



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:21 PM UTC

PDB ID : 4GMG / pdb_00004gmg
Title : NADP⁺ bound structure of a ThiazolinyI Imine Reductase from *Yersinia enterocolitica* (Irp3)
Authors : Lamb, A.L.; Meneely, K.M.
Deposited on : 2012-08-15
Resolution : 2.31 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

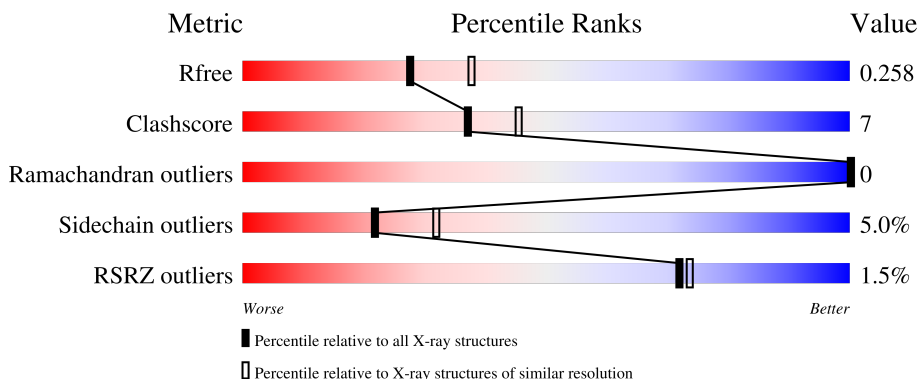
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

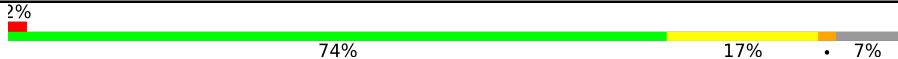
The reported resolution of this entry is 2.31 Å.

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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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 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	385	
1	B	385	
1	C	385	
1	D	385	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11156 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 Yersiniabactin biosynthetic protein YbtU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2806	1784	511	495	16			
1	B	345	Total	C	N	O	S	0	0	0
			2715	1728	493	479	15			
1	C	336	Total	C	N	O	S	0	0	0
			2636	1679	476	466	15			
1	D	343	Total	C	N	O	S	0	0	0
			2699	1719	489	476	15			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP A1JTG0
A	-18	GLY	-	expression tag	UNP A1JTG0
A	-17	SER	-	expression tag	UNP A1JTG0
A	-16	SER	-	expression tag	UNP A1JTG0
A	-15	HIS	-	expression tag	UNP A1JTG0
A	-14	HIS	-	expression tag	UNP A1JTG0
A	-13	HIS	-	expression tag	UNP A1JTG0
A	-12	HIS	-	expression tag	UNP A1JTG0
A	-11	HIS	-	expression tag	UNP A1JTG0
A	-10	HIS	-	expression tag	UNP A1JTG0
A	-9	SER	-	expression tag	UNP A1JTG0
A	-8	SER	-	expression tag	UNP A1JTG0
A	-7	GLY	-	expression tag	UNP A1JTG0
A	-6	LEU	-	expression tag	UNP A1JTG0
A	-5	VAL	-	expression tag	UNP A1JTG0
A	-4	PRO	-	expression tag	UNP A1JTG0
A	-3	ARG	-	expression tag	UNP A1JTG0
A	-2	GLY	-	expression tag	UNP A1JTG0
A	-1	SER	-	expression tag	UNP A1JTG0
A	0	HIS	-	expression tag	UNP A1JTG0
B	-19	MET	-	expression tag	UNP A1JTG0

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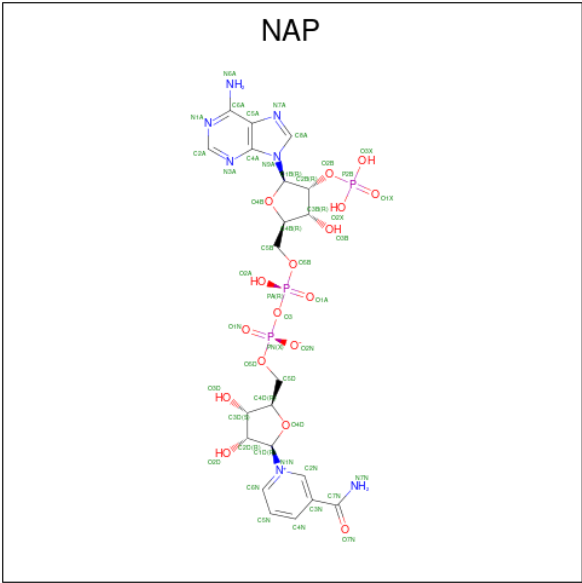
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP A1JTG0
B	-17	SER	-	expression tag	UNP A1JTG0
B	-16	SER	-	expression tag	UNP A1JTG0
B	-15	HIS	-	expression tag	UNP A1JTG0
B	-14	HIS	-	expression tag	UNP A1JTG0
B	-13	HIS	-	expression tag	UNP A1JTG0
B	-12	HIS	-	expression tag	UNP A1JTG0
B	-11	HIS	-	expression tag	UNP A1JTG0
B	-10	HIS	-	expression tag	UNP A1JTG0
B	-9	SER	-	expression tag	UNP A1JTG0
B	-8	SER	-	expression tag	UNP A1JTG0
B	-7	GLY	-	expression tag	UNP A1JTG0
B	-6	LEU	-	expression tag	UNP A1JTG0
B	-5	VAL	-	expression tag	UNP A1JTG0
B	-4	PRO	-	expression tag	UNP A1JTG0
B	-3	ARG	-	expression tag	UNP A1JTG0
B	-2	GLY	-	expression tag	UNP A1JTG0
B	-1	SER	-	expression tag	UNP A1JTG0
B	0	HIS	-	expression tag	UNP A1JTG0
C	-19	MET	-	expression tag	UNP A1JTG0
C	-18	GLY	-	expression tag	UNP A1JTG0
C	-17	SER	-	expression tag	UNP A1JTG0
C	-16	SER	-	expression tag	UNP A1JTG0
C	-15	HIS	-	expression tag	UNP A1JTG0
C	-14	HIS	-	expression tag	UNP A1JTG0
C	-13	HIS	-	expression tag	UNP A1JTG0
C	-12	HIS	-	expression tag	UNP A1JTG0
C	-11	HIS	-	expression tag	UNP A1JTG0
C	-10	HIS	-	expression tag	UNP A1JTG0
C	-9	SER	-	expression tag	UNP A1JTG0
C	-8	SER	-	expression tag	UNP A1JTG0
C	-7	GLY	-	expression tag	UNP A1JTG0
C	-6	LEU	-	expression tag	UNP A1JTG0
C	-5	VAL	-	expression tag	UNP A1JTG0
C	-4	PRO	-	expression tag	UNP A1JTG0
C	-3	ARG	-	expression tag	UNP A1JTG0
C	-2	GLY	-	expression tag	UNP A1JTG0
C	-1	SER	-	expression tag	UNP A1JTG0
C	0	HIS	-	expression tag	UNP A1JTG0
D	-19	MET	-	expression tag	UNP A1JTG0
D	-18	GLY	-	expression tag	UNP A1JTG0
D	-17	SER	-	expression tag	UNP A1JTG0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP A1JTG0
D	-15	HIS	-	expression tag	UNP A1JTG0
D	-14	HIS	-	expression tag	UNP A1JTG0
D	-13	HIS	-	expression tag	UNP A1JTG0
D	-12	HIS	-	expression tag	UNP A1JTG0
D	-11	HIS	-	expression tag	UNP A1JTG0
D	-10	HIS	-	expression tag	UNP A1JTG0
D	-9	SER	-	expression tag	UNP A1JTG0
D	-8	SER	-	expression tag	UNP A1JTG0
D	-7	GLY	-	expression tag	UNP A1JTG0
D	-6	LEU	-	expression tag	UNP A1JTG0
D	-5	VAL	-	expression tag	UNP A1JTG0
D	-4	PRO	-	expression tag	UNP A1JTG0
D	-3	ARG	-	expression tag	UNP A1JTG0
D	-2	GLY	-	expression tag	UNP A1JTG0
D	-1	SER	-	expression tag	UNP A1JTG0
D	0	HIS	-	expression tag	UNP A1JTG0

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: 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

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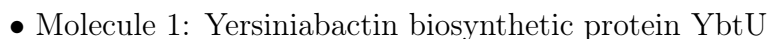
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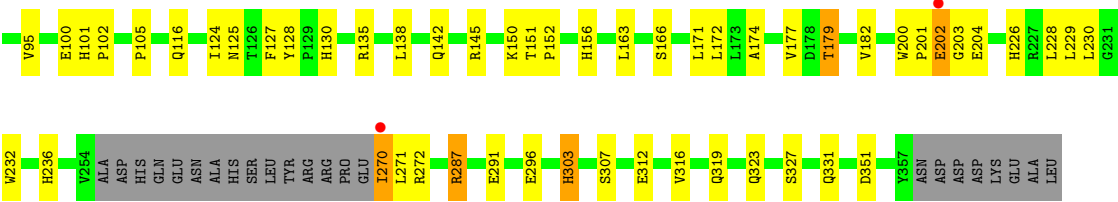
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is water.

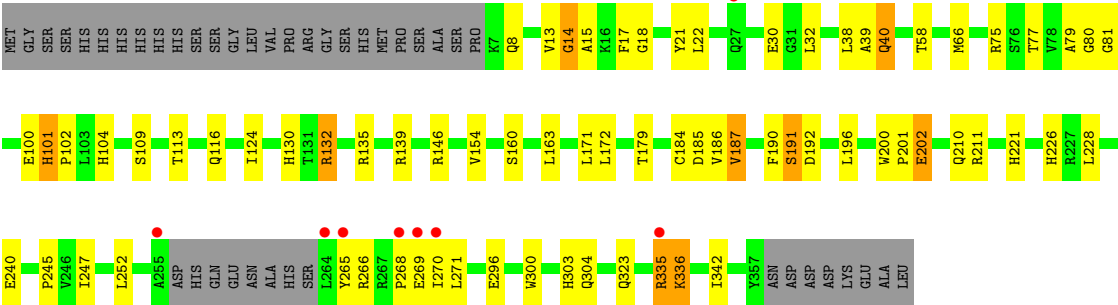
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	29	Total	O	0	0
			29	29		
3	B	34	Total	O	0	0
			34	34		
3	C	23	Total	O	0	0
			23	23		
3	D	22	Total	O	0	0
			22	22		

- Molecule 1: Yersiniabactin biosynthetic protein YbtU





● Molecule 1: Yersiniabactin biosynthetic protein YbtU



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.42Å 93.82Å 181.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.89 – 2.31 39.89 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.89-2.31) 99.7 (39.89-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.39	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.197 , 0.260 0.196 , 0.258	Depositor DCC
R_{free} test set	3227 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	29.6	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 29.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11156	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.76 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.5938e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: NAP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.24	8/2885 (0.3%)	1.20	11/3933 (0.3%)
1	B	1.19	7/2790 (0.3%)	1.18	19/3803 (0.5%)
1	C	1.29	12/2708 (0.4%)	1.18	13/3692 (0.4%)
1	D	1.14	5/2773 (0.2%)	1.19	12/3780 (0.3%)
All	All	1.22	32/11156 (0.3%)	1.19	55/15208 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	D	0	1
All	All	0	4

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	128	TYR	C-O	-8.39	1.16	1.24
1	C	125	ASN	C-O	-7.70	1.14	1.24
1	C	130	HIS	CG-ND1	-7.38	1.30	1.38
1	C	130	HIS	CD2-NE2	-6.94	1.30	1.37
1	C	39	ALA	C-O	-6.44	1.18	1.24
1	B	156	HIS	CG-CD2	6.36	1.42	1.35
1	A	39	ALA	C-O	-6.28	1.18	1.24
1	C	303	HIS	CG-CD2	6.01	1.42	1.35
1	C	236	HIS	CG-CD2	5.99	1.42	1.35
1	C	17	PHE	C-O	-5.85	1.16	1.24
1	C	226	HIS	CG-CD2	5.82	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	101	HIS	CG-CD2	5.81	1.42	1.35
1	B	240	GLU	N-CA	5.70	1.53	1.46
1	B	221	HIS	CG-CD2	5.69	1.42	1.35
1	A	156	HIS	CG-CD2	5.66	1.42	1.35
1	B	134	GLY	N-CA	5.55	1.52	1.45
1	A	128	TYR	C-O	-5.51	1.17	1.24
1	A	125	ASN	C-O	-5.51	1.17	1.24
1	A	152	PRO	C-O	-5.50	1.18	1.24
1	B	156	HIS	ND1-CE1	5.30	1.37	1.32
1	D	221	HIS	CG-CD2	5.30	1.41	1.35
1	B	104	HIS	CG-CD2	5.29	1.41	1.35
1	C	127	PHE	C-O	-5.28	1.17	1.24
1	A	129	PRO	C-O	-5.28	1.17	1.24
1	A	16	LYS	C-O	-5.21	1.17	1.24
1	C	179	THR	C-O	-5.21	1.18	1.24
1	D	130	HIS	CG-CD2	5.21	1.41	1.35
1	C	156	HIS	CG-CD2	5.11	1.41	1.35
1	D	104	HIS	CG-CD2	5.05	1.41	1.35
1	B	221	HIS	ND1-CE1	5.05	1.37	1.32
1	A	194	HIS	CE1-NE2	5.02	1.37	1.32
1	D	226	HIS	CG-CD2	5.01	1.41	1.35

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	15	ALA	N-CA-C	9.44	125.06	113.17
1	A	15	ALA	N-CA-C	8.23	124.55	112.94
1	D	265	TYR	N-CA-C	-8.02	102.55	113.30
1	A	40	GLN	N-CA-C	-7.42	98.15	109.95
1	B	80	GLY	N-CA-C	7.26	124.32	115.31
1	A	151	THR	CB-CA-C	6.94	118.66	108.87
1	D	190	PHE	N-CA-C	-6.91	98.91	109.41
1	A	152	PRO	CA-C-N	-6.89	111.88	119.19
1	A	152	PRO	C-N-CA	-6.89	111.88	119.19
1	A	273	ASP	CA-C-N	6.53	127.11	120.38
1	A	273	ASP	C-N-CA	6.53	127.11	120.38
1	A	79	ALA	N-CA-C	-6.49	100.31	110.36
1	D	40	GLN	N-CA-C	-6.39	101.33	110.59
1	C	15	ALA	N-CA-C	6.38	121.94	112.94
1	C	130	HIS	N-CA-C	6.27	120.94	113.16
1	B	81	GLY	N-CA-C	6.23	127.95	113.18
1	B	15	ALA	N-CA-C	6.16	120.68	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	187	VAL	CB-CA-C	6.05	118.51	111.55
1	D	81	GLY	N-CA-C	5.92	119.90	112.79
1	D	13	VAL	CA-C-N	5.84	132.22	121.70
1	D	13	VAL	C-N-CA	5.84	132.22	121.70
1	C	13	VAL	CA-C-N	5.83	132.19	121.70
1	C	13	VAL	C-N-CA	5.83	132.19	121.70
1	B	106	ASP	N-CA-C	5.82	117.62	111.28
1	B	78	VAL	CB-CA-C	-5.76	104.36	112.14
1	C	202	GLU	N-CA-C	5.76	119.41	112.38
1	B	347	PRO	N-CA-C	5.76	117.72	110.70
1	B	40	GLN	N-CA-C	-5.73	101.72	110.14
1	C	40	GLN	N-CA-C	5.70	120.24	112.88
1	C	203	GLY	N-CA-C	5.63	119.35	111.19
1	A	217	ASP	CA-C-N	5.62	125.30	119.56
1	A	217	ASP	C-N-CA	5.62	125.30	119.56
1	D	13	VAL	CB-CA-C	-5.62	102.84	110.42
1	A	26	MET	N-CA-C	-5.61	106.43	113.28
1	B	172	LEU	N-CA-C	5.61	117.47	111.36
1	D	80	GLY	N-CA-C	5.50	120.82	114.16
1	B	35	VAL	N-CA-C	5.43	118.37	113.10
1	B	346	THR	CA-C-N	-5.41	114.80	120.38
1	B	346	THR	C-N-CA	-5.41	114.80	120.38
1	B	172	LEU	CA-CB-CG	-5.39	97.42	116.30
1	D	17	PHE	N-CA-C	-5.38	105.98	112.54
1	B	152	PRO	CA-C-N	-5.32	114.34	119.87
1	B	152	PRO	C-N-CA	-5.32	114.34	119.87
1	C	35	VAL	CB-CA-C	-5.28	105.47	110.70
1	C	13	VAL	CA-C-O	-5.24	115.06	120.25
1	C	152	PRO	CA-C-N	-5.24	113.29	119.84
1	C	152	PRO	C-N-CA	-5.24	113.29	119.84
1	D	13	VAL	O-C-N	-5.18	117.79	123.18
1	B	153	PRO	CA-C-N	-5.16	116.79	123.19
1	B	153	PRO	C-N-CA	-5.16	116.79	123.19
1	B	311	GLY	N-CA-C	5.14	120.81	114.69
1	B	13	VAL	O-C-N	-5.11	117.68	123.20
1	B	291	GLU	N-CA-C	-5.04	107.26	113.41
1	C	232	TRP	CA-C-N	-5.02	114.44	119.56
1	C	232	TRP	C-N-CA	-5.02	114.44	119.56

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	VAL	Peptide
1	B	13	VAL	Peptide
1	B	14	GLY	Peptide
1	D	14	GLY	Peptide

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	2806	0	2785	42	1
1	B	2715	0	2691	46	0
1	C	2636	0	2615	34	1
1	D	2699	0	2679	41	0
2	A	48	0	25	3	0
2	B	48	0	25	4	0
2	C	48	0	25	4	0
2	D	48	0	25	4	0
3	A	29	0	0	0	0
3	B	34	0	0	1	0
3	C	23	0	0	0	0
3	D	22	0	0	1	0
All	All	11156	0	10870	155	1

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 (155) 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:151:THR:HG21	1:C:202:GLU:OE1	1.36	1.23
1:C:151:THR:CG2	1:C:202:GLU:OE1	1.94	1.15
1:A:40:GLN:O	2:A:401:NAP:O1X	1.77	1.00
1:D:171:LEU:HD13	1:D:228:LEU:HD23	1.49	0.95
1:A:124:ILE:H	1:A:323:GLN:HE22	1.14	0.93
1:A:172:LEU:CD2	1:A:179:THR:HG23	1.99	0.93
1:D:132:ARG:HH11	1:D:132:ARG:HG2	1.38	0.89
1:D:172:LEU:HD13	1:D:179:THR:HG23	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:HIS:HD2	1:A:106:ASP:H	1.27	0.83
1:B:40:GLN:O	2:B:401:NAP:O3X	1.98	0.81
1:A:172:LEU:HD22	1:A:179:THR:HG23	1.60	0.81
1:B:124:ILE:H	1:B:323:GLN:HE22	1.30	0.80
1:D:184:CYS:O	1:D:336:LYS:HE2	1.82	0.79
1:A:96:HIS:HD2	1:A:121:CYS:H	1.27	0.79
1:D:124:ILE:H	1:D:323:GLN:HE22	1.32	0.78
1:B:171:LEU:HD13	1:B:228:LEU:HD23	1.66	0.77
1:C:124:ILE:H	1:C:323:GLN:HE22	1.31	0.77
1:C:172:LEU:HD22	1:C:179:THR:HG23	1.70	0.74
1:A:8:GLN:HB2	1:A:32:LEU:HD23	1.70	0.73
1:D:132:ARG:HG2	1:D:132:ARG:NH1	2.04	0.72
1:A:74:VAL:HG21	1:A:86:LEU:HD12	1.71	0.71
1:C:105:PRO:HD3	1:C:327:SER:OG	1.92	0.68
1:B:16:LYS:HB3	2:B:401:NAP:O2N	1.93	0.67
1:B:7:LYS:HE2	1:B:31:GLY:HA2	1.76	0.67
1:D:171:LEU:CD1	1:D:228:LEU:HD23	2.24	0.67
1:C:142:GLN:HG2	1:C:145:ARG:NH2	2.10	0.67
1:B:27:GLN:HE21	1:D:335:ARG:HE	1.41	0.66
1:A:104:HIS:CD2	1:A:106:ASP:H	2.11	0.65
1:D:75:ARG:HB3	1:D:79:ALA:HB3	1.79	0.64
1:D:8:GLN:HB2	1:D:32:LEU:HD23	1.79	0.64
1:D:270:ILE:O	1:D:271:LEU:HB2	1.97	0.63
1:C:307:SER:HB3	1:C:312:GLU:HG3	1.83	0.60
1:A:266:ARG:HG3	1:B:47:GLU:OE1	2.01	0.60
1:C:100:GLU:HG3	2:C:401:NAP:H1D	1.84	0.60
1:A:172:LEU:HD23	1:A:179:THR:HG23	1.83	0.59
1:D:40:GLN:O	2:D:401:NAP:O2X	2.19	0.59
1:A:312:GLU:HA	1:A:312:GLU:OE1	2.04	0.58
1:C:151:THR:HG23	1:C:202:GLU:OE1	1.98	0.56
1:A:96:HIS:CD2	1:A:120:CYS:HB2	2.40	0.56
1:B:20:MET:HE3	1:B:290:CYS:HA	1.88	0.56
1:C:151:THR:HG21	1:C:202:GLU:CD	2.26	0.56
1:B:29:PRO:HG2	1:B:32:LEU:HD13	1.88	0.55
1:B:172:LEU:HD22	1:B:179:THR:OG1	2.05	0.55
1:D:200:TRP:HB2	1:D:201:PRO:HD2	1.88	0.55
1:B:186:VAL:HA	1:B:196:LEU:HD23	1.89	0.55
1:B:46:ARG:HG2	1:B:56:LEU:HD22	1.89	0.55
1:C:16:LYS:HE2	2:C:401:NAP:H51A	1.89	0.55
1:B:108:ILE:HG12	1:B:124:ILE:HD11	1.87	0.54
1:D:132:ARG:HH11	1:D:132:ARG:CG	2.17	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:LEU:HD21	1:C:182:VAL:HG21	1.90	0.54
1:C:229:LEU:C	1:C:229:LEU:HD23	2.33	0.54
1:D:269:GLU:H	1:D:269:GLU:CD	2.16	0.54
1:A:187:VAL:CG1	1:B:188:GLY:HA3	2.37	0.54
1:D:300:TRP:O	1:D:304:GLN:HG2	2.08	0.53
1:A:3:SER:HB2	1:A:7:LYS:HE2	1.89	0.53
1:B:46:ARG:HG2	1:B:56:LEU:CD2	2.39	0.52
1:B:75:ARG:HG2	1:B:79:ALA:HB1	1.90	0.52
1:A:19:GLU:HA	1:A:22:LEU:HD12	1.91	0.52
1:B:229:LEU:C	1:B:229:LEU:HD23	2.35	0.52
1:A:100:GLU:HG3	2:A:401:NAP:H1D	1.91	0.51
1:D:135:ARG:NH2	1:D:296:GLU:OE1	2.44	0.50
1:B:126:THR:OG1	1:B:169:ASP:OD2	2.19	0.50
1:C:30:GLU:O	1:C:303:HIS:HE1	1.94	0.50
1:B:75:ARG:HD3	2:B:401:NAP:O2A	2.12	0.50
1:B:132:ARG:NH2	1:D:185:ASP:OD2	2.45	0.49
1:D:101:HIS:HB2	1:D:102:PRO:HA	1.94	0.49
1:D:160:SER:HA	1:D:210:GLN:HB3	1.94	0.49
1:A:74:VAL:CG2	1:A:83:GLY:HA2	2.43	0.49
1:A:245:PRO:HA	1:A:280:SER:O	2.12	0.49
1:A:14:GLY:O	1:A:18:GLY:HA3	2.12	0.48
1:B:20:MET:HE2	1:B:294:GLY:HA3	1.95	0.48
1:D:266:ARG:C	1:D:268:PRO:HD3	2.39	0.48
1:B:14:GLY:O	1:B:18:GLY:HA3	2.13	0.48
1:D:192:ASP:C	1:D:211:ARG:HG2	2.38	0.48
1:A:136:THR:HG21	1:A:280:SER:HB2	1.94	0.48
1:C:138:LEU:O	1:C:142:GLN:HG3	2.14	0.48
1:D:240:GLU:HB2	1:D:245:PRO:HD2	1.96	0.48
1:A:74:VAL:HG23	1:A:83:GLY:CA	2.44	0.47
1:D:75:ARG:HG3	2:D:401:NAP:O2A	2.14	0.47
1:C:101:HIS:HB2	1:C:102:PRO:HA	1.97	0.47
1:A:147:CYS:HB3	1:B:352:ARG:O	2.15	0.47
1:C:15:ALA:HB2	1:C:37:LEU:HD21	1.96	0.47
1:A:270:ILE:O	1:A:271:LEU:HB2	2.14	0.46
1:D:40:GLN:C	2:D:401:NAP:O2X	2.58	0.46
1:A:150:LYS:HE3	1:A:150:LYS:HA	1.97	0.46
1:A:74:VAL:HG23	1:A:83:GLY:HA2	1.97	0.46
1:B:77:THR:O	1:B:79:ALA:O	2.33	0.46
1:C:200:TRP:HB2	1:C:201:PRO:HD2	1.97	0.46
1:B:291:GLU:O	1:D:335:ARG:NH1	2.49	0.46
1:C:287:ARG:O	1:C:291:GLU:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:GLU:OE1	1:D:266:ARG:HG3	2.15	0.46
1:A:100:GLU:CG	2:A:401:NAP:H1D	2.47	0.45
1:B:40:GLN:C	2:B:401:NAP:O3X	2.58	0.45
1:D:39:ALA:O	1:D:58:THR:HA	2.15	0.45
1:B:215:PRO:CD	1:B:342:ILE:HG23	2.47	0.45
1:D:100:GLU:HG3	2:D:401:NAP:H1D	1.98	0.45
1:C:174:ALA:HB1	1:C:230:LEU:HD11	1.98	0.45
1:A:300:TRP:O	1:A:304:GLN:HG2	2.17	0.45
1:C:171:LEU:HD13	1:C:228:LEU:HD23	1.99	0.45
1:D:200:TRP:HB2	1:D:201:PRO:CD	2.47	0.45
1:B:29:PRO:HG2	1:B:32:LEU:CD1	2.47	0.45
1:A:29:PRO:HG2	1:A:32:LEU:HD12	1.98	0.44
1:D:14:GLY:HA2	1:D:38:LEU:O	2.16	0.44
1:A:77:THR:O	1:A:79:ALA:O	2.36	0.44
1:B:78:VAL:HG22	1:B:104:HIS:HB2	1.98	0.44
1:C:270:ILE:HG12	1:C:271:LEU:N	2.32	0.44
1:A:39:ALA:O	1:A:58:THR:HA	2.18	0.44
1:C:172:LEU:CD2	1:C:179:THR:HG23	2.44	0.44
1:C:22:LEU:HD11	1:C:37:LEU:HD22	1.98	0.44
1:D:14:GLY:O	1:D:18:GLY:HA3	2.17	0.44
1:D:186:VAL:HA	1:D:196:LEU:HD23	2.00	0.44
1:C:46:ARG:HA	1:C:56:LEU:HD22	1.99	0.43
1:B:283:PRO:HG3	1:B:293:VAL:HG21	2.00	0.43
1:B:13:VAL:O	1:B:73:VAL:N	2.36	0.43
1:B:192:ASP:C	1:B:211:ARG:HG2	2.43	0.43
1:C:14:GLY:O	1:C:18:GLY:HA3	2.18	0.43
1:D:66:MET:HA	1:D:66:MET:HE2	2.01	0.43
1:B:292:THR:C	1:B:295:PRO:HD2	2.43	0.43
1:D:21:TYR:O	1:D:22:LEU:C	2.61	0.43
1:B:213:LEU:C	1:B:213:LEU:HD12	2.44	0.43
1:A:22:LEU:CD1	1:A:48:LEU:HD13	2.48	0.43
1:C:46:ARG:HA	1:C:56:LEU:CD2	2.49	0.42
1:D:146:ARG:NH1	3:D:501:HOH:O	2.51	0.42
1:A:8:GLN:HB2	1:A:32:LEU:CD2	2.43	0.42
1:B:101:HIS:HB2	1:B:102:PRO:HA	2.01	0.42
1:B:192:ASP:O	1:B:211:ARG:HG2	2.18	0.42
1:C:90:PHE:HB3	1:C:95:VAL:HB	2.01	0.42
1:D:77:THR:O	1:D:79:ALA:O	2.37	0.42
1:B:183:GLU:O	1:B:198:LEU:HA	2.19	0.42
1:B:194:HIS:HD2	3:B:512:HOH:O	2.02	0.42
1:A:20:MET:HE3	1:A:20:MET:HB2	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:MET:O	1:A:221:HIS:HB2	2.19	0.42
1:A:267:ARG:O	1:A:270:ILE:HG22	2.20	0.42
1:A:213:LEU:C	1:A:213:LEU:HD12	2.45	0.42
1:B:160:SER:HA	1:B:210:GLN:HB3	2.02	0.41
1:B:200:TRP:HB2	1:B:201:PRO:HD2	2.03	0.41
1:B:300:TRP:O	1:B:304:GLN:HG2	2.20	0.41
1:C:42:SER:OG	2:C:401:NAP:O1X	2.28	0.41
1:C:135:ARG:NH2	1:C:296:GLU:OE1	2.41	0.41
1:D:30:GLU:HB2	1:D:303:HIS:CD2	2.54	0.41
1:A:148:LEU:HD21	1:B:353:LEU:HD21	2.03	0.41
1:A:160:SER:HA	1:A:210:GLN:HB3	2.03	0.41
1:A:319:GLN:O	1:A:323:GLN:HG3	2.21	0.41
1:A:104:HIS:CD2	1:A:106:ASP:HB2	2.54	0.41
1:B:347:PRO:HA	1:B:348:PRO:HD3	1.88	0.41
1:C:35:VAL:O	1:C:55:PRO:HG2	2.20	0.41
1:C:171:LEU:CD1	1:C:228:LEU:HD23	2.50	0.41
1:C:204:GLU:OE2	1:D:191:SER:N	2.48	0.41
1:A:90:PHE:HB3	1:A:95:VAL:HB	2.03	0.40
1:D:240:GLU:HG3	1:D:247:ILE:HD12	2.03	0.40
1:B:20:MET:HE2	1:B:127:PHE:HZ	1.86	0.40
1:B:171:LEU:HA	1:B:171:LEU:HD12	1.82	0.40
1:D:200:TRP:CD1	1:D:202:GLU:HG2	2.56	0.40
1:B:10:VAL:N	1:B:33:GLU:O	2.48	0.40
2:C:401:NAP:H6N	2:C:401:NAP:H2D	1.80	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:ASN:OD1	1:C:27:GLN:NE2[1_655]	2.17	0.03

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	354/385 (92%)	341 (96%)	13 (4%)	0	100	100
1	B	341/385 (89%)	329 (96%)	12 (4%)	0	100	100
1	C	332/385 (86%)	321 (97%)	11 (3%)	0	100	100
1	D	339/385 (88%)	329 (97%)	10 (3%)	0	100	100
All	All	1366/1540 (89%)	1320 (97%)	46 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	302/325 (93%)	289 (96%)	13 (4%)	26	38
1	B	291/325 (90%)	275 (94%)	16 (6%)	19	27
1	C	283/325 (87%)	268 (95%)	15 (5%)	20	29
1	D	289/325 (89%)	275 (95%)	14 (5%)	23	33
All	All	1165/1300 (90%)	1107 (95%)	58 (5%)	22	32

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	MET
1	A	73	VAL
1	A	139	ARG
1	A	142	GLN
1	A	150	LYS
1	A	151	THR
1	A	177	VAL
1	A	228	LEU
1	A	247	ILE
1	A	271	LEU
1	A	292	THR

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Mol	Chain	Res	Type
1	A	316	VAL
1	A	344	ARG
1	B	8	GLN
1	B	40	GLN
1	B	74	VAL
1	B	75	ARG
1	B	78	VAL
1	B	150	LYS
1	B	154	VAL
1	B	172	LEU
1	B	177	VAL
1	B	202	GLU
1	B	264	LEU
1	B	265	TYR
1	B	271	LEU
1	B	287	ARG
1	B	292	THR
1	B	347	PRO
1	C	16	LYS
1	C	40	GLN
1	C	73	VAL
1	C	116	GLN
1	C	150	LYS
1	C	163	LEU
1	C	166	SER
1	C	177	VAL
1	C	270	ILE
1	C	272	ARG
1	C	287	ARG
1	C	316	VAL
1	C	319	GLN
1	C	331	GLN
1	C	351	ASP
1	D	109	SER
1	D	113	THR
1	D	116	GLN
1	D	132	ARG
1	D	139	ARG
1	D	154	VAL
1	D	163	LEU
1	D	187	VAL
1	D	191	SER

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Mol	Chain	Res	Type
1	D	202	GLU
1	D	252	LEU
1	D	335	ARG
1	D	336	LYS
1	D	342	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	96	HIS
1	A	104	HIS
1	A	130	HIS
1	A	323	GLN
1	A	349	HIS
1	B	130	HIS
1	B	194	HIS
1	B	323	GLN
1	B	350	HIS
1	C	130	HIS
1	C	303	HIS
1	C	323	GLN
1	C	332	GLN
1	D	85	GLN
1	D	130	HIS
1	D	303	HIS
1	D	323	GLN
1	D	339	ASN
1	D	350	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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
2	NAP	A	401	-	50,52,52	2.19	16 (32%)	71,80,80	1.74	15 (21%)
2	NAP	C	401	-	50,52,52	2.05	16 (32%)	71,80,80	1.77	11 (15%)
2	NAP	D	401	-	50,52,52	1.99	14 (28%)	71,80,80	1.57	12 (16%)
2	NAP	B	401	-	50,52,52	1.50	6 (12%)	71,80,80	2.09	18 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	A	401	-	-	8/35/67/67	0/5/5/5
2	NAP	C	401	-	-	12/35/67/67	0/5/5/5
2	NAP	D	401	-	-	11/35/67/67	0/5/5/5
2	NAP	B	401	-	-	8/35/67/67	0/5/5/5

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	NAP	C5A-C4A	5.25	1.48	1.39
2	C	401	NAP	C5A-N7A	-5.19	1.29	1.39
2	A	401	NAP	C5A-N7A	-5.04	1.29	1.39
2	A	401	NAP	PA-O3	-4.61	1.54	1.59
2	A	401	NAP	PN-O3	-4.60	1.54	1.59
2	D	401	NAP	C5A-N7A	-4.38	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	NAP	C2N-N1N	-4.36	1.30	1.35
2	D	401	NAP	C4A-N9A	-4.03	1.29	1.37
2	C	401	NAP	C8A-N9A	-3.94	1.30	1.37
2	C	401	NAP	C4A-N9A	-3.86	1.29	1.37
2	B	401	NAP	PN-O3	3.85	1.63	1.59
2	C	401	NAP	PN-O1N	-3.81	1.37	1.50
2	B	401	NAP	C5A-C6A	3.78	1.51	1.41
2	D	401	NAP	C8A-N9A	-3.74	1.31	1.37
2	B	401	NAP	PA-O3	3.74	1.63	1.59
2	A	401	NAP	PA-O2A	-3.61	1.38	1.55
2	C	401	NAP	PN-O3	-3.53	1.55	1.59
2	D	401	NAP	P2B-O2X	-3.47	1.41	1.54
2	A	401	NAP	P2B-O2X	-3.39	1.42	1.54
2	A	401	NAP	C8A-N9A	-3.38	1.31	1.37
2	C	401	NAP	P2B-O2X	-3.28	1.42	1.54
2	A	401	NAP	P2B-O3X	-3.20	1.42	1.54
2	A	401	NAP	PN-O1N	-3.17	1.39	1.50
2	A	401	NAP	C5A-C4A	3.15	1.44	1.39
2	D	401	NAP	O7N-C7N	-3.12	1.18	1.24
2	C	401	NAP	PA-O3	-3.02	1.56	1.59
2	D	401	NAP	P2B-O3X	-3.01	1.43	1.54
2	C	401	NAP	PN-O2N	-2.99	1.41	1.55
2	C	401	NAP	P2B-O3X	-2.93	1.43	1.54
2	A	401	NAP	O4D-C4D	-2.93	1.38	1.45
2	A	401	NAP	PN-O2N	-2.92	1.41	1.55
2	C	401	NAP	C5A-C4A	2.92	1.44	1.39
2	A	401	NAP	P2B-O1X	-2.88	1.41	1.50
2	A	401	NAP	PA-O1A	-2.87	1.40	1.50
2	A	401	NAP	C4A-N9A	-2.82	1.31	1.37
2	C	401	NAP	C2N-N1N	-2.80	1.31	1.35
2	C	401	NAP	PA-O2A	-2.80	1.42	1.55
2	D	401	NAP	C5A-C4A	2.75	1.44	1.39
2	C	401	NAP	O4D-C4D	-2.53	1.39	1.45
2	B	401	NAP	C8A-N7A	2.51	1.36	1.31
2	C	401	NAP	PN-O5D	-2.48	1.49	1.59
2	D	401	NAP	PN-O2N	-2.48	1.43	1.55
2	D	401	NAP	PA-O1A	-2.48	1.42	1.50
2	D	401	NAP	PN-O3	-2.46	1.56	1.59
2	D	401	NAP	PA-O2A	-2.45	1.44	1.55
2	B	401	NAP	O4D-C1D	2.37	1.44	1.40
2	C	401	NAP	O7N-C7N	-2.36	1.19	1.24
2	D	401	NAP	C5A-C6A	2.31	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAP	O7N-C7N	-2.26	1.19	1.24
2	D	401	NAP	O2D-C2D	-2.12	1.37	1.43
2	A	401	NAP	PA-O5B	-2.08	1.51	1.59
2	C	401	NAP	C2N-C3N	-2.04	1.35	1.39

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	NAP	C5A-C4A-N3A	-6.24	118.12	126.72
2	C	401	NAP	C5A-C4A-N3A	-6.04	118.40	126.72
2	D	401	NAP	C5A-C4A-N3A	-5.64	118.95	126.72
2	A	401	NAP	C5A-C4A-N3A	-5.30	119.42	126.72
2	B	401	NAP	C4A-C5A-N7A	-4.98	104.89	110.58
2	B	401	NAP	C5D-C4D-C3D	-4.86	97.70	115.21
2	B	401	NAP	O2N-PN-O3	4.77	120.16	107.27
2	C	401	NAP	O2N-PN-O3	4.74	120.10	107.27
2	A	401	NAP	N3A-C4A-N9A	4.49	134.80	127.17
2	B	401	NAP	C2A-N3A-C4A	4.47	122.76	111.83
2	C	401	NAP	O3-PN-O1N	-4.47	97.25	110.70
2	C	401	NAP	N3A-C4A-N9A	4.41	134.66	127.17
2	A	401	NAP	N3A-C2A-N1A	-4.34	122.01	128.58
2	D	401	NAP	N3A-C4A-N9A	4.34	134.54	127.17
2	B	401	NAP	N3A-C2A-N1A	-4.24	122.17	128.58
2	B	401	NAP	N3A-C4A-N9A	4.19	134.30	127.17
2	A	401	NAP	O3-PN-O1N	-4.14	98.24	110.70
2	B	401	NAP	C6A-C5A-N7A	3.85	139.51	132.09
2	A	401	NAP	C2A-N3A-C4A	3.82	121.17	111.83
2	C	401	NAP	C2A-N3A-C4A	3.78	121.06	111.83
2	A	401	NAP	O2B-P2B-O1X	-3.74	96.00	109.33
2	C	401	NAP	N3A-C2A-N1A	-3.71	122.97	128.58
2	C	401	NAP	C4A-C5A-N7A	-3.54	106.54	110.58
2	D	401	NAP	C2A-N3A-C4A	3.53	120.45	111.83
2	B	401	NAP	C5A-N7A-C8A	3.49	108.93	103.45
2	A	401	NAP	C4A-C5A-N7A	-3.46	106.62	110.58
2	D	401	NAP	O2A-PA-O3	3.29	116.16	107.27
2	A	401	NAP	C5A-N7A-C8A	3.19	108.46	103.45
2	B	401	NAP	O2N-PN-O5D	-3.08	93.59	107.57
2	D	401	NAP	C4A-C5A-N7A	-3.05	107.10	110.58
2	B	401	NAP	C5N-C4N-C3N	-2.99	117.43	120.36
2	A	401	NAP	C2A-N1A-C6A	2.98	123.63	118.73
2	B	401	NAP	C2A-N1A-C6A	2.90	123.50	118.73
2	D	401	NAP	C4D-O4D-C1D	2.80	112.49	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NAP	O2N-PN-O3	2.79	114.81	107.27
2	B	401	NAP	O3-PN-O1N	-2.78	102.34	110.70
2	D	401	NAP	O3-PA-O1A	-2.57	102.96	110.70
2	B	401	NAP	C6N-N1N-C2N	-2.53	119.72	121.88
2	A	401	NAP	C6A-C5A-N7A	2.47	136.85	132.09
2	B	401	NAP	C2N-C3N-C4N	2.45	121.11	118.26
2	A	401	NAP	C4A-N9A-C8A	2.45	108.31	105.74
2	C	401	NAP	O2A-PA-O3	2.44	113.86	107.27
2	C	401	NAP	C2B-C3B-C4B	2.40	107.15	101.99
2	C	401	NAP	C2A-N1A-C6A	2.39	122.65	118.73
2	A	401	NAP	O3X-P2B-O2X	2.35	116.62	107.80
2	B	401	NAP	N9A-C8A-N7A	-2.31	110.66	113.94
2	C	401	NAP	C5A-N7A-C8A	2.30	107.06	103.45
2	B	401	NAP	C6N-N1N-C1D	2.29	124.23	119.73
2	D	401	NAP	O2N-PN-O3	-2.28	101.12	107.27
2	D	401	NAP	C5N-C4N-C3N	-2.26	118.14	120.36
2	D	401	NAP	N3A-C2A-N1A	-2.25	125.18	128.58
2	D	401	NAP	C6A-C5A-N7A	2.23	136.38	132.09
2	A	401	NAP	N9A-C8A-N7A	-2.19	110.82	113.94
2	A	401	NAP	P2B-O2B-C2B	2.13	129.12	123.43
2	D	401	NAP	C2N-C3N-C4N	2.13	120.73	118.26
2	B	401	NAP	C4A-N9A-C8A	2.09	107.94	105.74

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAP	C5B-O5B-PA-O1A
2	A	401	NAP	O4D-C1D-N1N-C6N
2	B	401	NAP	PA-O3-PN-O5D
2	B	401	NAP	O4D-C1D-N1N-C6N
2	C	401	NAP	C5B-O5B-PA-O1A
2	C	401	NAP	PN-O3-PA-O5B
2	C	401	NAP	C5D-O5D-PN-O3
2	C	401	NAP	O4D-C1D-N1N-C2N
2	C	401	NAP	O4D-C1D-N1N-C6N
2	C	401	NAP	C2D-C1D-N1N-C2N
2	D	401	NAP	PA-O3-PN-O5D
2	D	401	NAP	C5D-O5D-PN-O1N
2	D	401	NAP	O4D-C1D-N1N-C2N
2	D	401	NAP	O4D-C1D-N1N-C6N
2	D	401	NAP	C2D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
2	D	401	NAP	C2D-C1D-N1N-C6N
2	A	401	NAP	C3B-C2B-O2B-P2B
2	C	401	NAP	C1B-C2B-O2B-P2B
2	B	401	NAP	C3B-C2B-O2B-P2B
2	C	401	NAP	C3B-C2B-O2B-P2B
2	D	401	NAP	C3B-C2B-O2B-P2B
2	B	401	NAP	C1B-C2B-O2B-P2B
2	D	401	NAP	C1B-C2B-O2B-P2B
2	A	401	NAP	PN-O3-PA-O5B
2	B	401	NAP	PN-O3-PA-O5B
2	A	401	NAP	C1B-C2B-O2B-P2B
2	A	401	NAP	C5B-O5B-PA-O2A
2	B	401	NAP	C5D-O5D-PN-O1N
2	C	401	NAP	C5B-O5B-PA-O2A
2	C	401	NAP	C5D-O5D-PN-O1N
2	D	401	NAP	C5D-O5D-PN-O3
2	A	401	NAP	C2D-C1D-N1N-C2N
2	C	401	NAP	C2D-C1D-N1N-C6N
2	A	401	NAP	O4D-C1D-N1N-C2N
2	B	401	NAP	O4D-C1D-N1N-C2N
2	C	401	NAP	C2B-O2B-P2B-O1X
2	D	401	NAP	C2B-O2B-P2B-O1X
2	D	401	NAP	C2B-O2B-P2B-O2X
2	B	401	NAP	C3D-C4D-C5D-O5D

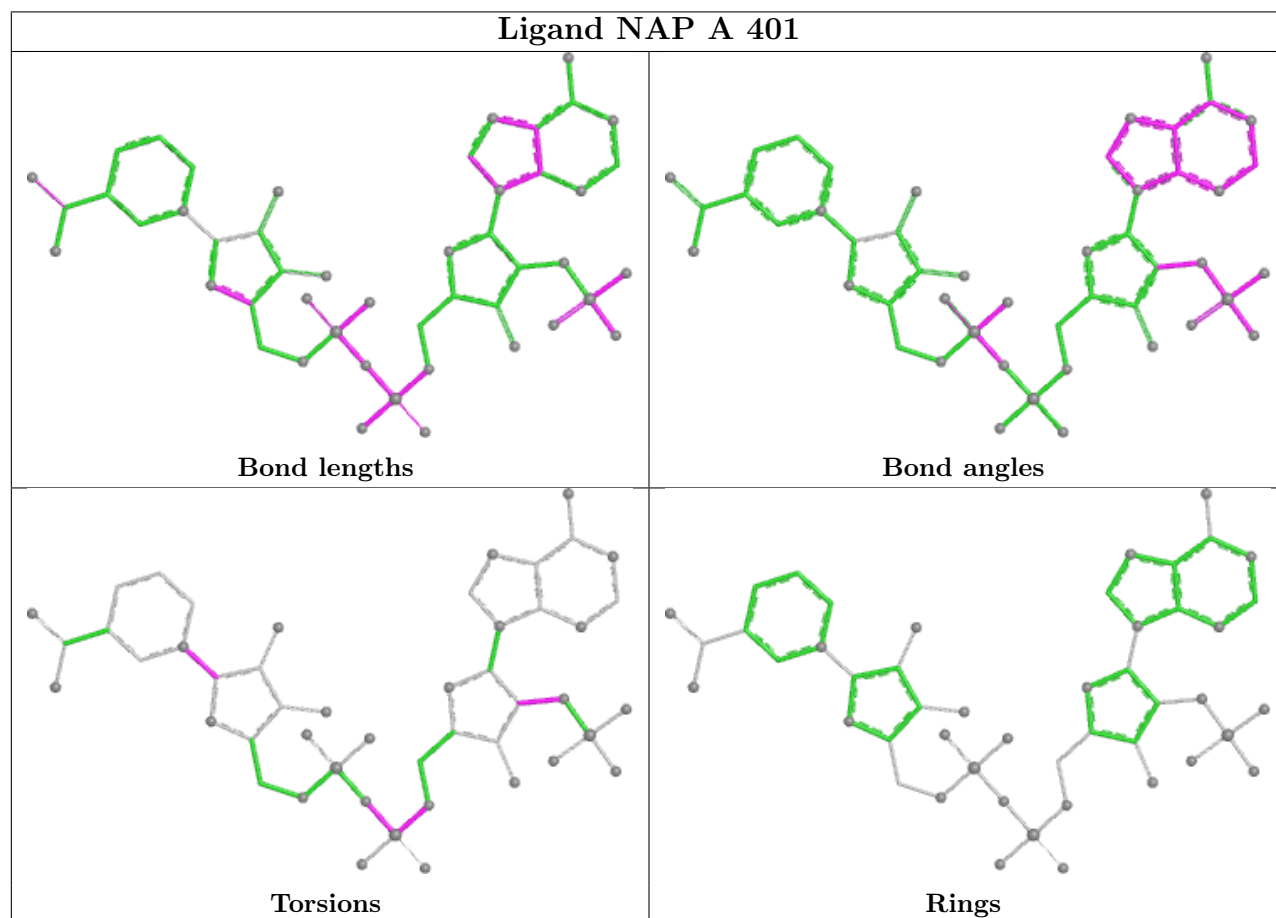
There are no ring outliers.

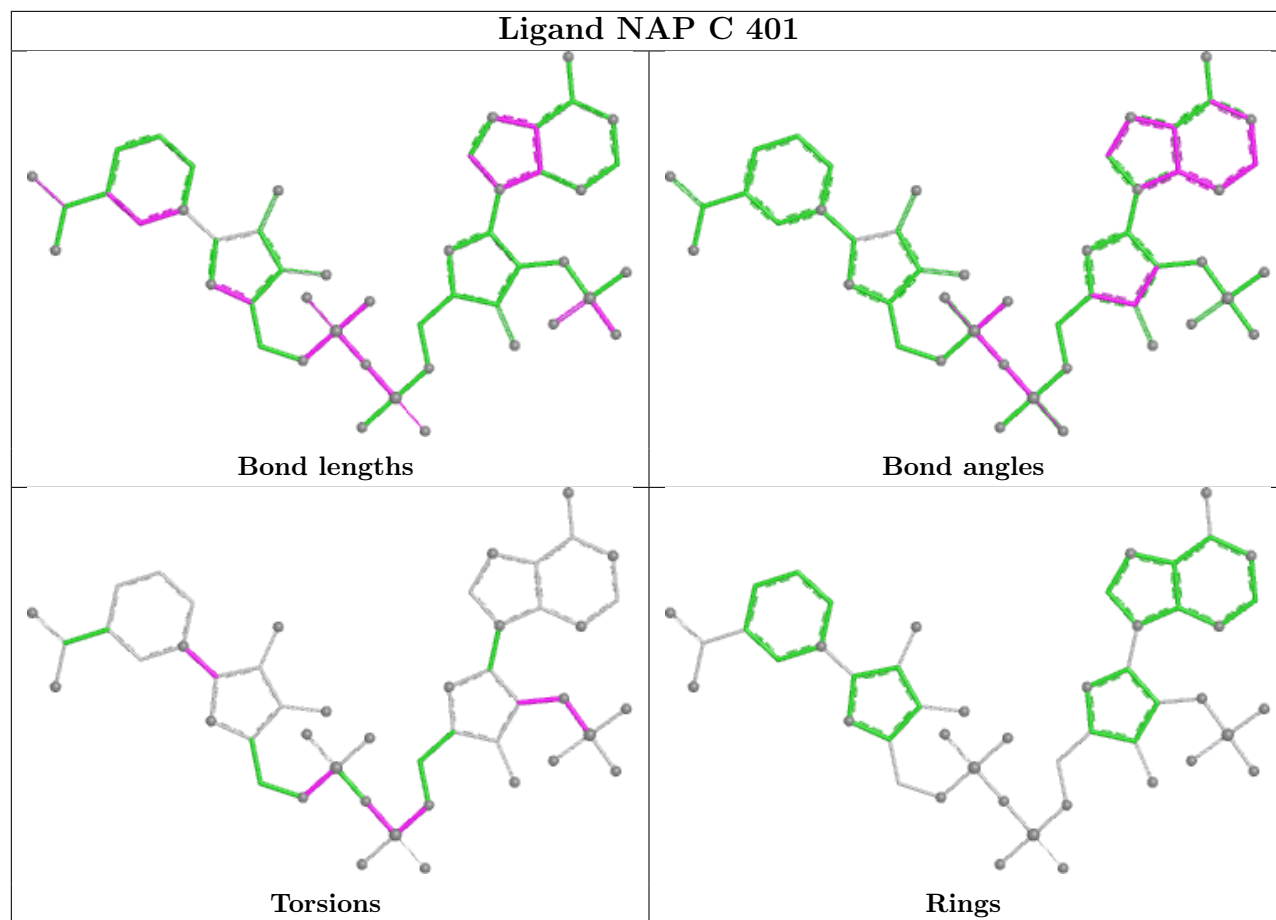
4 monomers are involved in 15 short contacts:

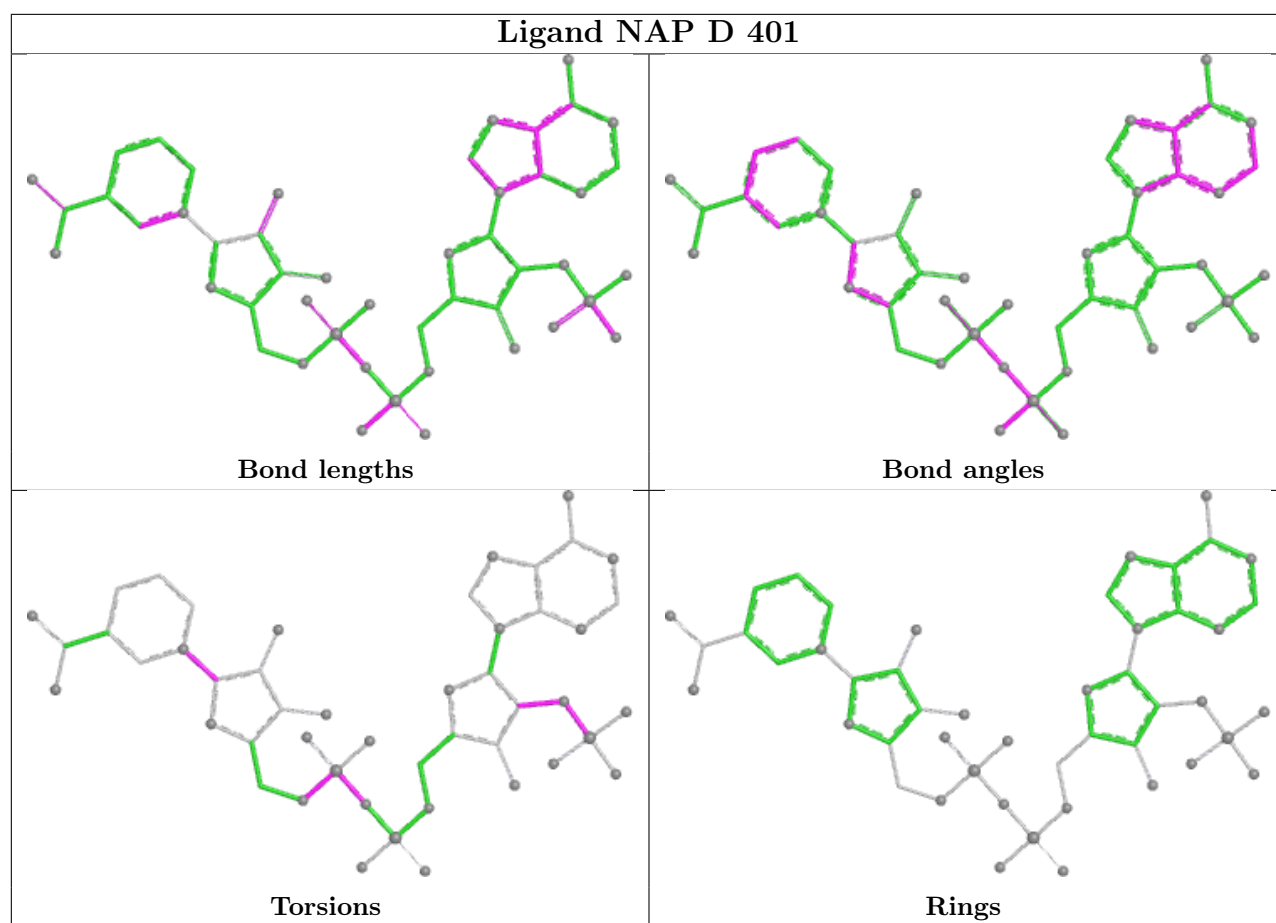
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NAP	3	0
2	C	401	NAP	4	0
2	D	401	NAP	4	0
2	B	401	NAP	4	0

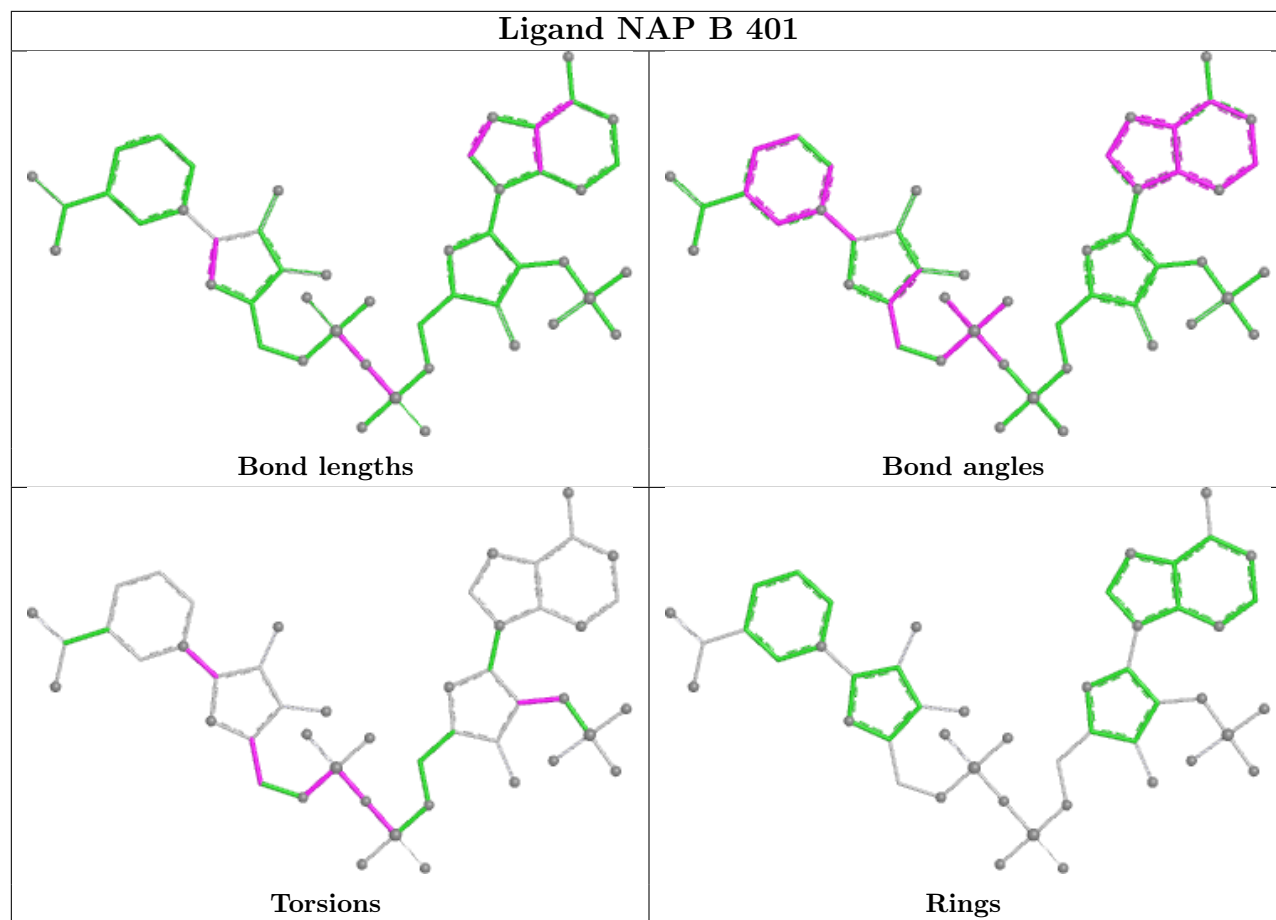
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	358/385 (92%)	-0.27	7 (1%) 65 67	13, 24, 49, 98	0
1	B	345/385 (89%)	-0.28	3 (0%) 81 82	12, 25, 48, 67	0
1	C	336/385 (87%)	-0.29	3 (0%) 81 82	14, 26, 44, 67	0
1	D	343/385 (89%)	-0.14	8 (2%) 61 63	13, 28, 52, 86	0
All	All	1382/1540 (89%)	-0.25	21 (1%) 72 73	12, 26, 49, 98	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	265	TYR	4.2
1	B	255	ALA	4.2
1	A	268	PRO	4.2
1	D	255	ALA	4.2
1	D	264	LEU	4.1
1	C	202	GLU	3.4
1	A	270	ILE	3.1
1	A	4	ALA	2.9
1	D	268	PRO	2.8
1	A	265	TYR	2.8
1	A	6	PRO	2.6
1	C	270	ILE	2.6
1	D	27	GLN	2.5
1	A	0	HIS	2.5
1	B	26	MET	2.5
1	C	29	PRO	2.3
1	D	270	ILE	2.3
1	D	269	GLU	2.2
1	B	7	LYS	2.1
1	D	335	ARG	2.1
1	A	262	HIS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

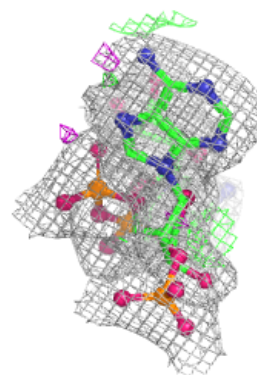
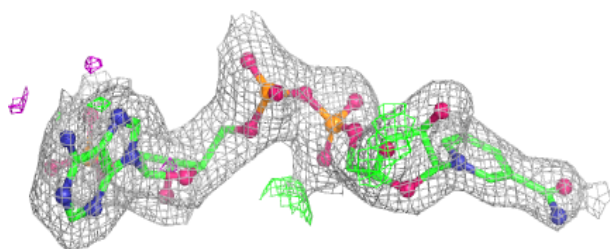
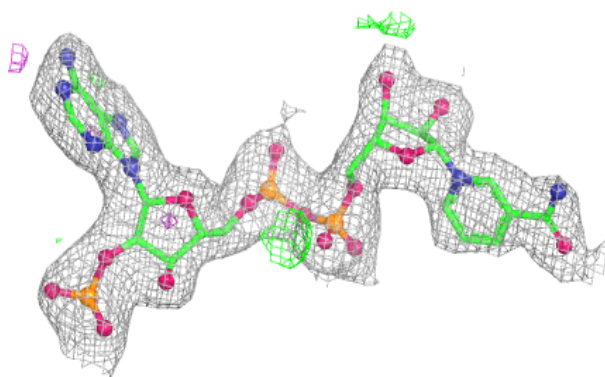
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAP	C	401	48/48	0.95	0.07	26,31,49,50	0
2	NAP	D	401	48/48	0.95	0.08	25,35,42,52	0
2	NAP	A	401	48/48	0.96	0.07	24,28,52,54	0
2	NAP	B	401	48/48	0.96	0.07	29,35,43,45	0

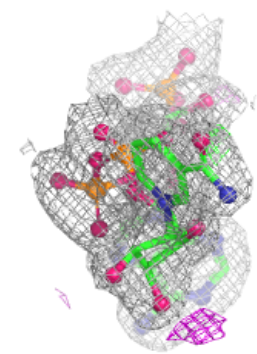
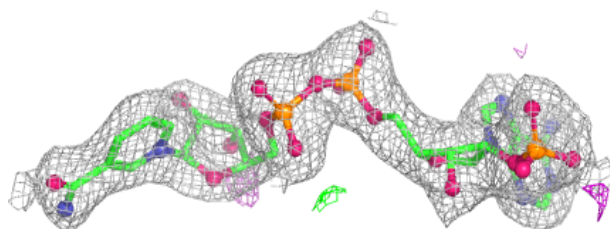
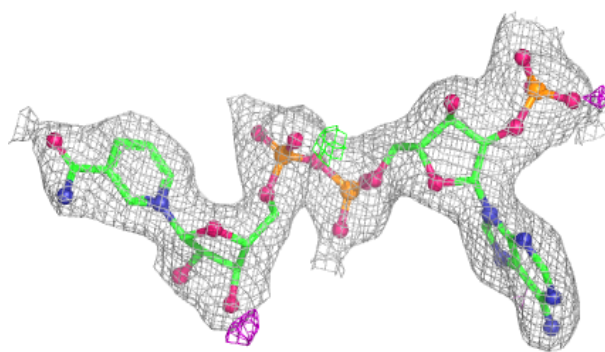
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP C 401:

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

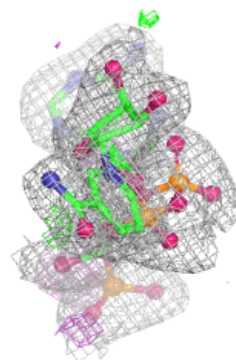
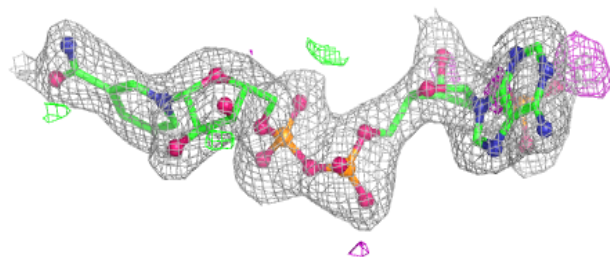
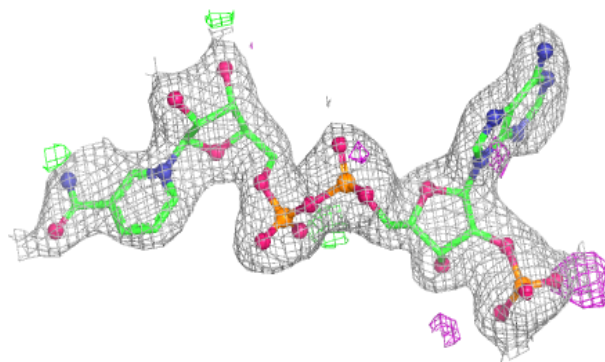
**Electron density around NAP D 401:**

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

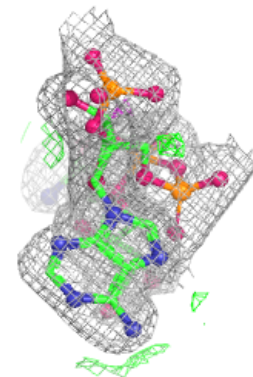
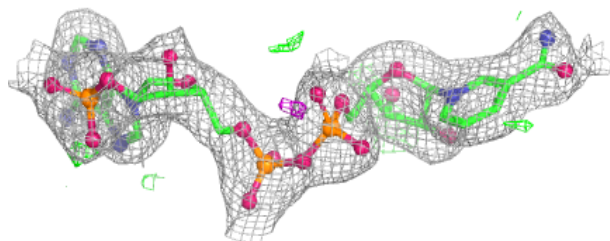
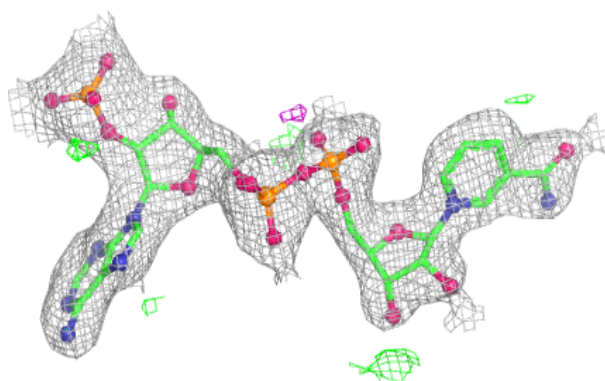


Electron density around NAP A 401:

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

**Electron density around NAP B 401:**

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



6.5 Other polymers

There are no such residues in this entry.