



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 02:13 pm BST

PDB ID : 4GNZ
Title : Crystal structure of the c707s mutant of c-terminal domain of 10'formyltetrahydrofolate dehydrogenase in complex with NADP
Authors : Tsybovsky, Y.
Deposited on : 2012-08-17
Resolution : 2.30 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 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 : 2.11
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) : 2.11

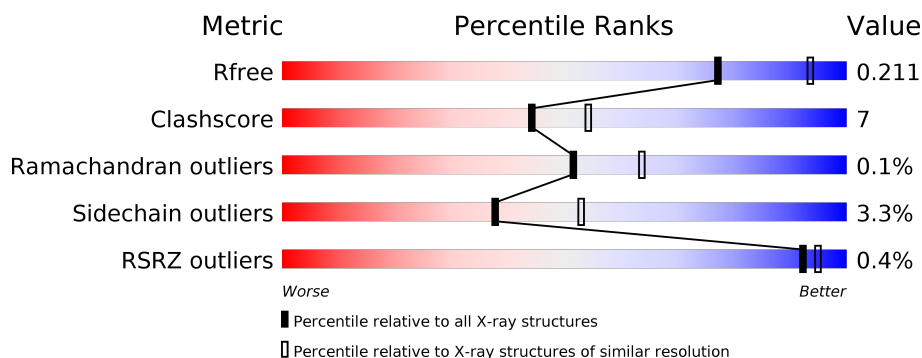
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 on 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	517	 82% 13% . .
1	B	517	 85% 11% .
1	C	517	 84% 11% . .
1	D	517	 82% 13% . .

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	1008	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 16989 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 Cytosolic 10-formyltetrahydrofolate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	15	0
			3904	2481	672	732	19			
1	B	498	Total	C	N	O	S	0	15	0
			3895	2474	672	730	19			
1	C	498	Total	C	N	O	S	0	13	0
			3886	2469	672	726	19			
1	D	498	Total	C	N	O	S	0	14	0
			3892	2473	669	731	19			

There are 48 discrepancies between the modelled and reference sequences:

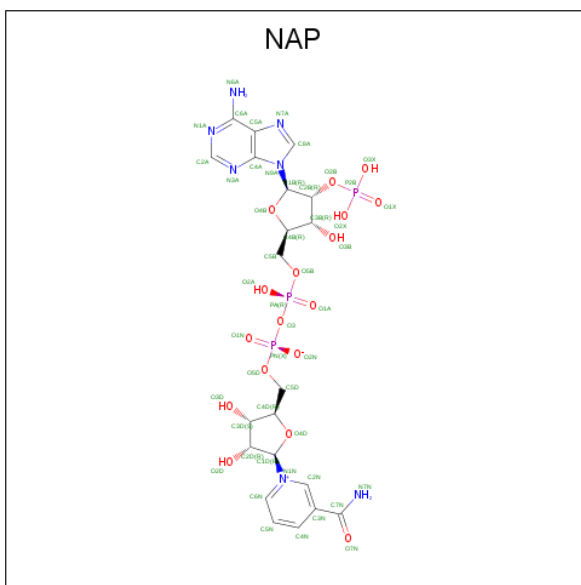
Chain	Residue	Modelled	Actual	Comment	Reference
A	386	MET	-	EXPRESSION TAG	UNP P28037
A	387	ARG	-	EXPRESSION TAG	UNP P28037
A	388	GLY	-	EXPRESSION TAG	UNP P28037
A	389	SER	-	EXPRESSION TAG	UNP P28037
A	390	HIS	-	EXPRESSION TAG	UNP P28037
A	391	HIS	-	EXPRESSION TAG	UNP P28037
A	392	HIS	-	EXPRESSION TAG	UNP P28037
A	393	HIS	-	EXPRESSION TAG	UNP P28037
A	394	HIS	-	EXPRESSION TAG	UNP P28037
A	395	THR	-	EXPRESSION TAG	UNP P28037
A	396	THR	-	EXPRESSION TAG	UNP P28037
A	707	SER	CYS	ENGINEERED MUTATION	UNP P28037
B	386	MET	-	EXPRESSION TAG	UNP P28037
B	387	ARG	-	EXPRESSION TAG	UNP P28037
B	388	GLY	-	EXPRESSION TAG	UNP P28037
B	389	SER	-	EXPRESSION TAG	UNP P28037
B	390	HIS	-	EXPRESSION TAG	UNP P28037
B	391	HIS	-	EXPRESSION TAG	UNP P28037
B	392	HIS	-	EXPRESSION TAG	UNP P28037
B	393	HIS	-	EXPRESSION TAG	UNP P28037
B	394	HIS	-	EXPRESSION TAG	UNP P28037

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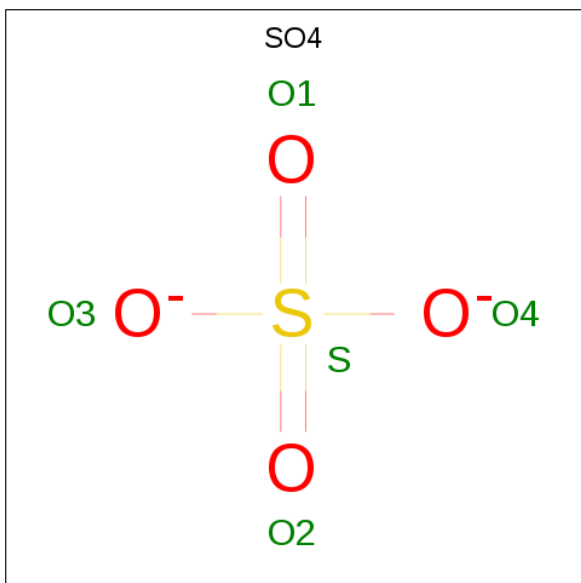
Chain	Residue	Modelled	Actual	Comment	Reference
B	395	THR	-	EXPRESSION TAG	UNP P28037
B	396	THR	-	EXPRESSION TAG	UNP P28037
B	707	SER	CYS	ENGINEERED MUTATION	UNP P28037
C	386	MET	-	EXPRESSION TAG	UNP P28037
C	387	ARG	-	EXPRESSION TAG	UNP P28037
C	388	GLY	-	EXPRESSION TAG	UNP P28037
C	389	SER	-	EXPRESSION TAG	UNP P28037
C	390	HIS	-	EXPRESSION TAG	UNP P28037
C	391	HIS	-	EXPRESSION TAG	UNP P28037
C	392	HIS	-	EXPRESSION TAG	UNP P28037
C	393	HIS	-	EXPRESSION TAG	UNP P28037
C	394	HIS	-	EXPRESSION TAG	UNP P28037
C	395	THR	-	EXPRESSION TAG	UNP P28037
C	396	THR	-	EXPRESSION TAG	UNP P28037
C	707	SER	CYS	ENGINEERED MUTATION	UNP P28037
D	386	MET	-	EXPRESSION TAG	UNP P28037
D	387	ARG	-	EXPRESSION TAG	UNP P28037
D	388	GLY	-	EXPRESSION TAG	UNP P28037
D	389	SER	-	EXPRESSION TAG	UNP P28037
D	390	HIS	-	EXPRESSION TAG	UNP P28037
D	391	HIS	-	EXPRESSION TAG	UNP P28037
D	392	HIS	-	EXPRESSION TAG	UNP P28037
D	393	HIS	-	EXPRESSION TAG	UNP P28037
D	394	HIS	-	EXPRESSION TAG	UNP P28037
D	395	THR	-	EXPRESSION TAG	UNP P28037
D	396	THR	-	EXPRESSION TAG	UNP P28037
D	707	SER	CYS	ENGINEERED MUTATION	UNP P28037

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



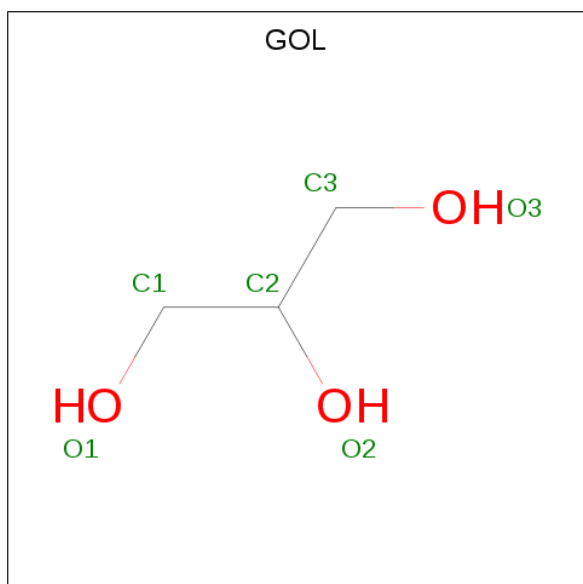
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0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

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

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



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

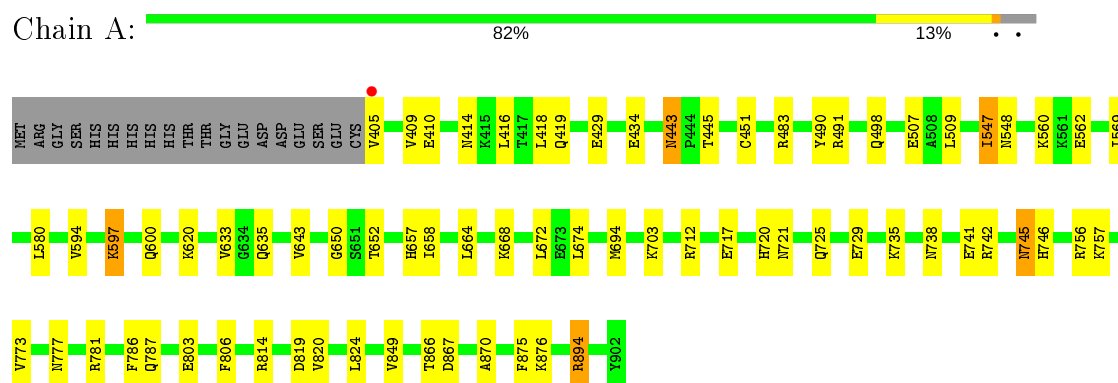
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	273	Total 273	O 273	0	0
5	B	245	Total 245	O 245	0	0
5	C	289	Total 289	O 289	0	0
5	D	249	Total 249	O 249	0	0

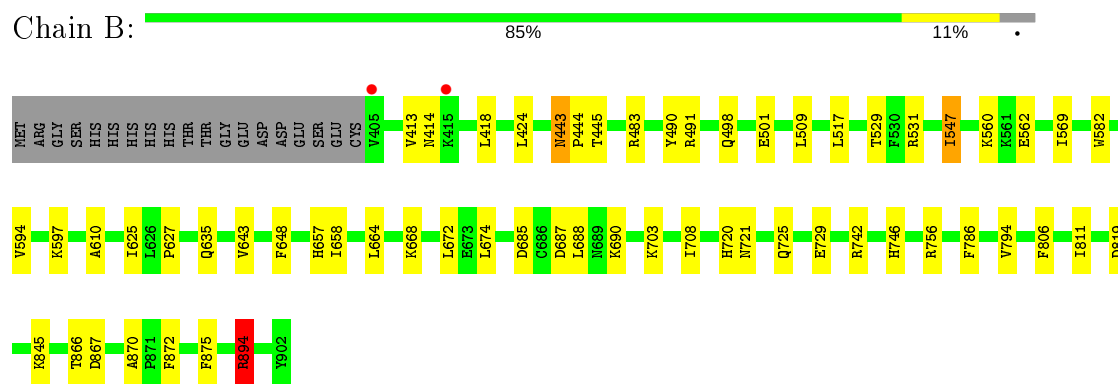
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

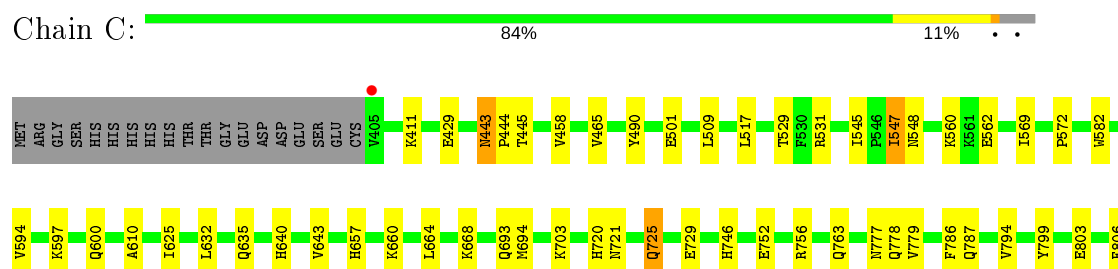
- Molecule 1: Cytosolic 10-formyltetrahydrofolate dehydrogenase



- Molecule 1: Cytosolic 10-formyltetrahydrofolate dehydrogenase

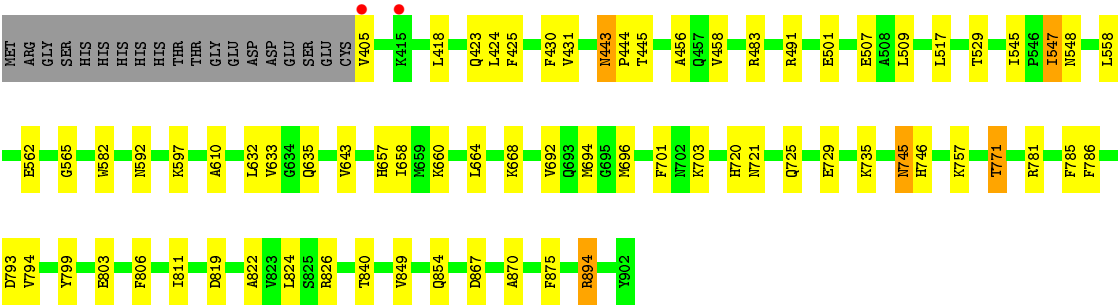
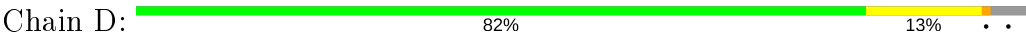


- Molecule 1: Cytosolic 10-formyltetrahydrofolate dehydrogenase





● Molecule 1: Cytosolic 10-formyltetrahydrofolate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	259.09 Å 194.25 Å 97.23 Å 90.00° 108.74° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 46.72 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.9 (50.00-2.30) 95.8 (46.72-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.29 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.180 , 0.210 0.181 , 0.211	Depositor DCC
R_{free} test set	9660 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16989	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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: GOL, NAP, SO4

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	0.57	0/4043	0.65	1/5466 (0.0%)
1	B	0.58	0/4043	0.65	2/5466 (0.0%)
1	C	0.62	0/4025	0.67	2/5442 (0.0%)
1	D	0.59	0/4032	0.66	1/5452 (0.0%)
All	All	0.59	0/16143	0.66	6/21826 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	894	ARG	NE-CZ-NH2	-7.79	116.40	120.30
1	C	894	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	B	894	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	B	894	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	712	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	D	826	ARG	NE-CZ-NH2	-5.11	117.75	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	3904	0	3933	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3895	0	3919	50	0
1	C	3886	0	3911	58	0
1	D	3892	0	3911	59	0
2	A	48	0	25	3	0
2	B	48	0	25	2	0
2	C	48	0	25	1	0
2	D	48	0	25	3	0
3	A	50	0	0	0	0
3	B	30	0	0	0	0
3	C	30	0	0	0	0
3	D	30	0	0	0	0
4	A	6	0	8	1	0
4	B	6	0	8	1	0
4	C	6	0	8	1	0
4	D	6	0	8	0	0
5	A	273	0	0	18	0
5	B	245	0	0	9	0
5	C	289	0	0	11	0
5	D	249	0	0	13	0
All	All	16989	0	15806	210	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 7.

All (210) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:694:MET:HG3	5:C:1202:HOH:O	1.44	1.15
1:B:501:GLU:HG2	5:B:1184:HOH:O	1.53	1.06
1:C:841[B]:ARG:HH11	1:C:841[B]:ARG:HG2	1.14	1.06
1:B:687:ASP:HB2	5:B:1199:HOH:O	1.59	1.01
1:D:501:GLU:HG2	5:D:1224:HOH:O	1.66	0.95
1:A:491[B]:ARG:HH12	1:A:498:GLN:HE22	1.16	0.88
1:C:501:GLU:HG2	5:C:1349:HOH:O	1.72	0.88
1:D:819:ASP:HB3	5:D:1125:HOH:O	1.73	0.88
1:A:547[A]:ILE:HG13	1:B:867:ASP:CG	1.94	0.87
1:C:547[A]:ILE:HG13	1:D:867:ASP:CG	1.94	0.87
1:C:429:GLU:HG2	5:C:1297:HOH:O	1.76	0.85
1:C:867:ASP:CG	1:D:547[A]:ILE:HG13	1.98	0.84
1:D:694:MET:HG3	5:D:1159:HOH:O	1.77	0.82
1:A:547[A]:ILE:HD11	1:B:870:ALA:HB2	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756[B]:ARG:HD3	5:A:1126:HOH:O	1.77	0.82
1:C:490[B]:TYR:CD2	5:C:1260:HOH:O	2.32	0.81
1:A:738:ASN:HB3	1:A:741[A]:GLU:HG3	1.59	0.81
1:D:771:THR:HG22	5:D:1243:HOH:O	1.79	0.81
1:A:870:ALA:HB2	1:B:547[A]:ILE:HD11	1.62	0.81
1:D:694:MET:CG	5:D:1159:HOH:O	2.31	0.79
1:A:725[A]:GLN:NE2	1:A:729:GLU:OE2	2.17	0.77
1:A:894:ARG:HD3	1:B:875:PHE:CZ	2.19	0.77
1:C:547[A]:ILE:HD11	1:D:870:ALA:HB2	1.65	0.77
1:B:443:ASN:C	1:B:443:ASN:HD22	1.89	0.77
1:A:490[A]:TYR:CD2	5:A:1230:HOH:O	2.38	0.76
1:C:866:THR:OG1	4:C:1008:GOL:H11	1.85	0.75
1:C:870:ALA:HB2	1:D:547[A]:ILE:HD11	1.71	0.72
1:B:443:ASN:ND2	1:B:445:THR:H	1.88	0.71
1:C:694:MET:CG	5:C:1202:HOH:O	2.18	0.71
1:C:490[B]:TYR:CE2	5:C:1260:HOH:O	2.43	0.71
1:C:560[A]:LYS:HD2	5:D:1147:HOH:O	1.91	0.71
1:A:720:HIS:HE1	5:A:1112:HOH:O	1.74	0.70
1:A:635:GLN:OE1	1:A:657:HIS:HE1	1.75	0.69
1:C:547[A]:ILE:HG13	1:D:867:ASP:CB	2.22	0.69
1:A:490[A]:TYR:CE2	5:A:1230:HOH:O	2.45	0.69
1:B:414:ASN:OD1	1:B:742:ARG:NH2	2.25	0.69
1:D:562:GLU:HB2	1:D:894:ARG:HD2	1.74	0.68
1:A:867:ASP:CG	1:B:547[A]:ILE:HG13	2.14	0.68
1:C:799:TYR:CE2	1:C:803[A]:GLU:HG3	2.28	0.67
1:D:771:THR:CG2	1:D:793:ASP:OD1	2.43	0.67
1:C:867:ASP:CB	1:D:547[A]:ILE:HG13	2.25	0.66
1:C:875:PHE:CZ	1:D:894:ARG:HD3	2.31	0.66
1:A:491[B]:ARG:HH12	1:A:498:GLN:NE2	1.91	0.65
1:C:746:HIS:HD2	5:C:1158:HOH:O	1.79	0.65
1:A:694:MET:HG3	5:A:1106:HOH:O	1.96	0.65
1:A:819:ASP:HB3	5:A:1151:HOH:O	1.95	0.64
1:C:841[B]:ARG:NH1	1:C:841[B]:ARG:HG2	1.94	0.64
1:D:635:GLN:OE1	1:D:657:HIS:HE1	1.81	0.64
1:C:562:GLU:HB2	1:C:894:ARG:HD2	1.79	0.64
1:D:799:TYR:CE2	1:D:803[A]:GLU:HG3	2.32	0.64
1:A:443:ASN:ND2	1:A:445:THR:H	1.95	0.64
1:A:410:GLU:OE1	1:A:419[B]:GLN:NE2	2.26	0.63
1:B:562:GLU:HB2	1:B:894:ARG:HD2	1.78	0.63
1:C:443:ASN:ND2	1:C:445:THR:H	1.96	0.63
1:A:600:GLN:NE2	5:A:1251:HOH:O	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:875:PHE:CZ	1:B:894:ARG:HD3	2.34	0.63
1:C:756[A]:ARG:HH12	1:C:778:GLN:HE22	1.46	0.63
1:D:771:THR:HG21	1:D:793:ASP:OD1	1.97	0.63
1:D:735:LYS:H	1:D:745:ASN:HD21	1.47	0.62
1:A:547[A]:ILE:HG13	1:B:867:ASP:CB	2.29	0.62
1:A:735:LYS:H	1:A:745:ASN:HD21	1.46	0.62
1:A:725[A]:GLN:HE21	1:A:729:GLU:CD	2.02	0.62
1:C:635:GLN:OE1	1:C:657:HIS:HE1	1.83	0.62
1:A:443:ASN:HD22	1:A:445:THR:H	1.48	0.61
1:D:720:HIS:HE1	5:D:1107:HOH:O	1.83	0.61
1:D:658:ILE:HD11	2:D:1001:NAP:C2A	2.31	0.61
1:A:720:HIS:CE1	5:A:1112:HOH:O	2.51	0.61
1:D:458:VAL:HG23	1:D:632:LEU:HD21	1.83	0.61
1:D:692:VAL:O	1:D:696:MET:HG2	2.01	0.60
1:C:894:ARG:HD3	1:D:875:PHE:CZ	2.38	0.59
1:D:443:ASN:C	1:D:443:ASN:HD22	2.06	0.58
1:B:491[B]:ARG:HH12	1:B:498:GLN:HE22	1.51	0.58
1:A:569:ILE:HD12	1:A:594:VAL:HG21	1.85	0.57
1:C:569:ILE:HD12	1:C:594:VAL:HG21	1.86	0.57
1:C:610:ALA:HB2	1:C:625:ILE:HD12	1.85	0.57
1:C:560[A]:LYS:CD	5:D:1147:HOH:O	2.49	0.57
1:C:725[A]:GLN:OE1	1:C:729:GLU:OE2	2.21	0.57
1:A:819:ASP:CB	5:A:1151:HOH:O	2.53	0.57
1:D:735:LYS:N	1:D:745:ASN:HD21	2.03	0.56
1:B:725[A]:GLN:NE2	1:B:729:GLU:OE2	2.38	0.56
1:B:648:PHE:CD1	1:B:658:ILE:HD13	2.40	0.56
1:B:443:ASN:ND2	1:B:443:ASN:C	2.59	0.56
1:C:720:HIS:HD2	1:C:721:ASN:OD1	1.89	0.56
1:A:443:ASN:C	1:A:443:ASN:HD22	2.09	0.56
1:A:434:GLU:HG3	5:A:1314:HOH:O	2.05	0.56
1:B:643:VAL:O	1:B:668:LYS:HE3	2.07	0.55
1:B:756[A]:ARG:NE	5:B:1343:HOH:O	2.40	0.55
1:A:429:GLU:HB3	5:A:1260:HOH:O	2.06	0.55
1:B:443:ASN:HD22	1:B:444:PRO:N	2.04	0.55
1:B:708:ILE:HG21	1:B:872:PHE:HE1	1.72	0.55
1:C:443:ASN:HD22	1:C:445:THR:H	1.53	0.54
1:C:779:VAL:HG22	1:C:787:GLN:HG3	1.89	0.54
1:C:752:GLU:OE2	1:C:756[B]:ARG:NH2	2.40	0.54
1:B:746:HIS:HE1	1:B:786:PHE:O	1.90	0.54
1:D:720:HIS:CE1	5:D:1107:HOH:O	2.59	0.54
1:C:443:ASN:HD22	1:C:443:ASN:C	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:735:LYS:N	1:A:745:ASN:HD21	2.06	0.53
1:C:756[B]:ARG:HG3	1:C:756[B]:ARG:HH11	1.72	0.53
1:C:867:ASP:CB	1:D:547[A]:ILE:CG1	2.86	0.53
1:B:529:THR:HG21	1:B:582:TRP:HA	1.91	0.53
1:D:725[A]:GLN:NE2	1:D:729:GLU:OE2	2.36	0.53
1:A:483:ARG:HB3	1:D:548:ASN:HD21	1.73	0.52
1:A:820:VAL:N	5:A:1151:HOH:O	2.42	0.52
1:C:458:VAL:HG23	1:C:632:LEU:HD21	1.92	0.52
1:A:894:ARG:HD3	1:B:875:PHE:CE2	2.44	0.52
1:B:483:ARG:HB3	1:C:548:ASN:HD21	1.75	0.52
1:B:720:HIS:HE1	5:B:1127:HOH:O	1.94	0.51
1:B:443:ASN:HD22	1:B:445:THR:H	1.56	0.51
1:A:547[A]:ILE:CG1	1:B:867:ASP:CB	2.88	0.51
1:B:806:PHE:CE1	2:B:1001:NAP:H2D	2.46	0.51
1:A:548:ASN:HD21	1:D:483:ARG:HB3	1.74	0.51
1:C:867:ASP:HB3	1:D:547[A]:ILE:CG1	2.41	0.51
1:D:854:GLN:HG3	5:D:1201:HOH:O	2.11	0.51
1:B:635:GLN:OE1	1:B:657:HIS:HE1	1.94	0.50
1:D:771:THR:HG23	1:D:793:ASP:OD1	2.09	0.50
1:C:529:THR:HG21	1:C:582:TRP:HA	1.93	0.50
1:D:545:ILE:HG22	1:D:547[A]:ILE:HD12	1.92	0.50
1:C:806:PHE:CE1	2:C:1001:NAP:H2D	2.47	0.50
1:C:756[A]:ARG:HH12	1:C:778:GLN:NE2	2.10	0.50
1:A:735:LYS:HD2	5:A:1294:HOH:O	2.11	0.50
1:D:771:THR:HG23	1:D:793:ASP:HB2	1.93	0.49
2:B:1001:NAP:H8A	5:B:1132:HOH:O	2.12	0.49
1:D:781[B]:ARG:HD2	1:D:785:PHE:CD2	2.47	0.49
1:A:875:PHE:CE2	1:B:894:ARG:HD3	2.48	0.49
1:C:632:LEU:HD23	1:C:632:LEU:C	2.34	0.48
1:D:806:PHE:CE1	2:D:1001:NAP:H2D	2.47	0.48
1:C:600:GLN:NE2	5:C:1226:HOH:O	2.43	0.48
1:A:635:GLN:OE1	1:A:657:HIS:CE1	2.62	0.48
1:C:794:VAL:HG21	1:C:811:ILE:HG23	1.96	0.47
1:D:443:ASN:HD22	1:D:444:PRO:N	2.12	0.47
1:A:867:ASP:CB	1:B:547[A]:ILE:HG13	2.44	0.47
1:A:717:GLU:OE2	1:A:814:ARG:HD3	2.13	0.47
1:A:560[A]:LYS:HD2	5:B:1181:HOH:O	2.14	0.47
1:B:866:THR:OG1	4:B:1008:GOL:H11	2.15	0.47
1:C:867:ASP:HB3	1:D:547[A]:ILE:HG13	1.96	0.47
1:D:794:VAL:HG21	1:D:811:ILE:HG23	1.96	0.47
1:A:416:LEU:CD1	1:A:418:LEU:CD1	2.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:763:GLN:NE2	5:C:1294:HOH:O	2.41	0.47
1:D:443:ASN:ND2	1:D:445:THR:H	2.12	0.47
1:B:490[A]:TYR:CE1	1:B:531:ARG:HG2	2.50	0.46
1:B:756[B]:ARG:HD3	5:B:1108:HOH:O	2.14	0.46
1:D:746:HIS:HE1	1:D:786:PHE:O	1.99	0.46
1:A:738:ASN:HB3	1:A:741[B]:GLU:HG3	1.97	0.46
5:A:1167:HOH:O	1:B:560[A]:LYS:HE2	2.15	0.46
1:A:562:GLU:HB2	1:A:894:ARG:HD2	1.98	0.46
1:D:643:VAL:O	1:D:668:LYS:HE3	2.16	0.46
1:C:547[A]:ILE:CG1	1:D:867:ASP:CB	2.92	0.46
1:A:806:PHE:CE1	2:A:1001:NAP:H2D	2.50	0.46
1:C:746:HIS:HE1	1:C:786:PHE:O	1.99	0.46
1:C:465:VAL:HG11	1:C:640:HIS:CE1	2.51	0.46
1:C:490[B]:TYR:CE1	1:C:531:ARG:HG2	2.51	0.46
1:A:866:THR:OG1	4:A:1012:GOL:H11	2.16	0.46
1:A:409:VAL:HG21	1:A:451:CYS:HB2	1.97	0.46
1:A:824:LEU:HD21	1:A:849:VAL:HG13	1.97	0.45
1:B:708:ILE:CG2	1:B:872:PHE:HE1	2.29	0.45
1:C:660:LYS:HG3	1:D:660:LYS:HG3	1.98	0.45
1:C:411:LYS:HD2	5:C:1239:HOH:O	2.15	0.45
1:A:777:ASN:H	1:A:787:GLN:NE2	2.13	0.45
1:D:894:ARG:NH2	5:D:1252:HOH:O	2.48	0.45
1:B:424:LEU:HD23	1:B:627:PRO:HD2	1.99	0.45
1:D:822:ALA:HB3	5:D:1125:HOH:O	2.16	0.45
1:D:529:THR:HG21	1:D:582:TRP:HA	1.99	0.45
1:B:491[B]:ARG:NH1	1:B:498:GLN:HE22	2.14	0.45
1:A:414:ASN:OD1	1:A:742:ARG:NH2	2.50	0.45
1:C:814:ARG:NH1	5:C:1375:HOH:O	2.41	0.45
1:C:443:ASN:HD22	1:C:444:PRO:N	2.15	0.44
1:C:875:PHE:CE1	1:D:894:ARG:HB2	2.53	0.44
1:A:720:HIS:HD2	1:A:721:ASN:OD1	2.01	0.44
1:A:597:LYS:HG3	1:A:633:VAL:HG12	2.00	0.44
1:B:491[B]:ARG:HD3	5:B:1219:HOH:O	2.17	0.44
1:B:569:ILE:HD12	1:B:594:VAL:HG21	2.00	0.44
1:B:720:HIS:CE1	5:B:1127:HOH:O	2.68	0.44
1:A:777:ASN:HD22	1:A:787:GLN:HE22	1.63	0.44
1:A:405:VAL:HA	5:A:1239:HOH:O	2.17	0.43
1:A:650:GLY:O	1:A:674:LEU:HA	2.18	0.43
1:D:824:LEU:HD21	1:D:849:VAL:HG13	1.99	0.43
1:B:794:VAL:HG21	1:B:811:ILE:HG23	2.00	0.43
1:A:491[B]:ARG:CZ	5:A:1317:HOH:O	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:648:PHE:CD1	1:B:658:ILE:CD1	3.02	0.42
1:A:547[A]:ILE:HG13	1:B:867:ASP:OD1	2.18	0.42
1:D:558:LEU:HD12	1:D:558:LEU:C	2.40	0.42
1:A:876:LYS:NZ	5:A:1339:HOH:O	2.48	0.42
1:C:643:VAL:O	1:C:668:LYS:HE3	2.19	0.42
1:D:635:GLN:OE1	1:D:657:HIS:CE1	2.68	0.42
1:A:735:LYS:H	1:A:745:ASN:ND2	2.16	0.41
1:D:425:PHE:CG	1:D:610:ALA:HB1	2.55	0.41
1:A:620:LYS:HG3	1:A:620:LYS:O	2.20	0.41
1:D:565:GLY:O	1:D:592:ASN:HB3	2.20	0.41
1:A:416:LEU:HD11	1:A:418:LEU:CD1	2.49	0.41
1:B:685:ASP:OD2	1:B:845:LYS:NZ	2.53	0.41
2:A:1001:NAP:H8A	5:A:1179:HOH:O	2.21	0.41
1:B:610:ALA:HB2	1:B:625:ILE:HD12	2.01	0.41
1:C:545:ILE:HG22	1:C:547[A]:ILE:HD12	2.01	0.41
1:A:777:ASN:H	1:A:787:GLN:HE21	1.67	0.41
2:D:1001:NAP:H8A	5:D:1161:HOH:O	2.20	0.41
1:A:674:LEU:O	2:A:1001:NAP:H2N	2.21	0.41
1:A:580:LEU:C	1:A:580:LEU:HD23	2.41	0.41
1:A:672:LEU:HB3	1:A:674:LEU:HD21	2.02	0.41
1:D:456:ALA:HB3	1:D:633:VAL:HG21	2.02	0.41
1:A:643:VAL:O	1:A:668:LYS:HE3	2.21	0.40
1:A:746:HIS:HE1	1:A:786:PHE:O	2.04	0.40
1:B:672:LEU:HB3	1:B:674:LEU:HD21	2.03	0.40
1:B:720:HIS:HD2	1:B:721:ASN:OD1	2.04	0.40
1:D:720:HIS:HD2	1:D:721:ASN:OD1	2.03	0.40
1:A:652:THR:HA	1:A:674:LEU:HD13	2.03	0.40
1:D:424:LEU:O	1:D:430:PHE:HA	2.21	0.40
1:A:867:ASP:OD1	1:B:547[A]:ILE:HG13	2.20	0.40
1:D:423:GLN:HB3	1:D:431:VAL:O	2.22	0.40
1:D:517:LEU:HD11	1:D:701:PHE:CZ	2.57	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	511/517 (99%)	492 (96%)	19 (4%)	0	100	100
1	B	511/517 (99%)	496 (97%)	15 (3%)	0	100	100
1	C	509/517 (98%)	493 (97%)	15 (3%)	1 (0%)	47	58
1	D	510/517 (99%)	490 (96%)	20 (4%)	0	100	100
All	All	2041/2068 (99%)	1971 (97%)	69 (3%)	1 (0%)	51	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	572	PRO

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	424/426 (100%)	407 (96%)	17 (4%)	31	44
1	B	424/426 (100%)	410 (97%)	14 (3%)	38	53
1	C	422/426 (99%)	407 (96%)	15 (4%)	35	49
1	D	423/426 (99%)	406 (96%)	17 (4%)	31	44
All	All	1693/1704 (99%)	1630 (96%)	63 (4%)	38	48

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	443	ASN
1	A	507	GLU
1	A	509	LEU
1	A	547[A]	ILE
1	A	547[B]	ILE
1	A	597	LYS
1	A	658	ILE

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Mol	Chain	Res	Type
1	A	664	LEU
1	A	703	LYS
1	A	745	ASN
1	A	757	LYS
1	A	773	VAL
1	A	781[A]	ARG
1	A	781[B]	ARG
1	A	803[A]	GLU
1	A	803[B]	GLU
1	A	894	ARG
1	B	413	VAL
1	B	418	LEU
1	B	443	ASN
1	B	509	LEU
1	B	517	LEU
1	B	547[A]	ILE
1	B	547[B]	ILE
1	B	597	LYS
1	B	664	LEU
1	B	688	LEU
1	B	690	LYS
1	B	703	LYS
1	B	819	ASP
1	B	894	ARG
1	C	443	ASN
1	C	509	LEU
1	C	517	LEU
1	C	547[A]	ILE
1	C	547[B]	ILE
1	C	597	LYS
1	C	664	LEU
1	C	693[A]	GLN
1	C	693[B]	GLN
1	C	703	LYS
1	C	725[A]	GLN
1	C	725[B]	GLN
1	C	777	ASN
1	C	819	ASP
1	C	894	ARG
1	D	405	VAL
1	D	418	LEU
1	D	443	ASN

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Mol	Chain	Res	Type
1	D	491[A]	ARG
1	D	491[B]	ARG
1	D	507	GLU
1	D	509	LEU
1	D	547[A]	ILE
1	D	547[B]	ILE
1	D	597	LYS
1	D	664	LEU
1	D	703	LYS
1	D	745	ASN
1	D	757	LYS
1	D	771	THR
1	D	840	THR
1	D	894	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	443	ASN
1	A	457	GLN
1	A	498	GLN
1	A	548	ASN
1	A	657	HIS
1	A	706	ASN
1	A	720	HIS
1	A	745	ASN
1	A	746	HIS
1	A	778	GLN
1	A	787	GLN
1	A	797	HIS
1	A	844	ASN
1	B	443	ASN
1	B	548	ASN
1	B	600	GLN
1	B	657	HIS
1	B	706	ASN
1	B	720	HIS
1	B	746	HIS
1	B	750	ASN
1	B	778	GLN
1	B	787	GLN
1	C	443	ASN

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Mol	Chain	Res	Type
1	C	548	ASN
1	C	600	GLN
1	C	657	HIS
1	C	706	ASN
1	C	720	HIS
1	C	746	HIS
1	C	778	GLN
1	C	787	GLN
1	C	844	ASN
1	D	443	ASN
1	D	457	GLN
1	D	548	ASN
1	D	600	GLN
1	D	657	HIS
1	D	706	ASN
1	D	720	HIS
1	D	745	ASN
1	D	746	HIS
1	D	844	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

36 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	C	1005	-	4,4,4	0.13	0	6,6,6	0.27	0
3	SO4	A	1006	-	4,4,4	0.22	0	6,6,6	0.19	0
3	SO4	A	1009	-	4,4,4	0.19	0	6,6,6	0.13	0
2	NAP	C	1001	-	45,52,52	1.64	4 (8%)	56,80,80	1.34	5 (8%)
3	SO4	C	1003	-	4,4,4	0.15	0	6,6,6	0.18	0
3	SO4	A	1008	-	4,4,4	0.18	0	6,6,6	0.26	0
3	SO4	A	1002	-	4,4,4	0.15	0	6,6,6	0.25	0
2	NAP	A	1001	-	45,52,52	1.70	4 (8%)	56,80,80	1.25	6 (10%)
3	SO4	A	1005	-	4,4,4	0.13	0	6,6,6	0.12	0
3	SO4	D	1007	-	4,4,4	0.14	0	6,6,6	0.52	0
4	GOL	B	1008	-	5,5,5	0.30	0	5,5,5	0.30	0
4	GOL	C	1008	-	5,5,5	0.31	0	5,5,5	0.34	0
3	SO4	A	1004	-	4,4,4	0.12	0	6,6,6	0.40	0
3	SO4	D	1004	-	4,4,4	0.24	0	6,6,6	0.23	0
3	SO4	D	1003	-	4,4,4	0.15	0	6,6,6	0.14	0
4	GOL	A	1012	-	5,5,5	0.30	0	5,5,5	0.43	0
3	SO4	A	1007	-	4,4,4	0.12	0	6,6,6	0.13	0
4	GOL	D	1008	-	5,5,5	0.34	0	5,5,5	0.35	0
3	SO4	A	1003	-	4,4,4	0.19	0	6,6,6	0.40	0
3	SO4	D	1005	-	4,4,4	0.14	0	6,6,6	0.18	0
2	NAP	D	1001	-	45,52,52	1.55	3 (6%)	56,80,80	1.34	7 (12%)
3	SO4	D	1006	-	4,4,4	0.14	0	6,6,6	0.20	0
3	SO4	B	1007	-	4,4,4	0.16	0	6,6,6	0.18	0
3	SO4	C	1004	-	4,4,4	0.13	0	6,6,6	0.20	0
3	SO4	B	1006	-	4,4,4	0.23	0	6,6,6	0.23	0
3	SO4	A	1011	-	4,4,4	0.11	0	6,6,6	0.51	0
3	SO4	B	1002	-	4,4,4	0.21	0	6,6,6	0.18	0
3	SO4	B	1005	-	4,4,4	0.15	0	6,6,6	0.14	0
3	SO4	B	1003	-	4,4,4	0.13	0	6,6,6	0.09	0
3	SO4	B	1004	-	4,4,4	0.20	0	6,6,6	0.38	0
3	SO4	C	1007	-	4,4,4	0.19	0	6,6,6	0.38	0
3	SO4	A	1010	-	4,4,4	0.24	0	6,6,6	0.37	0
3	SO4	D	1002	-	4,4,4	0.17	0	6,6,6	0.30	0
3	SO4	C	1006	-	4,4,4	0.18	0	6,6,6	0.37	0
2	NAP	B	1001	-	45,52,52	1.65	4 (8%)	56,80,80	1.32	6 (10%)
3	SO4	C	1002	-	4,4,4	0.17	0	6,6,6	0.53	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
4	GOL	C	1008	-	-	2/4/4/4	-
4	GOL	A	1012	-	-	3/4/4/4	-
4	GOL	B	1008	-	-	2/4/4/4	-
4	GOL	D	1008	-	-	2/4/4/4	-
2	NAP	C	1001	-	-	8/31/67/67	0/5/5/5
2	NAP	A	1001	-	-	6/31/67/67	0/5/5/5
2	NAP	D	1001	-	-	6/31/67/67	0/5/5/5
2	NAP	B	1001	-	-	6/31/67/67	0/5/5/5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	NAP	O7N-C7N	8.77	1.40	1.24
2	B	1001	NAP	O7N-C7N	8.45	1.40	1.24
2	C	1001	NAP	O7N-C7N	7.99	1.39	1.24
2	D	1001	NAP	O7N-C7N	7.84	1.39	1.24
2	A	1001	NAP	C2A-N3A	3.54	1.37	1.32
2	C	1001	NAP	C2A-N3A	3.52	1.37	1.32
2	B	1001	NAP	C2A-N3A	3.42	1.37	1.32
2	D	1001	NAP	C2A-N3A	2.99	1.36	1.32
2	A	1001	NAP	C2N-N1N	2.82	1.38	1.35
2	D	1001	NAP	C2N-N1N	2.63	1.38	1.35
2	C	1001	NAP	C2A-N1A	2.36	1.38	1.33
2	B	1001	NAP	C2N-N1N	2.27	1.37	1.35
2	C	1001	NAP	C2N-N1N	2.26	1.37	1.35
2	A	1001	NAP	C2A-N1A	2.21	1.38	1.33
2	B	1001	NAP	C2A-N1A	2.06	1.37	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1001	NAP	N3A-C2A-N1A	-5.73	119.72	128.68
2	C	1001	NAP	N3A-C2A-N1A	-5.40	120.24	128.68
2	A	1001	NAP	N3A-C2A-N1A	-5.17	120.59	128.68
2	B	1001	NAP	N3A-C2A-N1A	-5.02	120.83	128.68
2	A	1001	NAP	O4D-C1D-C2D	-3.65	101.59	106.93
2	C	1001	NAP	O7N-C7N-C3N	-3.56	115.37	119.63
2	B	1001	NAP	O7N-C7N-C3N	-3.41	115.55	119.63
2	C	1001	NAP	C3N-C7N-N7N	3.31	121.72	117.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	NAP	C2N-C3N-C4N	3.09	121.76	118.26
2	C	1001	NAP	C2N-C3N-C4N	2.84	121.48	118.26
2	D	1001	NAP	O7N-C7N-C3N	-2.75	116.33	119.63
2	D	1001	NAP	O4B-C1B-C2B	-2.73	101.85	106.59
2	D	1001	NAP	C3N-C7N-N7N	2.66	120.94	117.75
2	C	1001	NAP	C3N-C2N-N1N	-2.59	117.89	120.43
2	A	1001	NAP	C3N-C7N-N7N	2.49	120.74	117.75
2	B	1001	NAP	C3N-C7N-N7N	2.18	120.37	117.75
2	B	1001	NAP	O4D-C1D-C2D	-2.17	103.75	106.93
2	A	1001	NAP	C4A-C5A-N7A	-2.17	107.14	109.40
2	D	1001	NAP	O4D-C1D-C2D	-2.13	103.81	106.93
2	B	1001	NAP	C4A-C5A-N7A	-2.10	107.21	109.40
2	A	1001	NAP	O4B-C1B-C2B	-2.09	102.96	106.59
2	D	1001	NAP	C4A-C5A-N7A	-2.09	107.22	109.40
2	D	1001	NAP	C1B-N9A-C4A	-2.02	123.10	126.64
2	A	1001	NAP	O2N-PN-O1N	2.00	122.14	112.24

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1001	NAP	C5D-O5D-PN-O1N
2	A	1001	NAP	C5D-O5D-PN-O1N
4	B	1008	GOL	O1-C1-C2-C3
4	C	1008	GOL	O1-C1-C2-C3
4	A	1012	GOL	O1-C1-C2-C3
2	D	1001	NAP	C5D-O5D-PN-O1N
2	B	1001	NAP	C5D-O5D-PN-O1N
4	B	1008	GOL	O1-C1-C2-O2
4	C	1008	GOL	O1-C1-C2-O2
4	A	1012	GOL	O1-C1-C2-O2
2	B	1001	NAP	PN-O3-PA-O1A
2	C	1001	NAP	C4D-C5D-O5D-PN
2	B	1001	NAP	C4D-C5D-O5D-PN
2	D	1001	NAP	C4D-C5D-O5D-PN
2	A	1001	NAP	C4D-C5D-O5D-PN
4	D	1008	GOL	O1-C1-C2-O2
2	D	1001	NAP	C5D-O5D-PN-O3
2	B	1001	NAP	C5D-O5D-PN-O3
2	C	1001	NAP	PN-O3-PA-O2A
2	D	1001	NAP	PN-O3-PA-O1A
2	C	1001	NAP	C5D-O5D-PN-O2N

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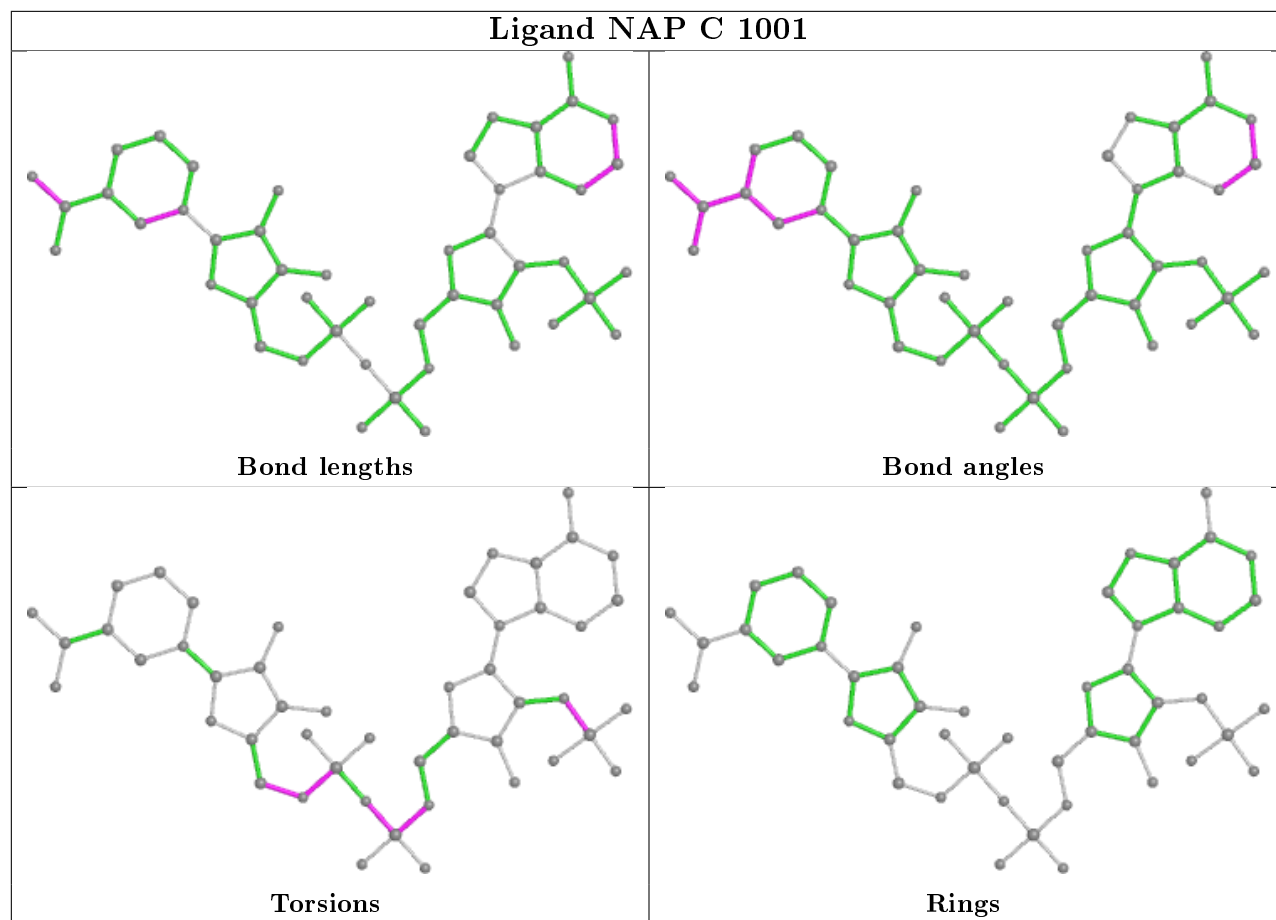
Mol	Chain	Res	Type	Atoms
2	D	1001	NAP	C5D-O5D-PN-O2N
2	B	1001	NAP	C5D-O5D-PN-O2N
2	A	1001	NAP	C3B-C2B-O2B-P2B
2	A	1001	NAP	C1B-C2B-O2B-P2B
4	D	1008	GOL	O1-C1-C2-C3
2	C	1001	NAP	C2B-O2B-P2B-O1X
2	D	1001	NAP	C2B-O2B-P2B-O1X
2	B	1001	NAP	C2B-O2B-P2B-O1X
2	C	1001	NAP	C5D-O5D-PN-O3
2	A	1001	NAP	C2B-O2B-P2B-O3X
2	A	1001	NAP	C5D-O5D-PN-O3
2	C	1001	NAP	PN-O3-PA-O1A
4	A	1012	GOL	C1-C2-C3-O3
2	C	1001	NAP	C5B-O5B-PA-O1A

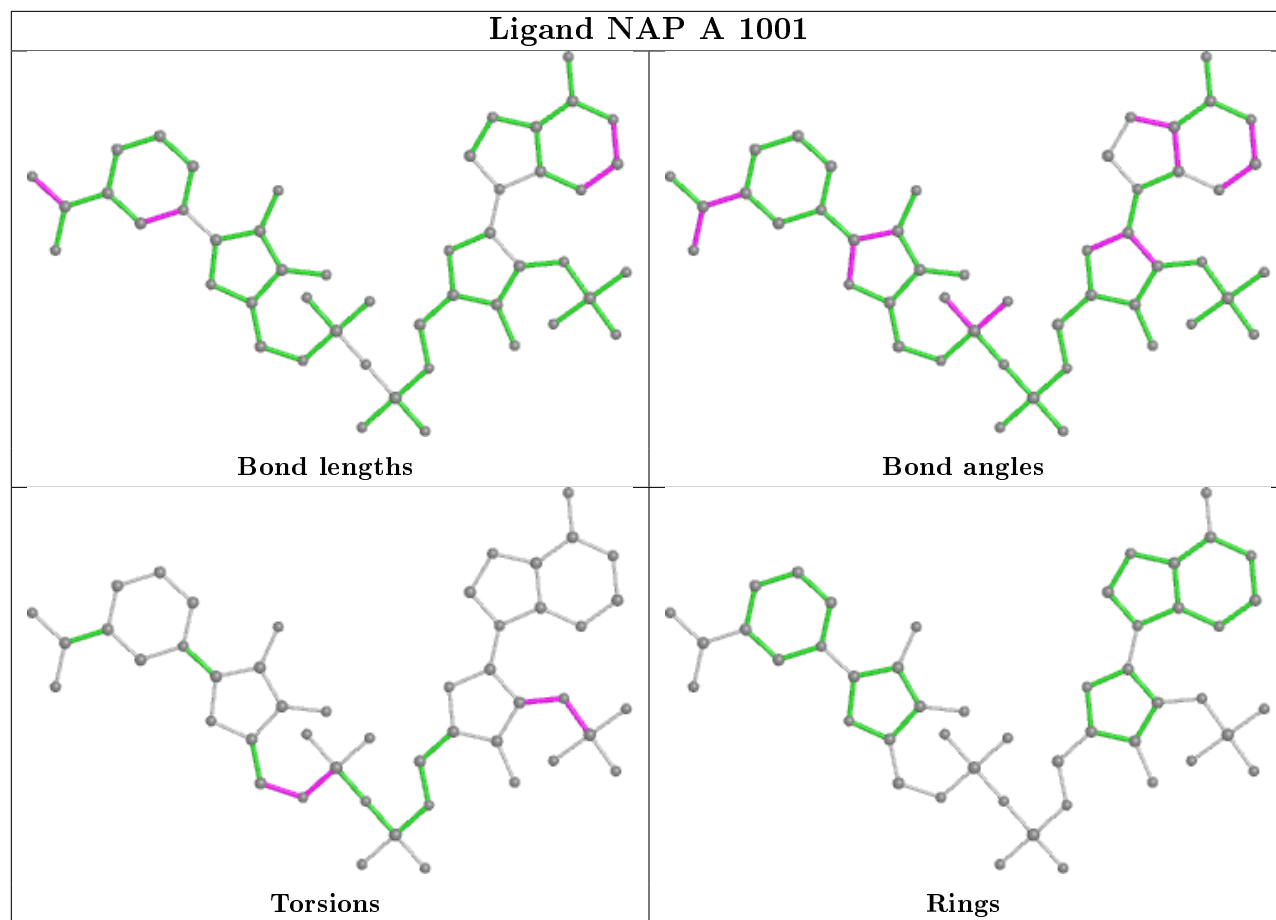
There are no ring outliers.

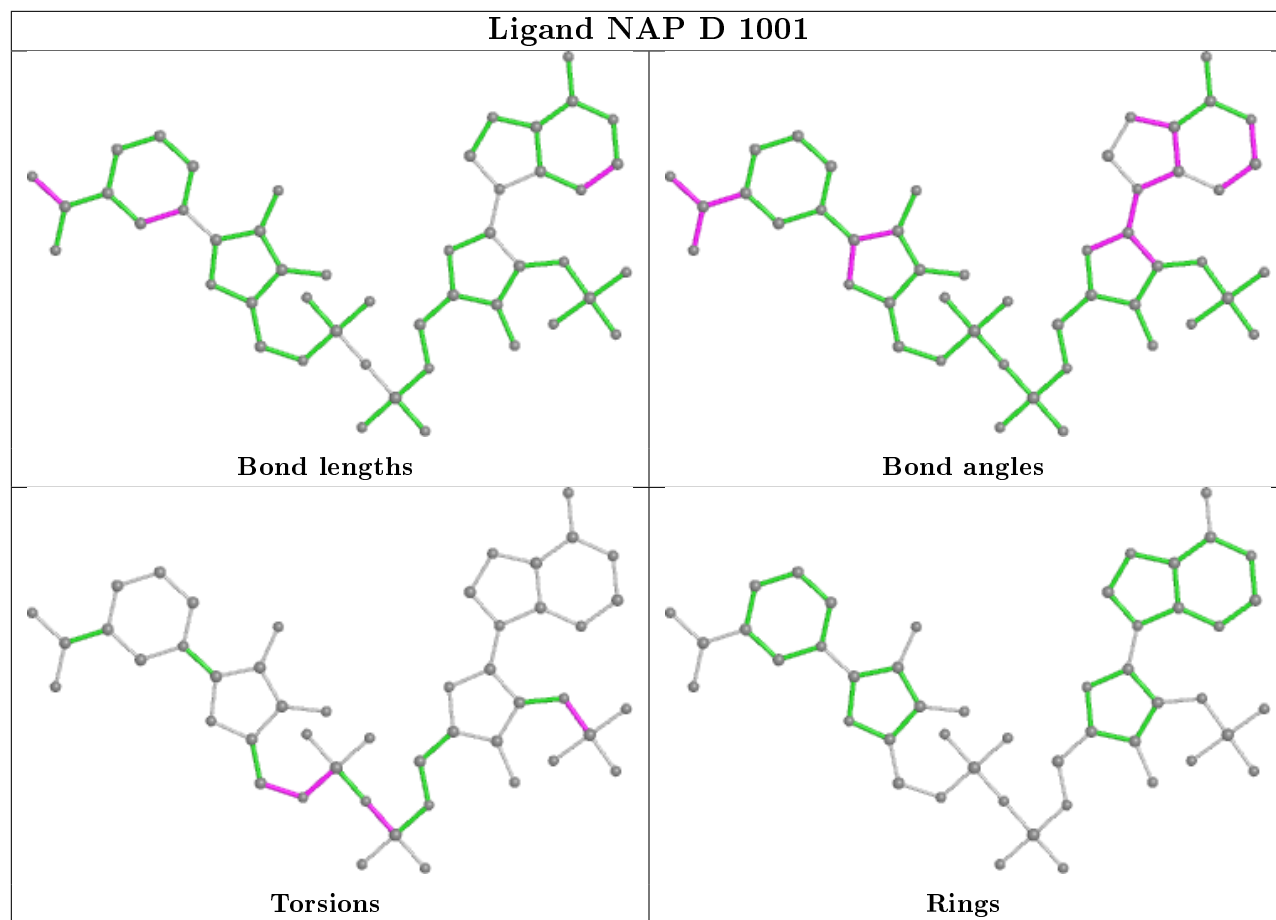
7 monomers are involved in 12 short contacts:

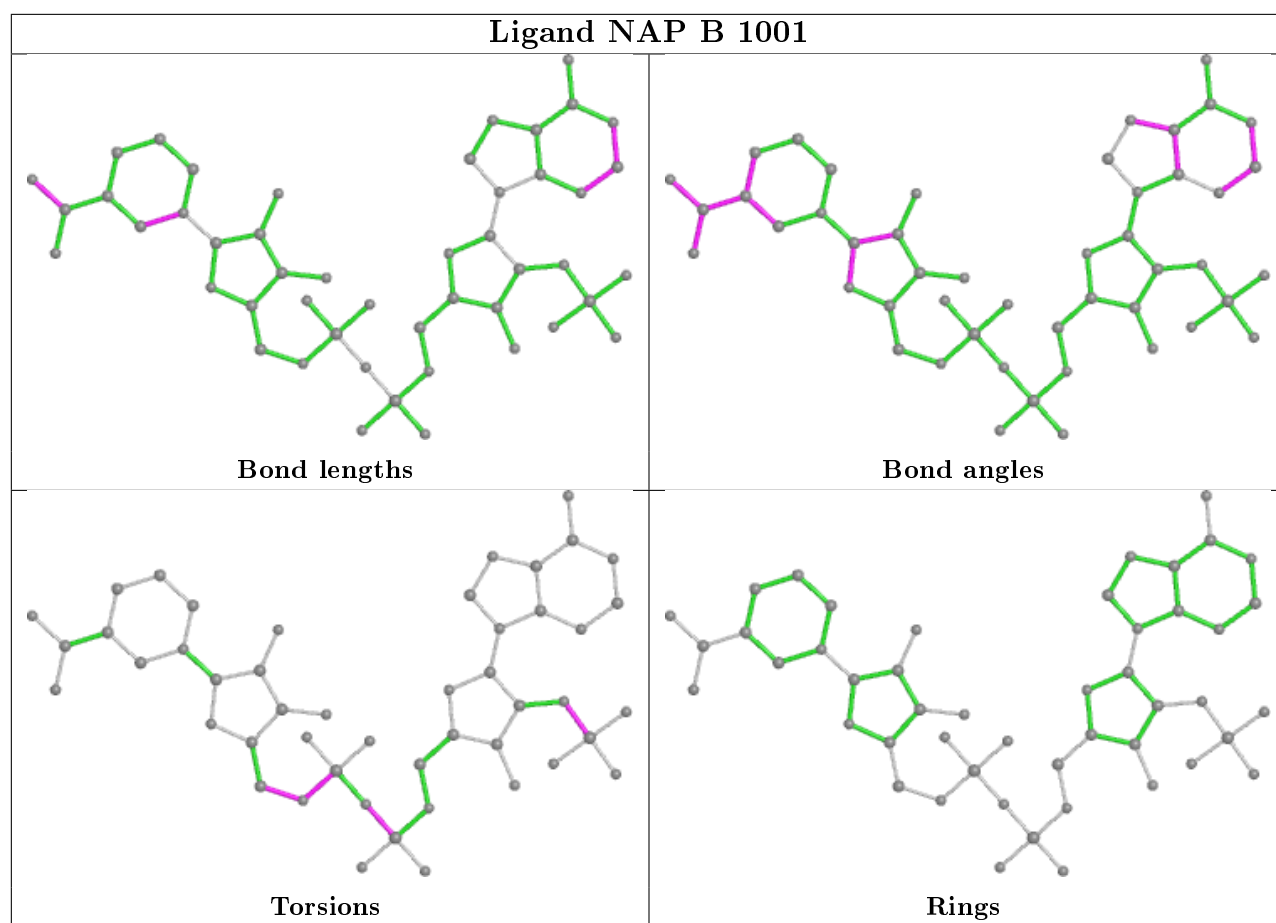
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1001	NAP	1	0
2	A	1001	NAP	3	0
4	B	1008	GOL	1	0
4	C	1008	GOL	1	0
4	A	1012	GOL	1	0
2	D	1001	NAP	3	0
2	B	1001	NAP	2	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	498/517 (96%)	-0.46	1 (0%) 95 96	9, 21, 33, 42	12 (2%)
1	B	498/517 (96%)	-0.47	2 (0%) 92 95	12, 22, 32, 49	12 (2%)
1	C	498/517 (96%)	-0.62	2 (0%) 92 95	10, 18, 28, 47	12 (2%)
1	D	498/517 (96%)	-0.51	2 (0%) 92 95	10, 21, 33, 45	13 (2%)
All	All	1992/2068 (96%)	-0.52	7 (0%) 92 95	9, 20, 32, 49	49 (2%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	405	VAL	4.8
1	D	405	VAL	4.2
1	C	405	VAL	3.6
1	C	819	ASP	3.3
1	D	415	LYS	2.8
1	B	405	VAL	2.6
1	B	415	LYS	2.4

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 carbohydrates in this entry.

6.4 Ligands ⓘ

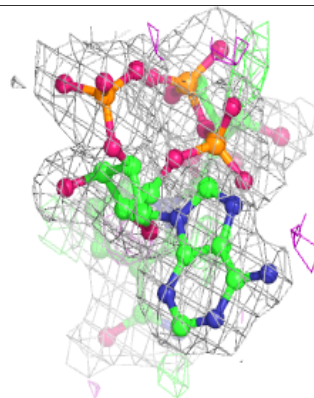
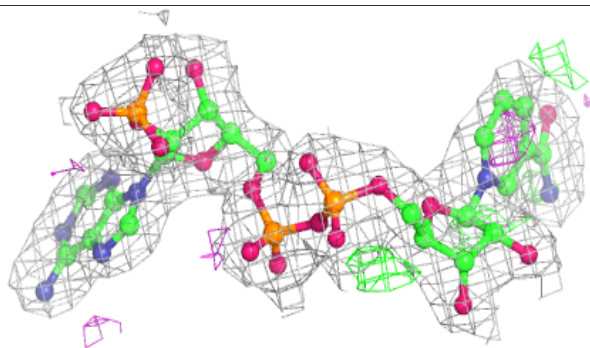
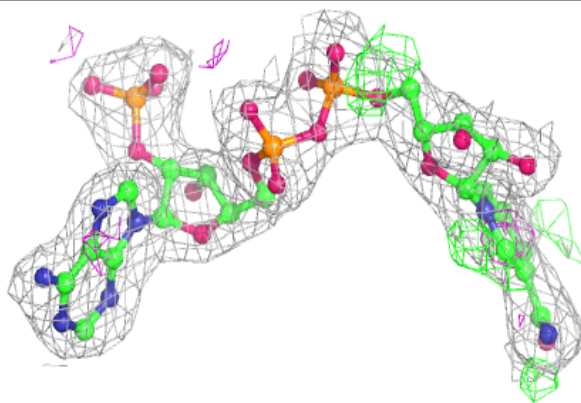
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	A	1008	5/5	0.65	0.41	45,48,48,49	5
3	SO4	D	1004	5/5	0.74	0.20	41,41,42,43	5
3	SO4	B	1006	5/5	0.78	0.24	39,39,41,41	5
3	SO4	D	1003	5/5	0.80	0.35	77,78,78,78	5
3	SO4	A	1006	5/5	0.82	0.21	43,44,45,46	5
3	SO4	A	1007	5/5	0.83	0.33	51,52,52,53	5
3	SO4	C	1003	5/5	0.83	0.27	70,71,72,72	5
3	SO4	D	1005	5/5	0.84	0.27	40,42,42,43	5
3	SO4	B	1005	5/5	0.84	0.28	96,96,97,97	0
3	SO4	A	1009	5/5	0.85	0.25	38,39,39,40	5
3	SO4	A	1005	5/5	0.86	0.34	81,81,82,82	5
4	GOL	D	1008	6/6	0.90	0.20	38,39,40,42	0
3	SO4	C	1004	5/5	0.90	0.27	44,45,46,46	5
3	SO4	D	1006	5/5	0.91	0.20	42,42,43,43	5
4	GOL	B	1008	6/6	0.93	0.20	39,41,41,43	0
3	SO4	B	1004	5/5	0.93	0.17	38,38,41,41	5
4	GOL	A	1012	6/6	0.94	0.21	40,42,42,42	0
3	SO4	A	1003	5/5	0.94	0.17	31,32,33,34	5
3	SO4	C	1005	5/5	0.95	0.14	33,34,34,34	5
3	SO4	B	1007	5/5	0.95	0.15	34,35,35,36	5
4	GOL	C	1008	6/6	0.96	0.17	34,39,39,40	0
3	SO4	A	1004	5/5	0.96	0.12	25,27,29,30	5
3	SO4	A	1002	5/5	0.96	0.10	31,32,33,33	5
3	SO4	C	1002	5/5	0.96	0.11	30,31,32,33	5
3	SO4	B	1002	5/5	0.97	0.12	19,21,21,22	5
2	NAP	A	1001	48/48	0.97	0.11	16,22,32,35	0
3	SO4	B	1003	5/5	0.97	0.11	33,34,34,35	5
2	NAP	D	1001	48/48	0.97	0.11	14,20,28,31	0
3	SO4	C	1007	5/5	0.97	0.10	28,30,32,32	5
3	SO4	A	1010	5/5	0.97	0.19	26,28,32,32	5
3	SO4	D	1002	5/5	0.97	0.13	27,28,29,30	5
2	NAP	B	1001	48/48	0.97	0.11	19,24,32,32	0
3	SO4	A	1011	5/5	0.97	0.17	22,27,28,29	5
3	SO4	C	1006	5/5	0.98	0.17	20,22,24,24	5
3	SO4	D	1007	5/5	0.98	0.17	22,24,26,27	5
2	NAP	C	1001	48/48	0.98	0.10	13,17,28,30	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.

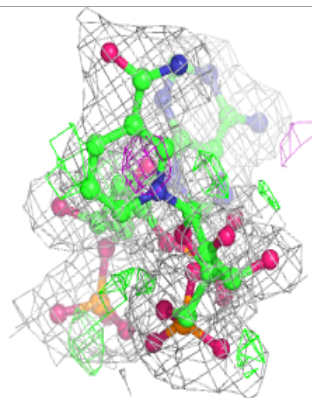
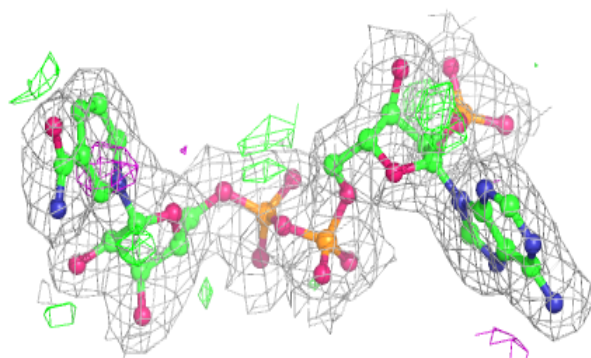
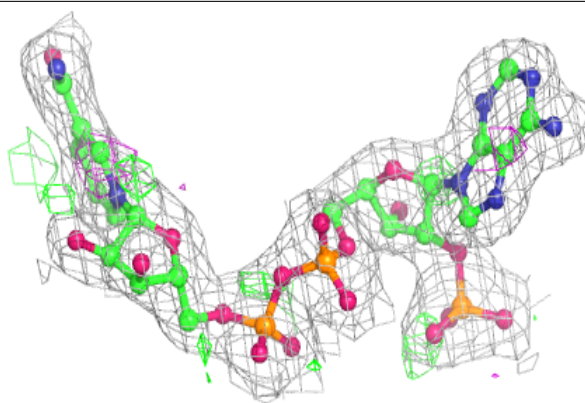
Electron density around NAP A 1001:

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

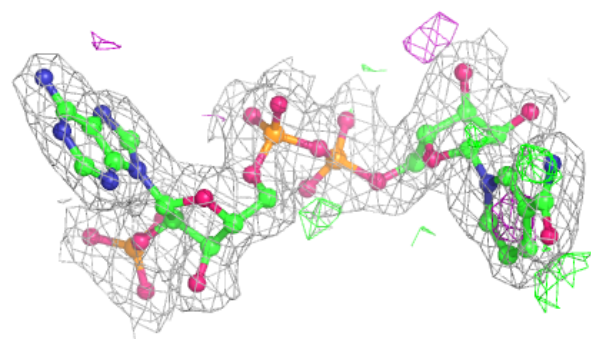
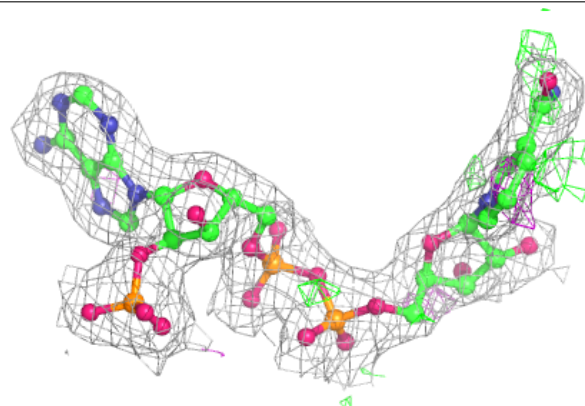


Electron density around NAP D 1001:

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

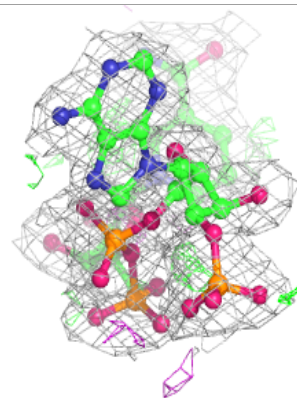
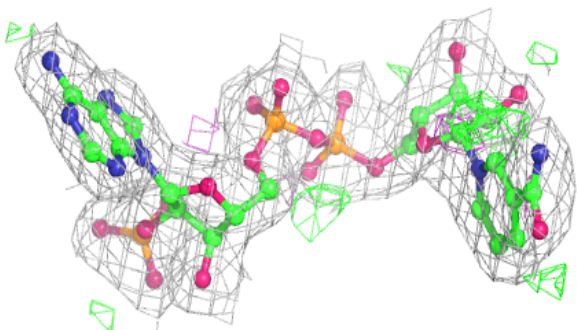
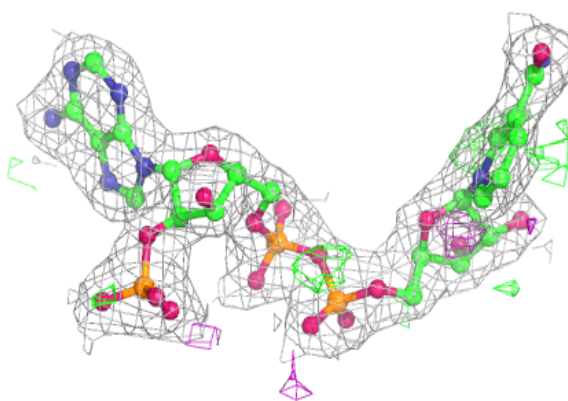
**Electron density around NAP B 1001:**

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



Electron density around NAP C 1001:

$2mF_o-DF_c$ (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.