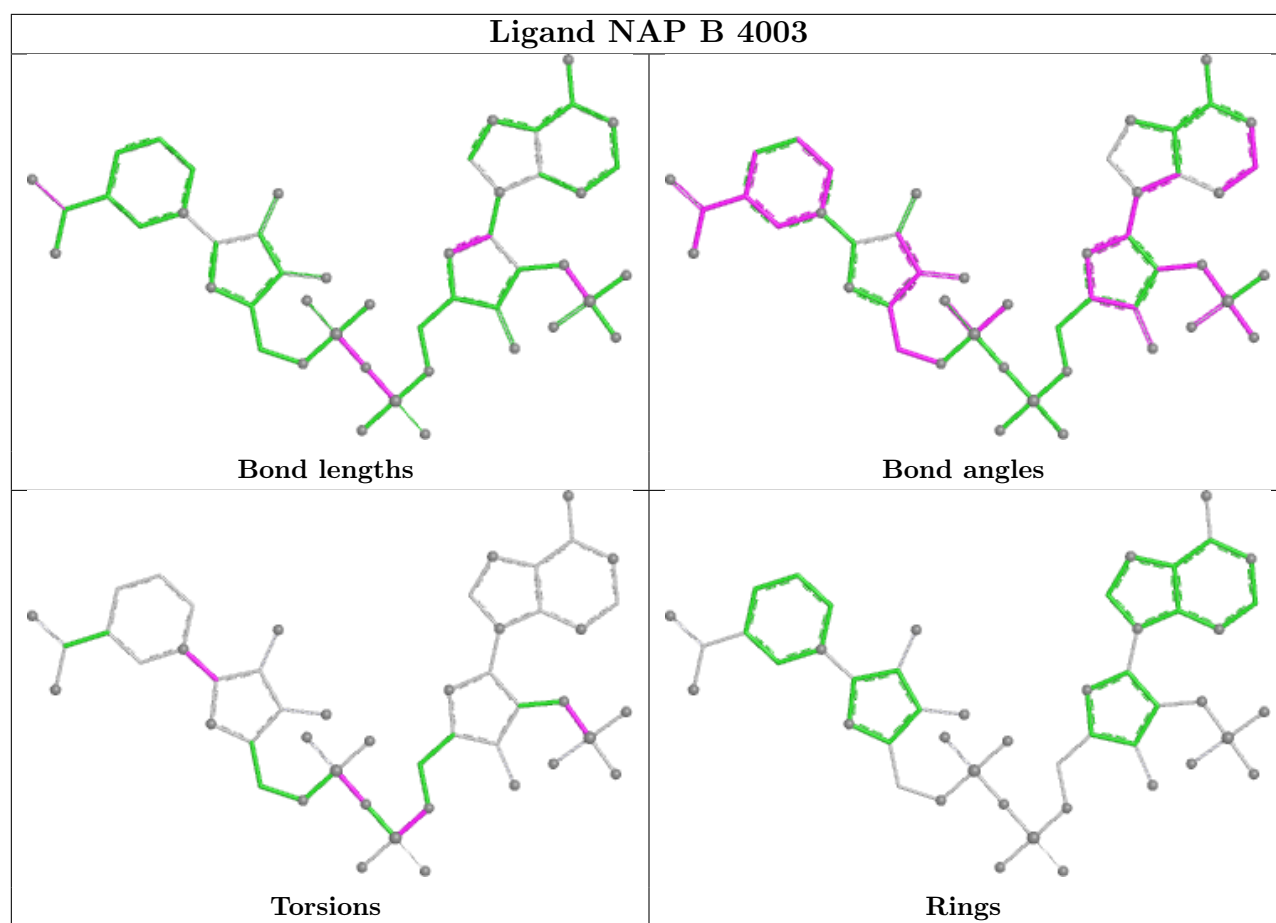
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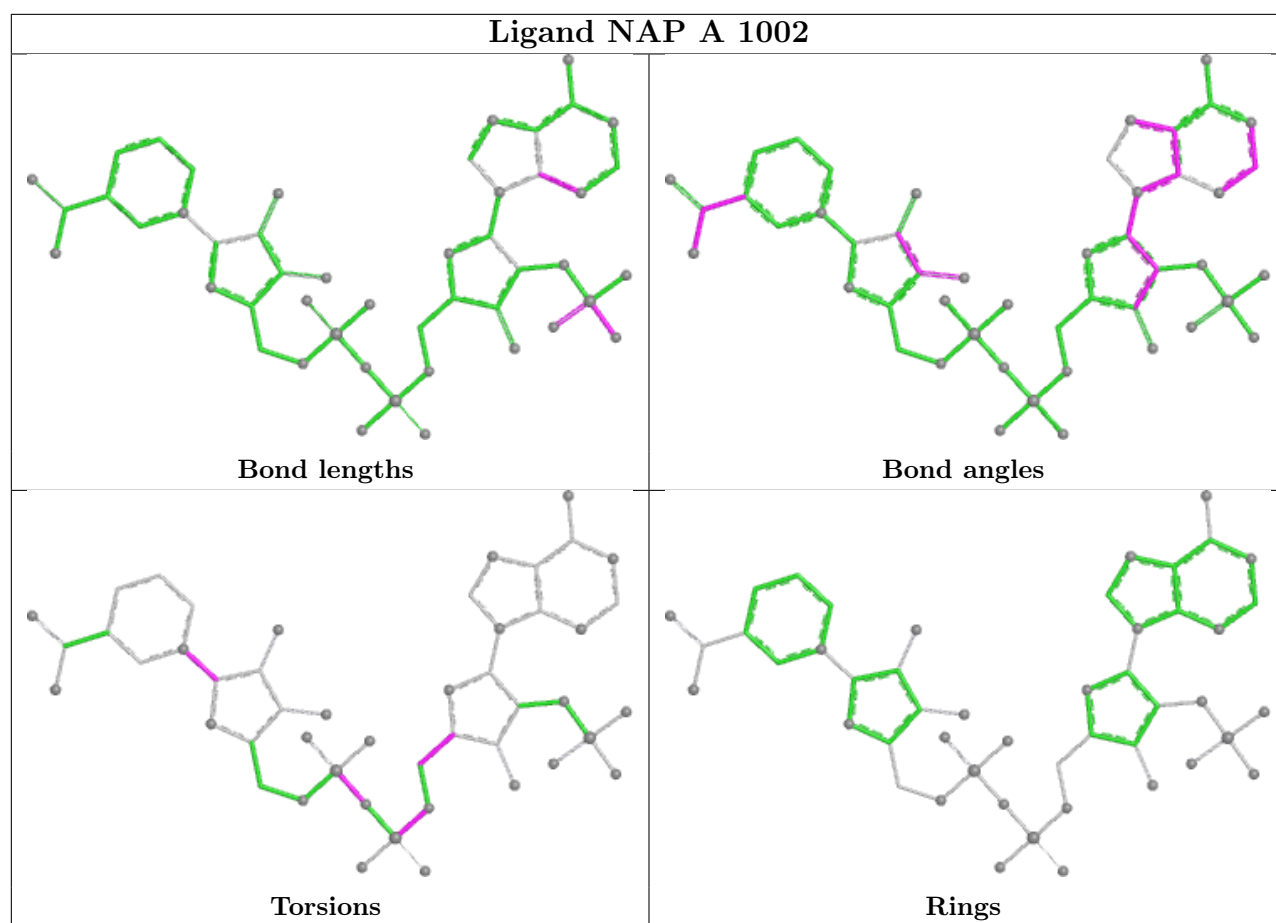
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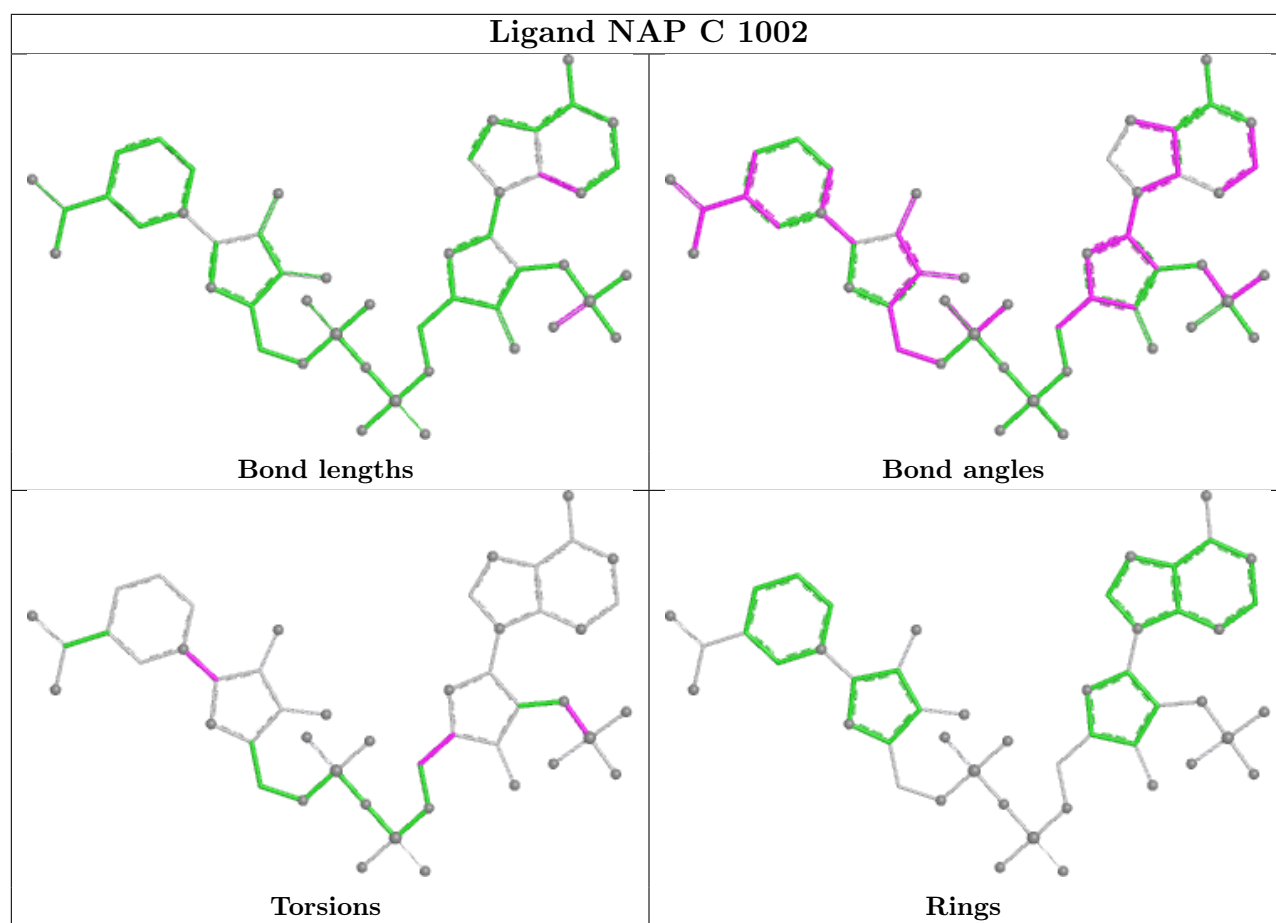
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1003	PGO	3	0
5	C	1004	1PE	8	0

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	360/369 (97%)	0.16	16 (4%) 34 37	27, 43, 64, 82	0
1	B	360/369 (97%)	-0.01	14 (3%) 39 42	24, 39, 61, 93	0
1	C	358/369 (97%)	0.00	10 (2%) 53 55	31, 50, 78, 104	0
1	D	360/369 (97%)	0.54	39 (10%) 5 5	26, 52, 85, 99	0
All	All	1438/1476 (97%)	0.18	79 (5%) 25 27	24, 45, 76, 104	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	62	ASN	5.5
1	D	26	PRO	4.8
1	D	24	PRO	4.0
1	D	3	THR	3.9
1	D	60	GLY	3.9
1	D	21	ILE	3.7
1	D	85	ARG	3.7
1	D	29	TYR	3.7
1	A	351	LYS	3.6
1	B	28	LYS	3.5
1	D	241	ASP	3.4
1	D	132	VAL	3.3
1	D	25	GLU	3.3
1	D	79	ASP	3.3
1	D	28	LYS	3.2
1	D	351	LYS	3.2
1	C	29	TYR	3.1
1	C	60	GLY	3.1
1	D	27	GLU	3.1
1	B	165	PHE	3.1
1	C	351	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	241	ASP	3.1
1	D	22	ASP	3.0
1	D	154	LEU	3.0
1	D	2	SER	3.0
1	D	63	PHE	3.0
1	D	20	LYS	3.0
1	B	351	LYS	3.0
1	D	5	ASN	2.9
1	D	134	TYR	2.9
1	D	84	LYS	2.8
1	A	165	PHE	2.7
1	B	170	VAL	2.6
1	D	76	ASP	2.6
1	C	17	LYS	2.6
1	B	310	ILE	2.6
1	A	239	LEU	2.6
1	C	352	GLY	2.5
1	A	240	LYS	2.5
1	D	222	GLU	2.5
1	A	352	GLY	2.5
1	B	348	GLN	2.4
1	A	241	ASP	2.4
1	B	167	VAL	2.4
1	D	157	PRO	2.4
1	C	240	LYS	2.4
1	B	171	VAL	2.4
1	D	242	MET	2.4
1	D	131	ASP	2.4
1	A	60	GLY	2.3
1	D	77	VAL	2.3
1	A	161	VAL	2.3
1	A	79	ASP	2.3
1	D	239	LEU	2.3
1	C	26	PRO	2.3
1	C	22	ASP	2.3
1	D	348	GLN	2.3
1	B	78	SER	2.2
1	D	41	CYS	2.2
1	A	168	PHE	2.2
1	A	222	GLU	2.2
1	C	2	SER	2.2
1	D	4	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	79	ASP	2.2
1	A	336	TYR	2.2
1	B	164	ALA	2.2
1	B	273	ILE	2.2
1	A	170	VAL	2.2
1	B	82	TYR	2.1
1	B	168	PHE	2.1
1	D	23	MET	2.1
1	D	171	VAL	2.1
1	A	164	ALA	2.1
1	D	153	VAL	2.1
1	A	171	VAL	2.1
1	A	204	VAL	2.1
1	D	74	VAL	2.0
1	D	82	TYR	2.0
1	D	352	GLY	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.

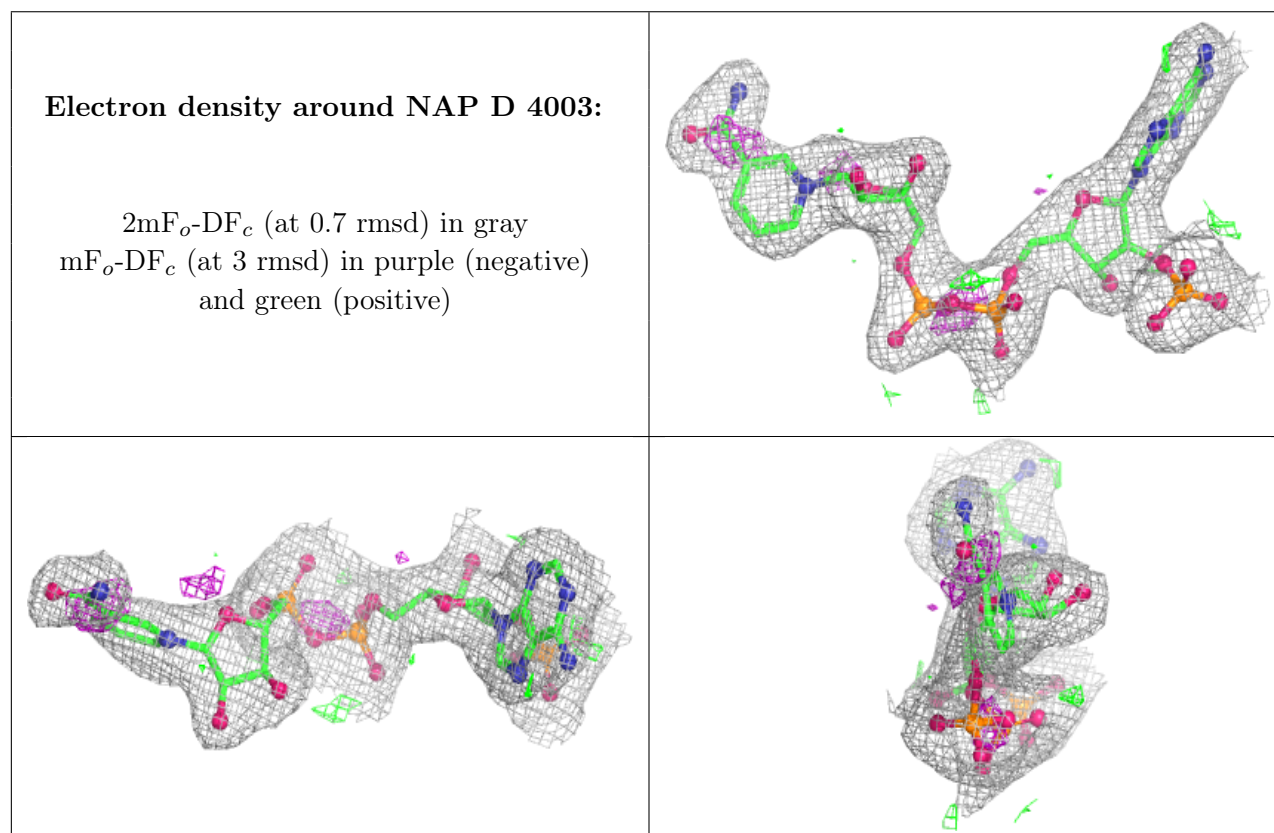
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	1PE	B	4005	16/16	0.74	0.32	43,56,63,64	0
5	1PE	B	4001	16/16	0.77	0.26	44,52,56,57	0
5	1PE	D	4001	16/16	0.79	0.23	37,51,61,62	0
5	1PE	C	1005	16/16	0.80	0.25	34,50,62,62	0
5	1PE	A	1004	16/16	0.83	0.26	42,50,61,64	0
5	1PE	B	4006	16/16	0.83	0.20	38,47,53,55	0
5	1PE	D	4005	16/16	0.87	0.27	46,54,69,72	0

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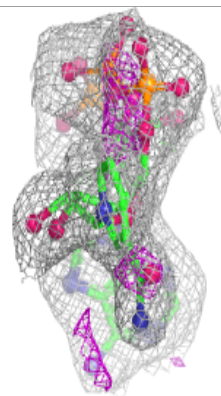
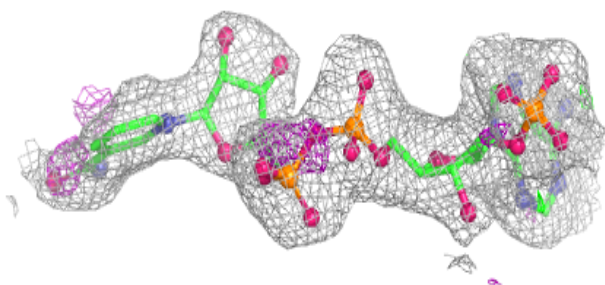
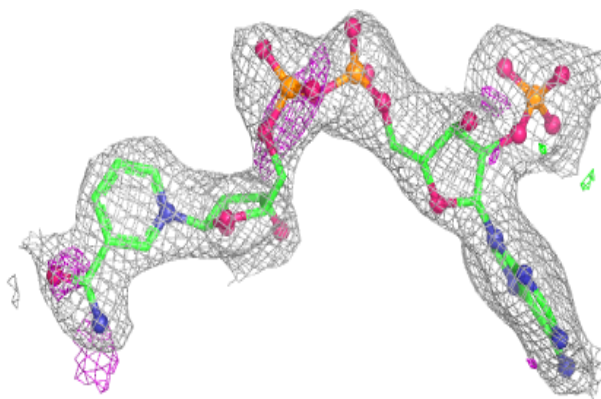
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	1PE	C	1004	16/16	0.88	0.20	41,55,63,65	0
4	PGO	C	1003	5/5	0.89	0.12	42,48,54,59	0
4	PGO	D	4004	5/5	0.89	0.27	48,52,57,61	0
3	NAP	D	4003	48/48	0.90	0.13	37,54,66,68	0
3	NAP	C	1002	48/48	0.91	0.13	43,62,75,78	0
3	NAP	A	1002	48/48	0.91	0.12	42,55,61,66	0
3	NAP	B	4003	48/48	0.92	0.13	39,50,68,71	0
4	PGO	A	1003	5/5	0.97	0.12	45,47,49,51	0
4	PGO	B	4004	5/5	0.98	0.15	43,43,47,51	0
2	ZN	B	4002	1/1	0.99	0.08	31,31,31,31	0
2	ZN	C	1001	1/1	0.99	0.09	34,34,34,34	0
2	ZN	A	1001	1/1	0.99	0.08	36,36,36,36	0
2	ZN	D	4002	1/1	1.00	0.08	38,38,38,38	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.

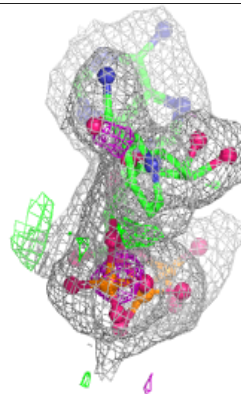
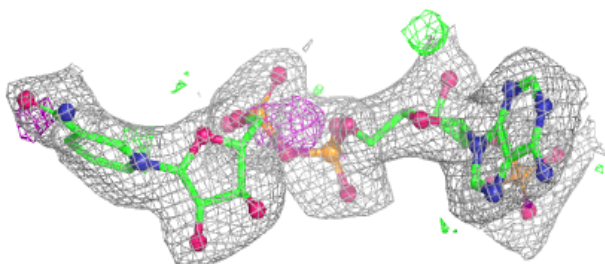
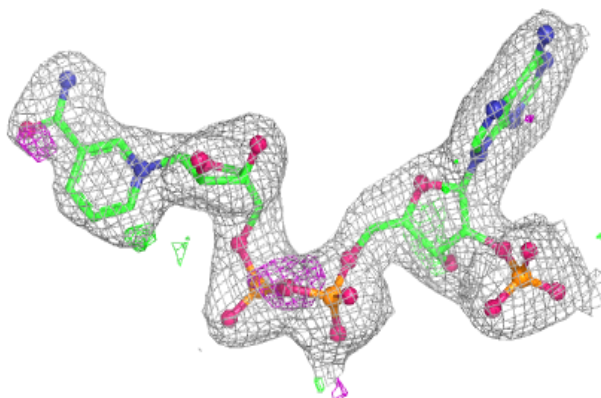


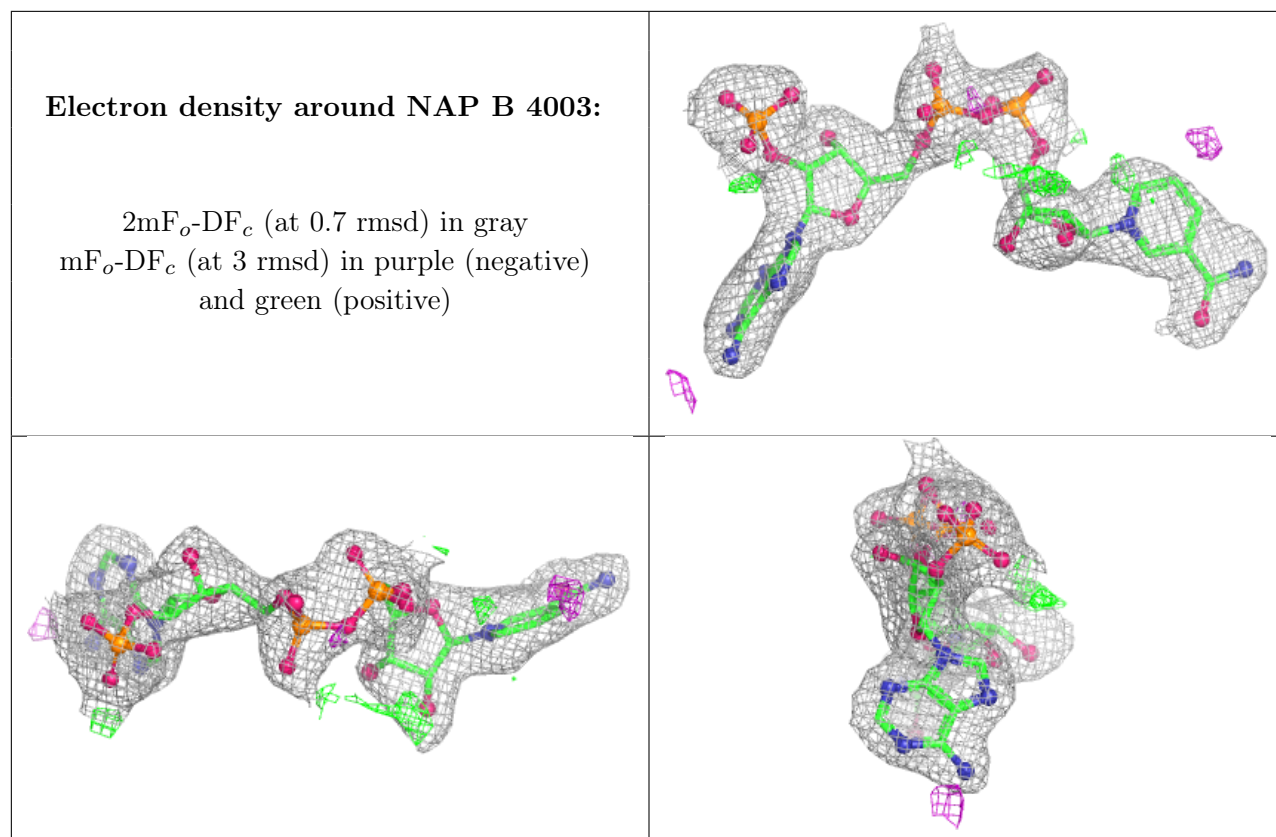
**Electron density around NAP C 1002:**

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

**Electron density around NAP A 1002:**

$2mF_o-DF_c$  (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.