



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:10 PM UTC

PDB ID : 3WID / pdb_00003wid
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

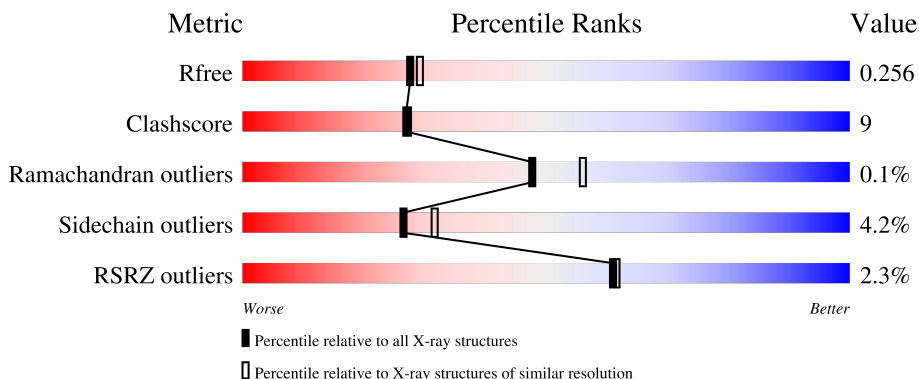
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (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 ≥ 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	 80% 16% ..
1	B	369	 81% 14% ..
1	C	369	 4% 80% 16% ..
1	D	369	 5% 77% 18% ..

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 [i](#)

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
			Total	C	N	O	S			
1	A	360	2827	1804	473	537	13	0	0	0
1	B	360	2827	1804	473	537	13	0	0	0
1	C	358	2809	1793	470	533	13	0	0	0
1	D	360	2827	1804	473	537	13	0	0	0

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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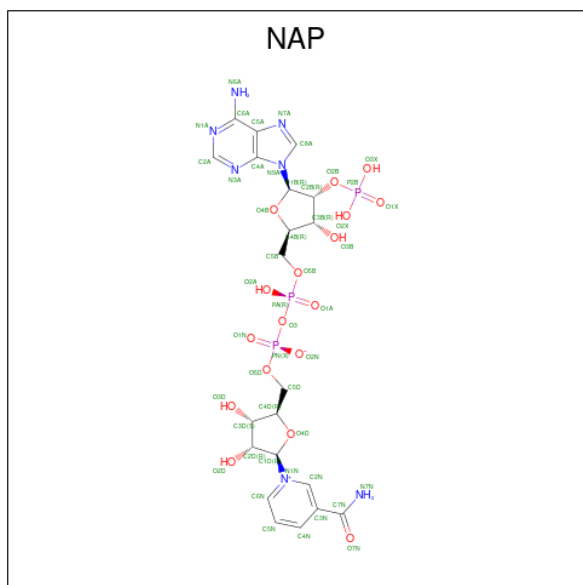
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Chain	Residue	Modelled	Actual	Comment	Reference
C	364	HIS	-	expression tag	UNP Q979W2
C	365	HIS	-	expression tag	UNP Q979W2
C	366	HIS	-	expression tag	UNP Q979W2
C	367	HIS	-	expression tag	UNP Q979W2
C	368	HIS	-	expression tag	UNP Q979W2
C	369	HIS	-	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 (CCD ID: ZN) (formula: Zn).

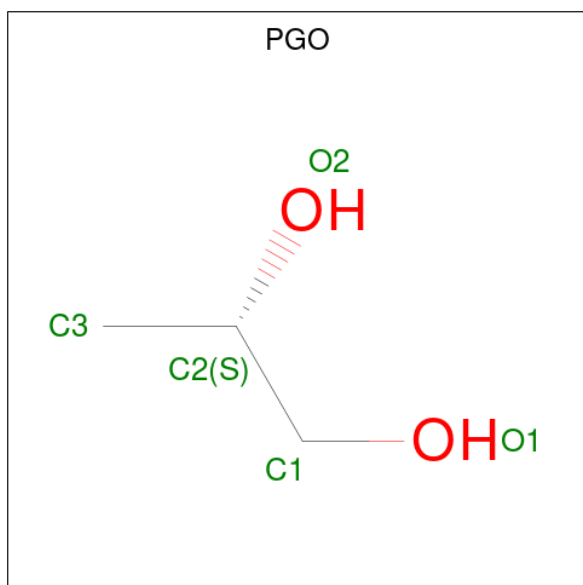
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



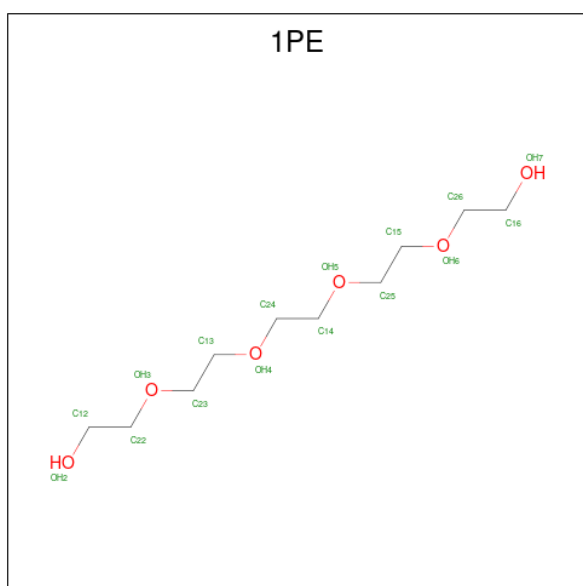
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	C	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	D	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 4 is S-1,2-PROPANEDIOL (CCD ID: PGO) (formula: $C_3H_8O_2$).



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

- Molecule 5 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



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

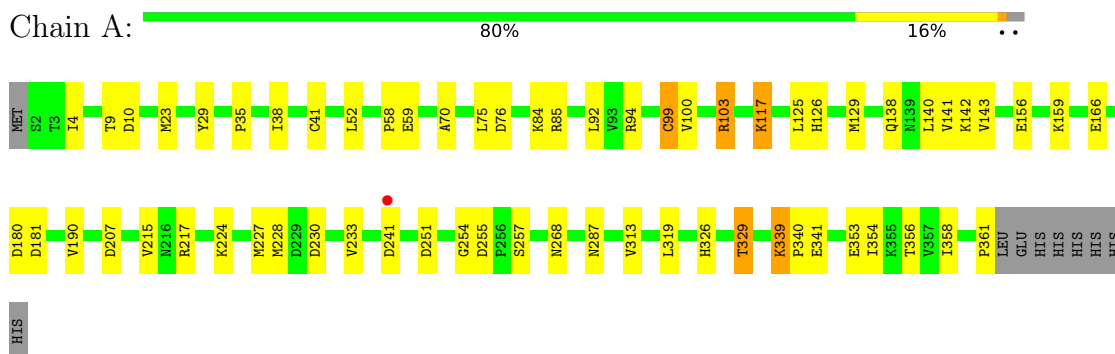
- Molecule 6 is water.

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

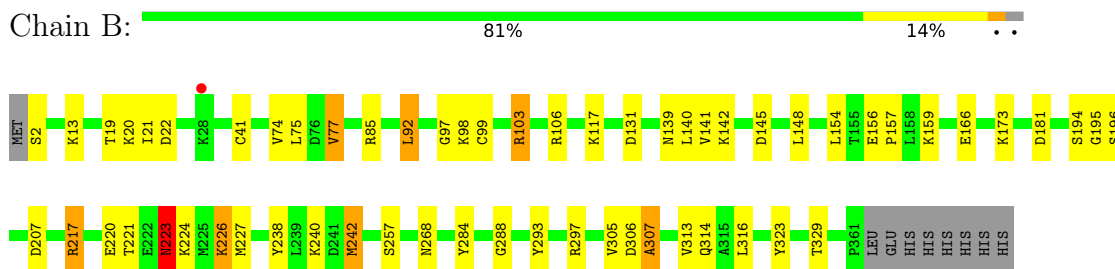
3 Residue-property plots [i](#)

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.

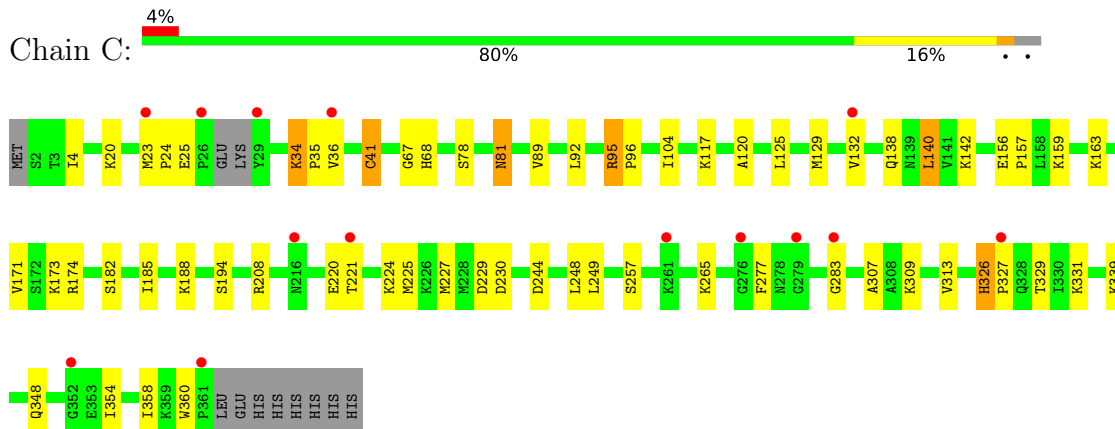
- Molecule 1: Glucose 1-dehydrogenase



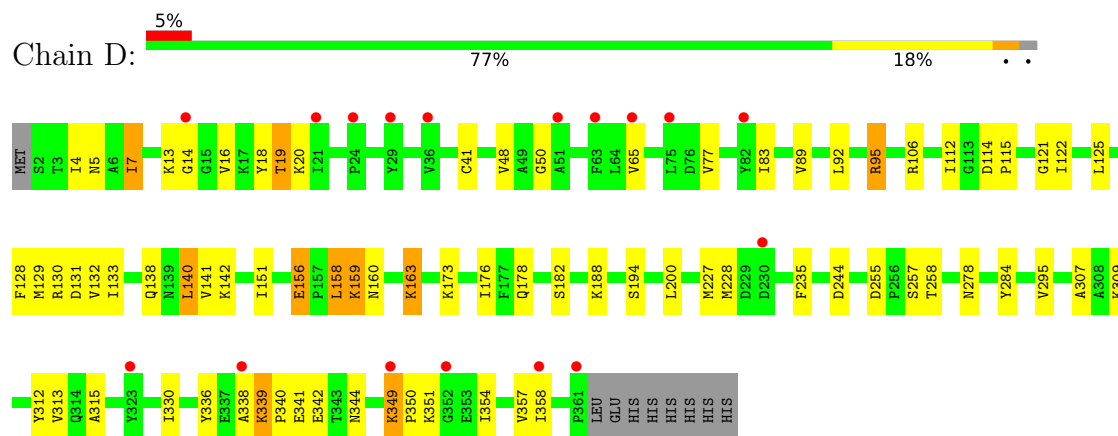
- Molecule 1: Glucose 1-dehydrogenase



- Molecule 1: Glucose 1-dehydrogenase



- Molecule 1: Glucose 1-dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.17Å 90.35Å 120.37Å 90.00° 90.84° 90.00°	Depositor
Resolution (Å)	39.27 – 2.25 39.27 – 2.25	Depositor EDS
% Data completeness (in resolution range)	94.3 (39.27-2.25) 94.3 (39.27-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.60 (at 2.24Å)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.197 , 0.251 (Not available) , 0.256	Depositor DCC
R_{free} test set	3881 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	39.1	Xtrriage
Anisotropy	0.478	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.012 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11962	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.21	5/2887 (0.2%)	1.10	5/3904 (0.1%)
1	B	1.29	7/2887 (0.2%)	1.14	3/3904 (0.1%)
1	C	1.09	4/2868 (0.1%)	1.11	5/3878 (0.1%)
1	D	1.07	2/2887 (0.1%)	1.12	5/3904 (0.1%)
All	All	1.17	18/11529 (0.2%)	1.12	18/15590 (0.1%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	70	ALA	CA-C	-6.81	1.44	1.52
1	A	207	ASP	C-O	-6.39	1.16	1.24
1	B	207	ASP	C-O	-6.23	1.16	1.24
1	B	145	ASP	C-O	-5.85	1.17	1.24
1	A	319	LEU	C-O	-5.83	1.17	1.24
1	C	326	HIS	C-N	5.79	1.41	1.33
1	B	223	ASN	CA-CB	5.72	1.62	1.53
1	C	95	ARG	C-N	5.51	1.40	1.33
1	B	195	GLY	C-O	-5.49	1.18	1.23
1	C	96	PRO	N-CD	5.46	1.55	1.47
1	D	200	LEU	CA-C	5.38	1.59	1.52
1	D	112	ILE	C-O	-5.31	1.17	1.23
1	B	103	ARG	CD-NE	-5.30	1.38	1.46
1	B	307	ALA	C-O	-5.22	1.17	1.23
1	B	131	ASP	CA-C	-5.22	1.45	1.52
1	A	190	VAL	N-CA	-5.19	1.40	1.46
1	C	327	PRO	N-CD	5.07	1.54	1.47
1	A	215	VAL	N-CA	-5.03	1.40	1.46

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	14	GLY	N-CA-C	7.39	119.84	110.38
1	B	240	LYS	N-CA-C	7.38	119.40	111.36
1	D	156	GLU	CA-C-N	-7.16	111.60	119.19
1	D	156	GLU	C-N-CA	-7.16	111.60	119.19
1	A	255	ASP	CA-C-N	6.66	126.17	119.24
1	A	255	ASP	C-N-CA	6.66	126.17	119.24
1	C	95	ARG	CA-C-N	-5.84	113.95	120.14
1	C	95	ARG	C-N-CA	-5.84	113.95	120.14
1	C	36	VAL	N-CA-C	-5.74	107.09	111.62
1	A	251	ASP	N-CA-C	5.67	118.20	109.07
1	B	323	TYR	N-CA-C	5.57	117.35	111.28
1	B	223	ASN	N-CA-C	-5.49	104.98	110.97
1	A	254	GLY	N-CA-C	-5.48	107.70	115.43
1	D	295	VAL	N-CA-C	5.46	115.91	110.23
1	D	163	LYS	N-CA-C	-5.32	105.49	111.28
1	A	166	GLU	N-CA-C	-5.14	105.75	111.36
1	C	326	HIS	CA-C-N	-5.08	113.69	119.28
1	C	326	HIS	C-N-CA	-5.08	113.69	119.28

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	2827	0	2808	42	0
1	B	2827	0	2808	50	0
1	C	2809	0	2788	46	0
1	D	2827	0	2808	65	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	18	0
6	A	92	0	0	3	0
6	B	109	0	0	5	0
6	C	58	0	0	8	0
6	D	69	0	0	3	0
All	All	11962	0	11520	212	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 (212) 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:D:227:MET:HE1	1:D:354:ILE:CD1	1.93	0.98
1:B:106:ARG:HD3	5:B:4005:1PE:H241	1.49	0.95
1:D:227:MET:HE1	1:D:354:ILE:HD11	1.48	0.91
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:A:224:LYS:HA	1:A:227:MET:HE3	1.59	0.84
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: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:D:309:LYS:HZ3	5:D:4005:1PE:H151	1.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:309:LYS:HZ1	5:C:1004:1PE:H152	1.57	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
1:A:227:MET:HE1	1:A:354:ILE:HD11	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: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:C:224:LYS:HA	1:C:227:MET:HE3	1.81	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: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
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:D:227:MET:HE1	1:D:354:ILE:HD13	1.84	0.56
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:309:LYS:NZ	5:D:4005:1PE:H151	2.21	0.54
1:B:154:LEU:C	1:B:157:PRO:HD2	2.33	0.54
1:D:313:VAL:HA	5:D:4005:1PE:H121	1.88	0.54
1:B:99:CYS:O	1:B:103:ARG:HD3	2.08	0.54
1:B:314:GLN:CD	6:B:4169:HOH:O	2.51	0.54
1:A:126:HIS:O	4:A:1003:PGO:O2	2.24	0.54
1:D:176:ILE:HG23	5:D:4001:1PE:H262	1.90	0.53
1:C:129:MET:HE2	1:C:358:ILE:HD12	1.89	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: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:A:29:TYR:OH	1:A:76:ASP:OD2	2.25	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:O	1:B:217:ARG:HG2	2.14	0.48
1:A:129:MET:HE2	1:A:358:ILE:HD12	1.95	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:C:309:LYS:HZ1	5:C:1004:1PE:C15	2.25	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
1:B:173:LYS:HE2	5:B:4001:1PE:C22	2.35	0.47
1:D:339:LYS:O	1:D:340:PRO:C	2.57	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:D:121:GLY:C	1:D:122:ILE:HG13	2.41	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:D:138:GLN:O	1:D:309:LYS:NZ	2.48	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:117:LYS:HD2	1:C:117:LYS:C	2.42	0.44
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:A:224:LYS:CA	1:A:227:MET:HE3	2.38	0.44
1:B:316:LEU:HB2	5:B:4006:1PE:H122	2.00	0.44
1:C:230:ASP:OD2	1:C:329:THR:OG1	2.22	0.44
1:A:227:MET:HE1	1:A:354:ILE:CD1	2.47	0.44
1:C:227:MET:HE1	1:C:354:ILE:HD11	2.00	0.43
1:D:5:ASN:HB3	1:D:18:TYR:CE1	2.53	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:84:LYS:O	1:A:85:ARG:C	2.61	0.42
1:D:349:LYS:O	1:D:350:PRO:C	2.61	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:A:180:ASP:OD1	1:A:180:ASP:C	2.61	0.42
1:D:158:LEU:HD13	1:D:315:ALA:CA	2.47	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:B:97:GLY:C	1:B:98:LYS:HD2	2.45	0.42
1:A:353:GLU:OE1	1:A:356:THR:OG1	2.30	0.41
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:23:MET:HE3	1:C:24:PRO:HD2	2.03	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:114:ASP:CG	1:D:115:PRO:HA	2.46	0.40
1:D:255:ASP:OD2	1:D:258:THR:OG1	2.21	0.40
1:D:284:TYR:CD1	1:D:284:TYR:C	2.99	0.40
1:B:220:GLU:CD	1:B:224:LYS:HD2	2.46	0.40
1:D:95:ARG:HD2	1:D:95:ARG:N	2.36	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 [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	358/369 (97%)	347 (97%)	10 (3%)	1 (0%)	36	40
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%)	48	56

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	CYS

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	313/322 (97%)	302 (96%)	11 (4%)	32	39
1	B	313/322 (97%)	302 (96%)	11 (4%)	32	39
1	C	311/322 (97%)	293 (94%)	18 (6%)	18	19
1	D	313/322 (97%)	300 (96%)	13 (4%)	26	31
All	All	1250/1288 (97%)	1197 (96%)	53 (4%)	26	31

All (53) 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	143	VAL
1	A	257	SER
1	A	268	ASN
1	A	329	THR
1	A	339	LYS

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Mol	Chain	Res	Type
1	A	341	GLU
1	B	13	LYS
1	B	77	VAL
1	B	92	LEU
1	B	117	LYS
1	B	148	LEU
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	20	LYS
1	C	25	GLU
1	C	34	LYS
1	C	41	CYS
1	C	78	SER
1	C	81	ASN
1	C	92	LEU
1	C	140	LEU
1	C	188	LYS
1	C	194	SER
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
1	C	348	GLN
1	D	7	ILE
1	D	19	THR
1	D	92	LEU
1	D	95	ARG
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

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Mol	Chain	Res	Type
1	D	351	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	GLN
1	A	268	ASN
1	A	298	ASN
1	A	326	HIS
1	B	81	ASN
1	B	139	ASN
1	B	178	GLN
1	B	223	ASN
1	B	268	ASN
1	B	321	ASN
1	B	348	GLN
1	C	144	ASN
1	C	267	ASN
1	C	269	ASN
1	C	326	HIS
1	C	328	GLN
1	C	348	GLN
1	D	5	ASN
1	D	118	HIS
1	D	138	GLN
1	D	144	ASN
1	D	321	ASN
1	D	348	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 oligosaccharides 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	C	1005	-	15,15,15	1.08	0	14,14,14	1.21	2 (14%)
4	PGO	D	4004	-	4,4,4	0.42	0	4,4,4	1.21	1 (25%)
3	NAP	A	1002	-	50,52,52	1.36	6 (12%)	71,80,80	1.72	12 (16%)
3	NAP	C	1002	-	50,52,52	1.29	5 (10%)	71,80,80	1.87	24 (33%)
3	NAP	B	4003	-	50,52,52	1.34	6 (12%)	71,80,80	2.20	24 (33%)
4	PGO	A	1003	-	4,4,4	0.48	0	4,4,4	1.13	1 (25%)
5	1PE	A	1004	-	15,15,15	0.90	0	14,14,14	1.16	1 (7%)
5	1PE	C	1004	-	15,15,15	0.74	0	14,14,14	0.74	0
5	1PE	B	4006	-	15,15,15	1.08	1 (6%)	14,14,14	0.98	0
3	NAP	D	4003	-	50,52,52	1.39	6 (12%)	71,80,80	1.78	12 (16%)
5	1PE	D	4001	-	15,15,15	0.87	0	14,14,14	0.59	0
5	1PE	B	4005	-	15,15,15	1.07	0	14,14,14	1.07	0
5	1PE	D	4005	-	15,15,15	0.72	0	14,14,14	0.89	1 (7%)
4	PGO	C	1003	-	4,4,4	0.67	0	4,4,4	0.75	0
5	1PE	B	4001	-	15,15,15	1.09	1 (6%)	14,14,14	0.99	0
4	PGO	B	4004	-	4,4,4	0.48	0	4,4,4	0.69	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	C	1005	-	-	7/13/13/13	-
4	PGO	D	4004	-	-	2/2/2/2	-
3	NAP	A	1002	-	-	10/35/67/67	0/5/5/5
3	NAP	C	1002	-	-	6/35/67/67	0/5/5/5
3	NAP	B	4003	-	-	9/35/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PGO	A	1003	-	-	0/2/2/2	-
5	1PE	A	1004	-	-	4/13/13/13	-
5	1PE	C	1004	-	-	9/13/13/13	-
5	1PE	B	4006	-	-	6/13/13/13	-
3	NAP	D	4003	-	-	8/35/67/67	0/5/5/5
5	1PE	D	4001	-	-	8/13/13/13	-
5	1PE	B	4005	-	-	6/13/13/13	-
5	1PE	D	4005	-	-	6/13/13/13	-
4	PGO	C	1003	-	-	0/2/2/2	-
5	1PE	B	4001	-	-	6/13/13/13	-
4	PGO	B	4004	-	-	0/2/2/2	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4003	NAP	C8A-N9A	-3.73	1.31	1.37
3	D	4003	NAP	C5A-N7A	-3.69	1.32	1.39
3	B	4003	NAP	PA-O3	3.68	1.63	1.59
3	A	1002	NAP	C4A-N9A	-3.59	1.30	1.37
3	B	4003	NAP	C5A-C4A	3.30	1.45	1.39
3	A	1002	NAP	C5A-N7A	-3.28	1.33	1.39
3	B	4003	NAP	O7N-C7N	3.26	1.30	1.24
3	C	1002	NAP	C5A-N7A	-3.24	1.33	1.39
3	C	1002	NAP	C4A-N9A	-3.12	1.31	1.37
3	B	4003	NAP	C4A-N9A	-3.04	1.31	1.37
3	C	1002	NAP	C5A-C4A	2.99	1.44	1.39
3	B	4003	NAP	PN-O3	2.84	1.62	1.59
3	A	1002	NAP	C8A-N9A	-2.73	1.32	1.37
3	A	1002	NAP	C5A-C4A	2.64	1.43	1.39
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	D	4003	NAP	C4A-N9A	-2.52	1.32	1.37
3	D	4003	NAP	C5A-C4A	2.52	1.43	1.39
3	D	4003	NAP	C2N-N1N	-2.34	1.32	1.35
3	C	1002	NAP	C8A-N9A	-2.29	1.33	1.37
3	A	1002	NAP	P2B-O3X	-2.13	1.46	1.54
3	A	1002	NAP	P2B-O2X	-2.11	1.47	1.54
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 (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4003	NAP	C5A-C4A-N3A	-6.78	117.38	126.72
3	B	4003	NAP	C4A-N9A-C8A	5.97	112.01	105.74
3	B	4003	NAP	O7N-C7N-C3N	5.73	126.60	119.60
3	D	4003	NAP	N3A-C4A-N9A	5.49	136.50	127.17
3	A	1002	NAP	C5A-C4A-N3A	-5.46	119.19	126.72
3	B	4003	NAP	C3N-C7N-N7N	-5.19	111.34	117.74
3	C	1002	NAP	C5A-C4A-N3A	-4.98	119.86	126.72
3	B	4003	NAP	N3A-C2A-N1A	-4.52	121.75	128.58
3	A	1002	NAP	N3A-C4A-N9A	4.42	134.69	127.17
3	D	4003	NAP	C2A-N3A-C4A	4.01	121.62	111.83
3	B	4003	NAP	O3X-P2B-O2X	3.99	122.75	107.80
3	A	1002	NAP	C2A-N3A-C4A	3.97	121.53	111.83
3	C	1002	NAP	N3A-C2A-N1A	-3.91	122.67	128.58
3	C	1002	NAP	C2A-N3A-C4A	3.87	121.28	111.83
3	A	1002	NAP	N3A-C2A-N1A	-3.85	122.75	128.58
3	C	1002	NAP	N3A-C4A-N9A	3.83	133.69	127.17
3	D	4003	NAP	C4A-C5A-N7A	-3.80	106.24	110.58
3	B	4003	NAP	C4A-N9A-C1B	-3.74	117.88	126.63
3	B	4003	NAP	N3A-C4A-N9A	3.69	133.44	127.17
3	B	4003	NAP	N9A-C8A-N7A	-3.63	108.78	113.94
3	D	4003	NAP	O4B-C1B-C2B	-3.58	100.42	106.59
3	B	4003	NAP	C5N-C6N-N1N	-3.57	115.52	120.38
3	A	1002	NAP	C4A-N9A-C8A	3.56	109.48	105.74
3	C	1002	NAP	C4A-C5A-N7A	-3.56	106.51	110.58
3	C	1002	NAP	O2D-C2D-C3D	-3.26	101.35	111.82
3	B	4003	NAP	C2A-N1A-C6A	3.23	124.03	118.73
3	C	1002	NAP	C4A-N9A-C8A	3.22	109.12	105.74
3	A	1002	NAP	C4A-C5A-N7A	-3.21	106.91	110.58
3	D	4003	NAP	N3A-C2A-N1A	-3.20	123.75	128.58
3	B	4003	NAP	C5A-C4A-N3A	-3.17	122.35	126.72
3	D	4003	NAP	C4A-N9A-C8A	3.16	109.06	105.74
3	D	4003	NAP	C5A-N7A-C8A	3.07	108.27	103.45
3	B	4003	NAP	C2A-N3A-C4A	2.97	119.08	111.83
3	C	1002	NAP	O2B-P2B-O1X	-2.96	98.78	109.33
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
3	C	1002	NAP	O4B-C1B-N9A	2.88	113.61	108.09
3	C	1002	NAP	C5A-N7A-C8A	2.84	107.92	103.45
5	C	1005	1PE	OH5-C25-C15	2.80	123.13	110.35
3	C	1002	NAP	N9A-C8A-N7A	-2.77	110.00	113.94
3	C	1002	NAP	O4B-C1B-C2B	-2.75	101.85	106.59
3	B	4003	NAP	C6A-C5A-N7A	2.74	137.36	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	C6A-C5A-N7A	2.61	137.13	132.09
3	A	1002	NAP	N9A-C8A-N7A	-2.61	110.23	113.94
3	D	4003	NAP	N9A-C8A-N7A	-2.56	110.31	113.94
3	C	1002	NAP	C3N-C7N-N7N	2.44	120.74	117.74
3	A	1002	NAP	C5A-N7A-C8A	2.42	107.26	103.45
3	C	1002	NAP	C5B-C4B-C3B	-2.42	106.50	115.21
3	B	4003	NAP	C4A-C5A-N7A	-2.42	107.82	110.58
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	B	4003	NAP	C5A-N7A-C8A	2.36	107.16	103.45
3	A	1002	NAP	C6A-C5A-N7A	2.25	136.44	132.09
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	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	C	1002	NAP	C2A-N1A-C6A	2.11	122.19	118.73
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	C	1002	NAP	C4A-N9A-C1B	-2.09	121.73	126.63
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	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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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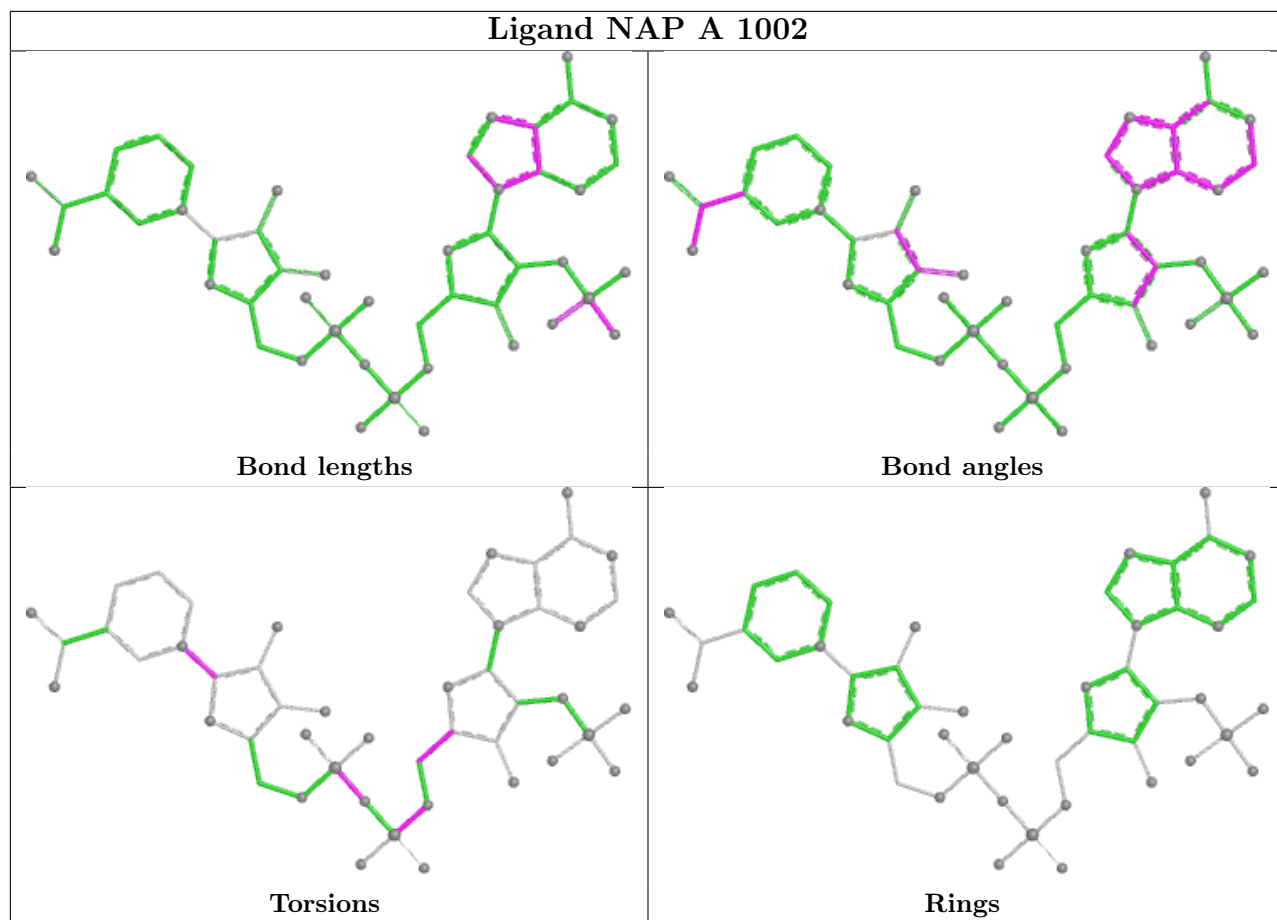
Mol	Chain	Res	Type	Atoms
5	C	1004	1PE	C15-C25-OH5-C14
3	C	1002	NAP	O4B-C4B-C5B-O5B

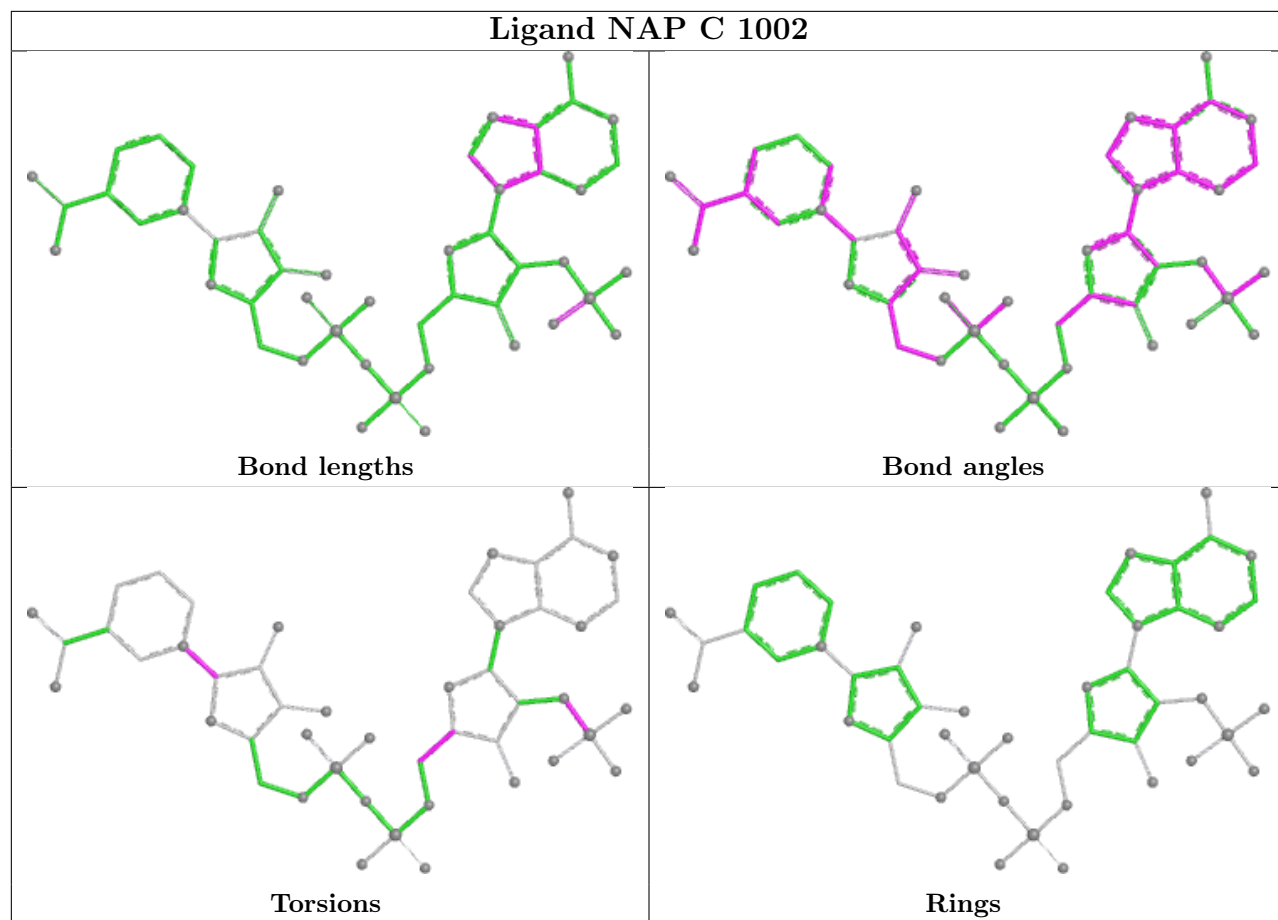
There are no ring outliers.

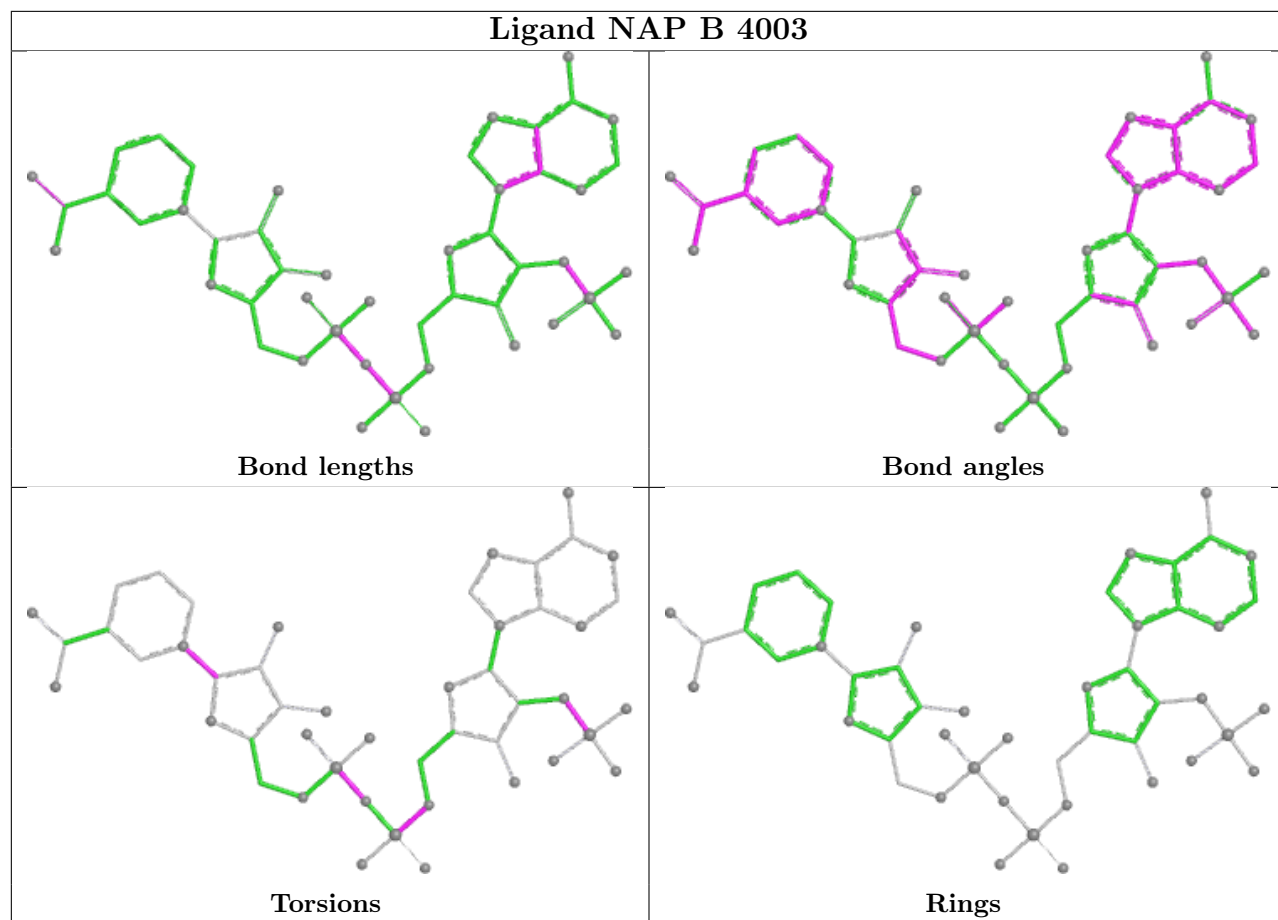
13 monomers are involved in 80 short contacts:

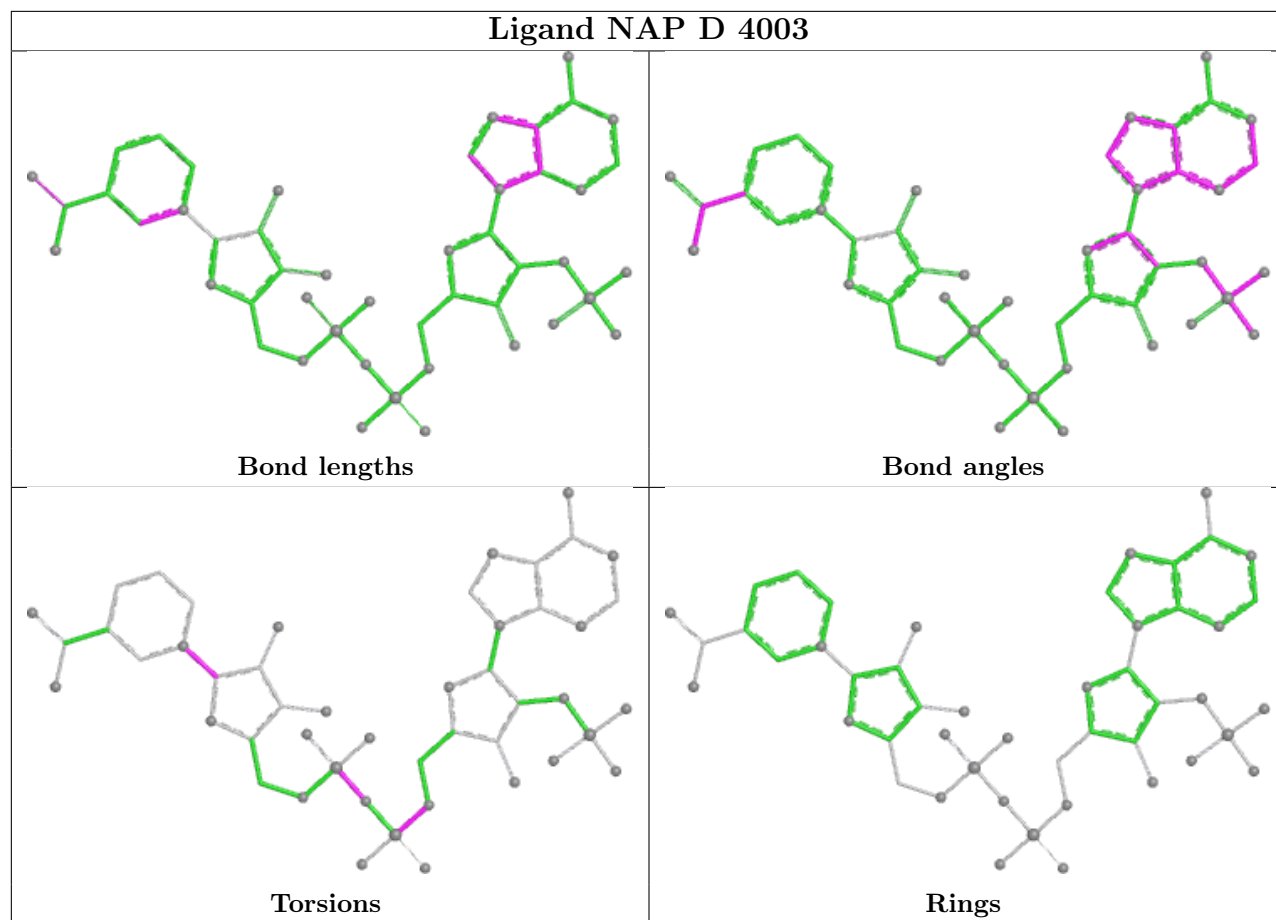
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1005	1PE	11	0
4	D	4004	PGO	3	0
3	A	1002	NAP	1	0
3	C	1002	NAP	1	0
3	B	4003	NAP	2	0
4	A	1003	PGO	3	0
5	A	1004	1PE	9	0
5	C	1004	1PE	8	0
5	B	4006	1PE	9	0
5	D	4001	1PE	7	0
5	B	4005	1PE	12	0
5	D	4005	1PE	11	0
5	B	4001	1PE	3	0

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









5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	360/369 (97%)	0.09	1 (0%) 90 90	27, 43, 64, 82	0
1	B	360/369 (97%)	-0.10	1 (0%) 90 90	24, 39, 61, 93	0
1	C	358/369 (97%)	0.43	14 (3%) 43 43	31, 50, 78, 104	0
1	D	360/369 (97%)	0.52	17 (4%) 36 35	26, 52, 85, 99	0
All	All	1438/1476 (97%)	0.23	33 (2%) 61 61	24, 45, 76, 104	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	352	GLY	3.9
1	D	14	GLY	3.8
1	C	279	GLY	3.6
1	C	26	PRO	3.2
1	C	352	GLY	2.9
1	D	361	PRO	2.8
1	C	216	ASN	2.7
1	D	24	PRO	2.6
1	C	261	LYS	2.6
1	C	132	VAL	2.6
1	D	349	LYS	2.5
1	C	283	GLY	2.5
1	C	29	TYR	2.4
1	C	361	PRO	2.4
1	D	338	ALA	2.4
1	D	63	PHE	2.4
1	C	23	MET	2.3
1	C	221	THR	2.3
1	D	36	VAL	2.3
1	B	28	LYS	2.3
1	C	276	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	21	ILE	2.3
1	D	82	TYR	2.2
1	D	75	LEU	2.2
1	D	29	TYR	2.2
1	C	327	PRO	2.2
1	D	65	VAL	2.1
1	D	358	ILE	2.1
1	D	230	ASP	2.1
1	C	36	VAL	2.1
1	D	51	ALA	2.1
1	A	241	ASP	2.1
1	D	323	TYR	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

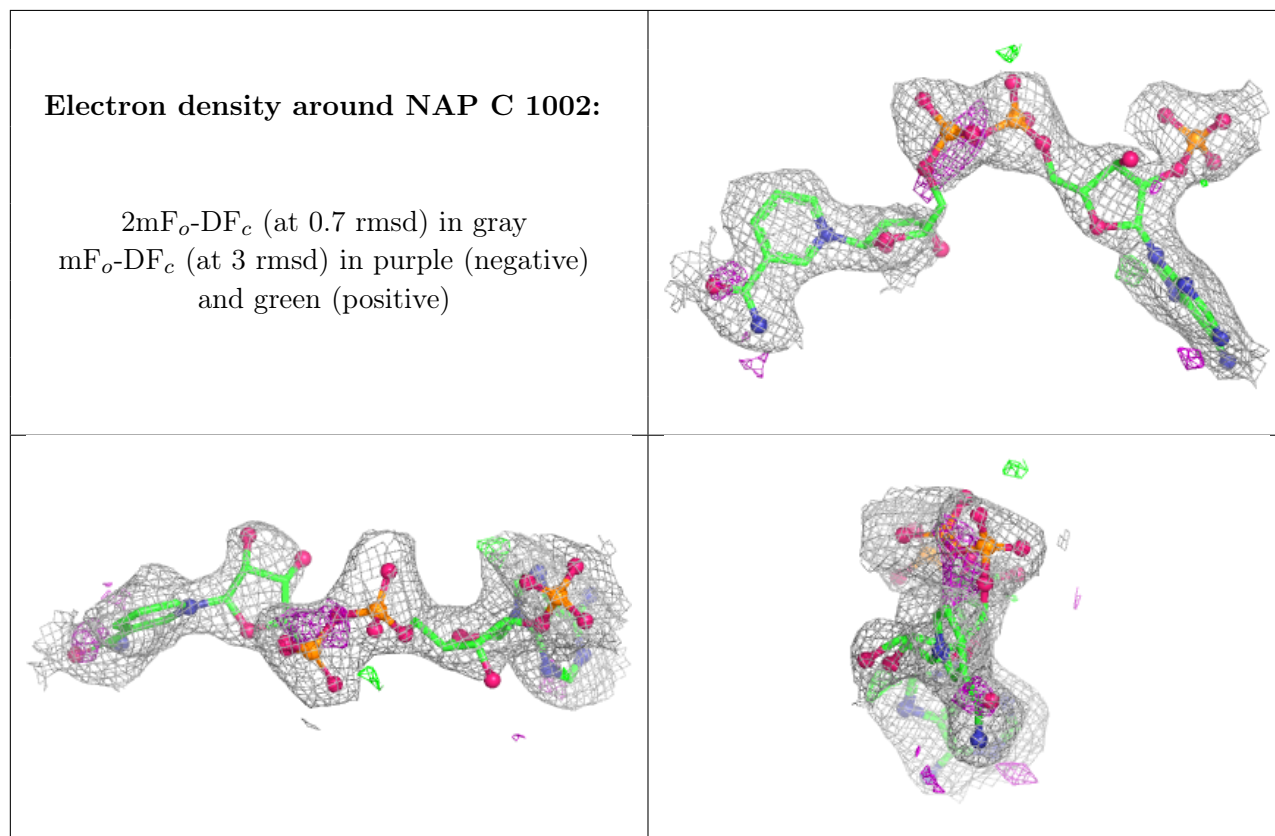
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	1PE	B	4005	16/16	0.75	0.17	43,56,63,64	0
5	1PE	D	4005	16/16	0.75	0.16	46,54,69,72	0
4	PGO	D	4004	5/5	0.80	0.12	48,52,57,61	0
5	1PE	B	4006	16/16	0.81	0.13	38,47,53,55	0
5	1PE	B	4001	16/16	0.82	0.13	44,52,56,57	0
4	PGO	C	1003	5/5	0.82	0.14	42,48,54,59	0
5	1PE	D	4001	16/16	0.83	0.14	37,51,61,62	0
5	1PE	A	1004	16/16	0.83	0.13	42,50,61,64	0
5	1PE	C	1005	16/16	0.85	0.14	34,50,62,62	0
5	1PE	C	1004	16/16	0.87	0.11	41,55,63,65	0
3	NAP	C	1002	48/48	0.88	0.13	43,62,75,78	0

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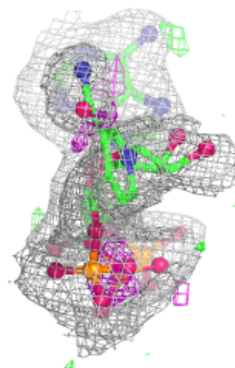
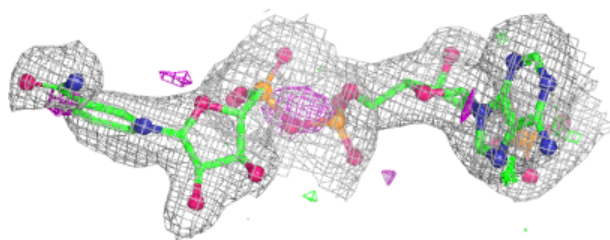
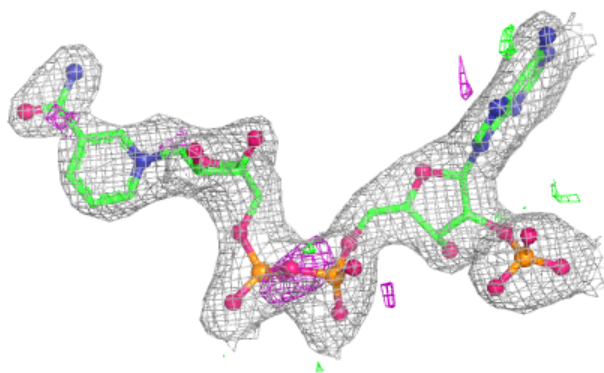
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAP	D	4003	48/48	0.89	0.12	37,54,66,68	0
3	NAP	A	1002	48/48	0.90	0.11	42,55,61,66	0
3	NAP	B	4003	48/48	0.93	0.10	39,50,68,71	0
4	PGO	A	1003	5/5	0.94	0.08	45,47,49,51	0
4	PGO	B	4004	5/5	0.96	0.10	43,43,47,51	0
2	ZN	A	1001	1/1	0.99	0.02	36,36,36,36	0
2	ZN	B	4002	1/1	0.99	0.02	31,31,31,31	0
2	ZN	C	1001	1/1	0.99	0.02	34,34,34,34	0
2	ZN	D	4002	1/1	0.99	0.02	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.

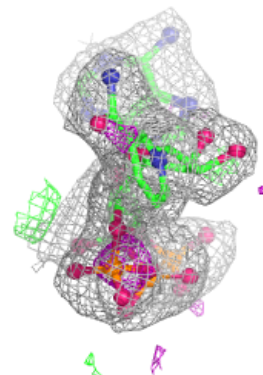
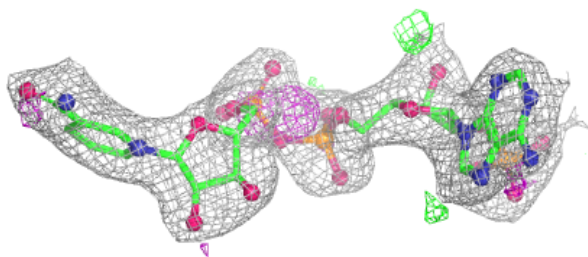
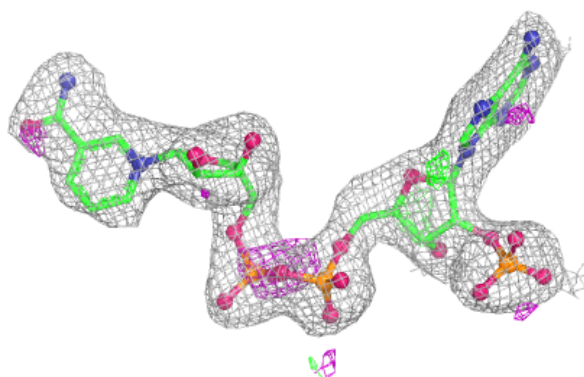


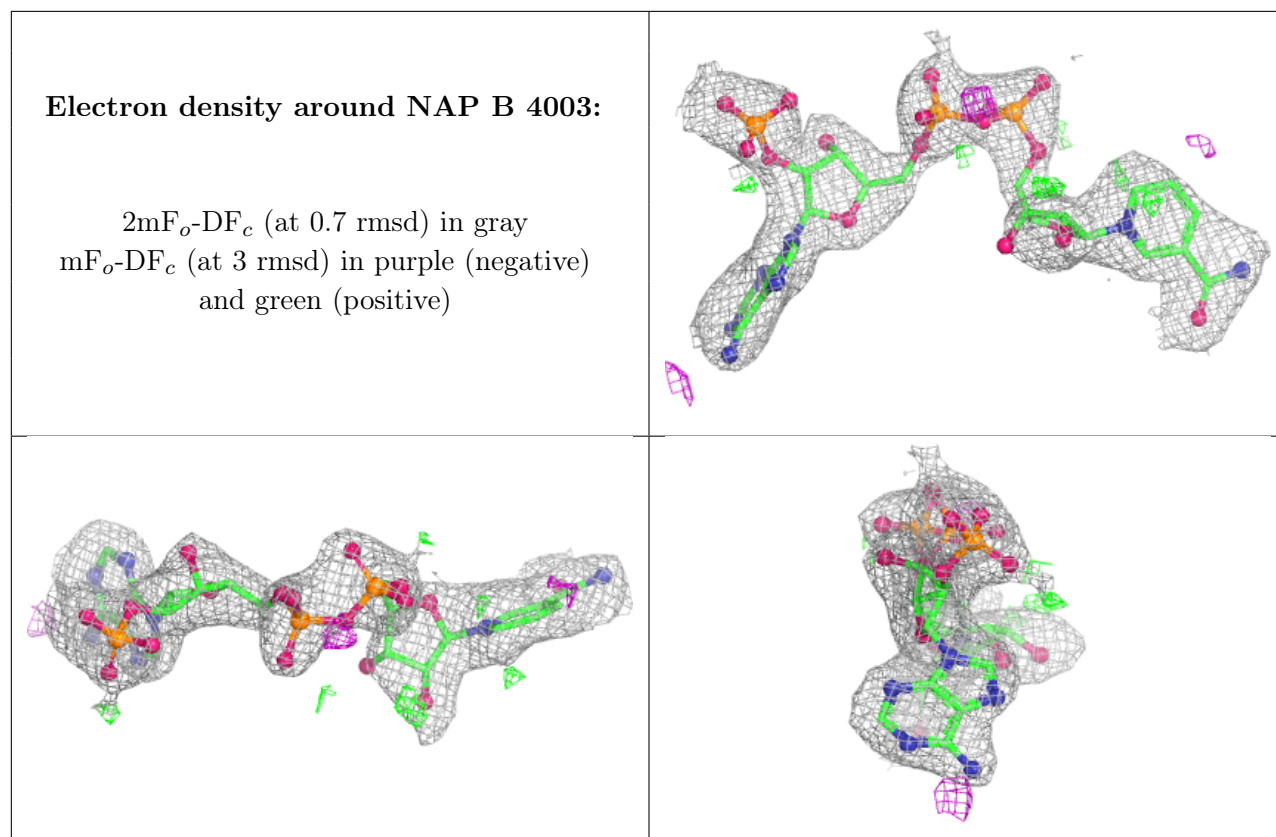
Electron density around NAP D 4003:

$2mF_o-DF_c$ (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.