



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 06:23 AM UTC

PDB ID : 6AJC / pdb_00006ajc
Title : Crystal structure of Trypanosoma cruzi cytosolic isocitrate dehydrogenase in complex with NADP⁺, isocitrate and ca²⁺
Authors : Wang, X.; Inaoka, D.K.; Shiba, T.; Balogun, E.O.; Ziebart, N.; Allman, S.; Watanabe, Y.; Nozaki, T.; Boshart, M.; Bringaud, F.; Harada, S.; Kita, K.
Deposited on : 2018-08-27
Resolution : 2.40 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

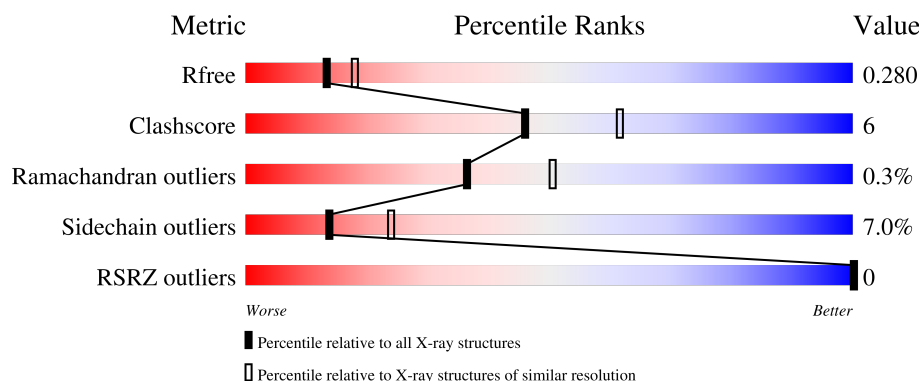
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	413	 81% 17% .
1	B	413	 80% 18% .
1	C	413	 83% 16% .
1	D	413	 80% 17% .

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Mol	Chain	Length	Quality of chain
1	E	413	 81% 17% .
1	F	413	 85% 13% .
1	G	413	 81% 18% .
1	H	413	 80% 17% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26905 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.

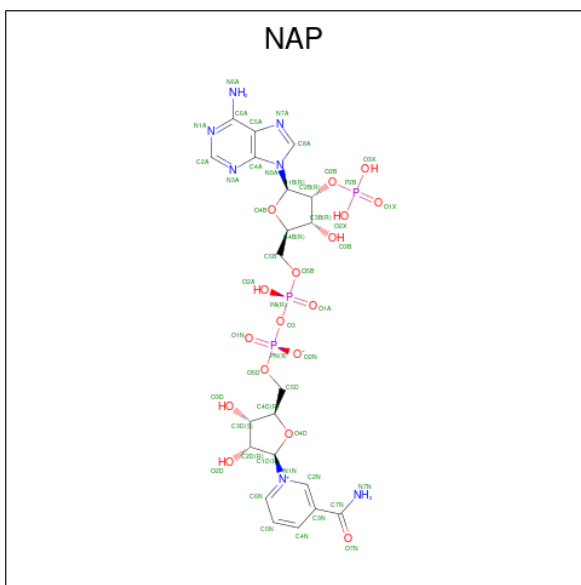
- Molecule 1 is a protein called Isocitrate dehydrogenase [NADP].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	0	0	0
			3289	2091	565	611	22			
1	B	412	Total	C	N	O	S	0	0	0
			3280	2085	563	610	22			
1	C	413	Total	C	N	O	S	0	0	0
			3289	2091	565	611	22			
1	D	413	Total	C	N	O	S	0	0	0
			3289	2091	565	611	22			
1	E	413	Total	C	N	O	S	0	0	0
			3289	2091	565	611	22			
1	F	413	Total	C	N	O	S	0	0	0
			3289	2091	565	611	22			
1	G	413	Total	C	N	O	S	0	0	0
			3289	2091	565	611	22			
1	H	411	Total	C	N	O	S	0	0	0
			3274	2083	562	607	22			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	MET	engineered mutation	UNP Q4E4L7
B	1	SER	MET	engineered mutation	UNP Q4E4L7
C	1	SER	MET	engineered mutation	UNP Q4E4L7
D	1	SER	MET	engineered mutation	UNP Q4E4L7
E	1	SER	MET	engineered mutation	UNP Q4E4L7
F	1	SER	MET	engineered mutation	UNP Q4E4L7
G	1	SER	MET	engineered mutation	UNP Q4E4L7
H	1	SER	MET	engineered mutation	UNP Q4E4L7

- 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
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
2	E	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	F	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	G	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	H	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

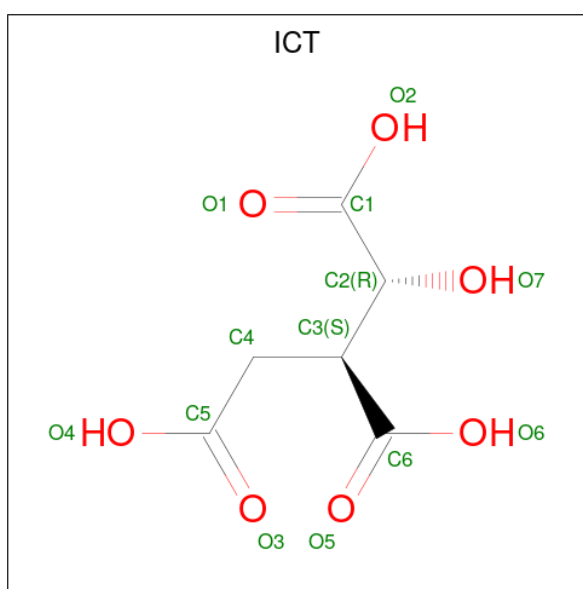
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0
3	D	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total	Ca	0	0
			1	1		
3	F	1	Total	Ca	0	0
			1	1		
3	G	1	Total	Ca	0	0
			1	1		
3	H	1	Total	Ca	0	0
			1	1		

- Molecule 4 is ISOCITRIC ACID (CCD ID: ICT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	6	7		
4	B	1	Total	C	O	0	0
			13	6	7		
4	C	1	Total	C	O	0	0
			13	6	7		
4	D	1	Total	C	O	0	0
			13	6	7		
4	E	1	Total	C	O	0	0
			13	6	7		
4	F	1	Total	C	O	0	0
			13	6	7		
4	G	1	Total	C	O	0	0
			13	6	7		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			13	6	7		

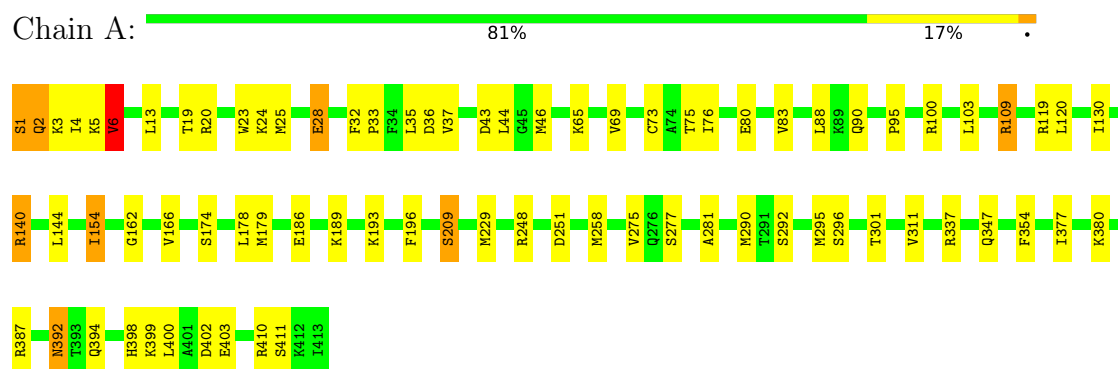
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	16	Total	O	0	0
			16	16		
5	B	24	Total	O	0	0
			24	24		
5	C	16	Total	O	0	0
			16	16		
5	D	14	Total	O	0	0
			14	14		
5	E	14	Total	O	0	0
			14	14		
5	F	15	Total	O	0	0
			15	15		
5	G	15	Total	O	0	0
			15	15		
5	H	7	Total	O	0	0
			7	7		

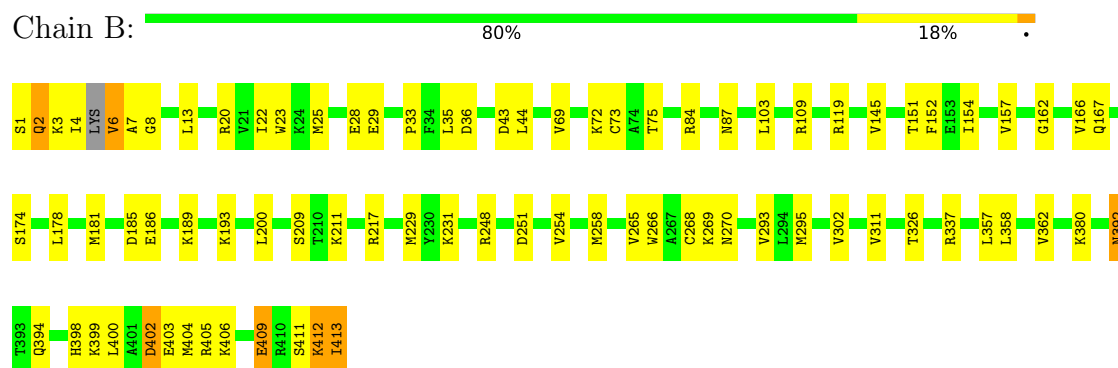
3 Residue-property plots

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.

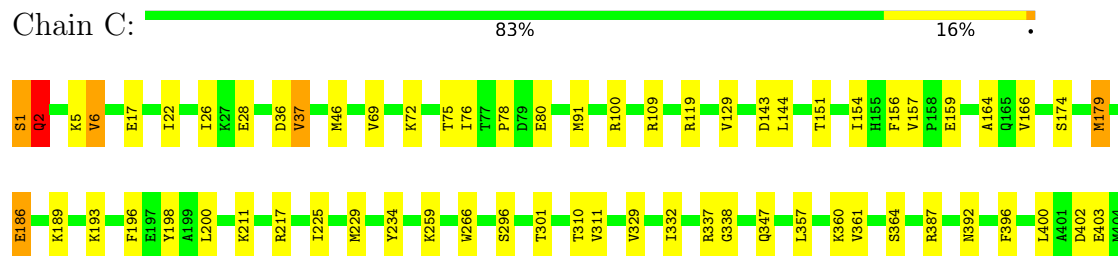
• Molecule 1: Isocitrate dehydrogenase [NADP]



• Molecule 1: Isocitrate dehydrogenase [NADP]



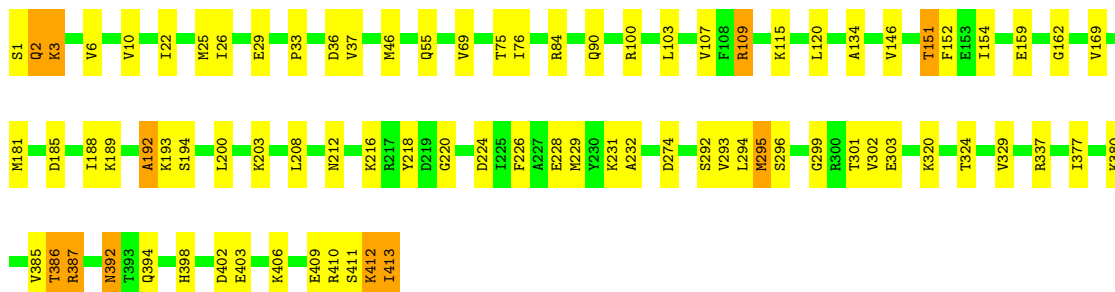
• Molecule 1: Isocitrate dehydrogenase [NADP]





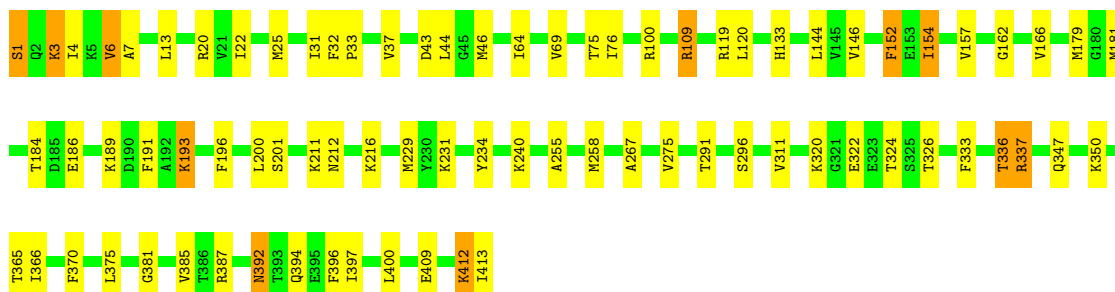
• Molecule 1: Isocitrate dehydrogenase [NADP]

Chain D:  80% 17%



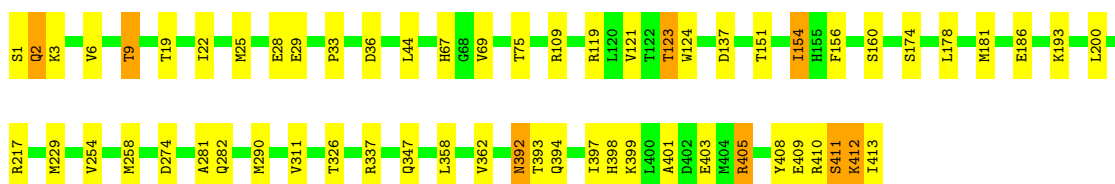
• Molecule 1: Isocitrate dehydrogenase [NADP]

Chain E:  81% 17%



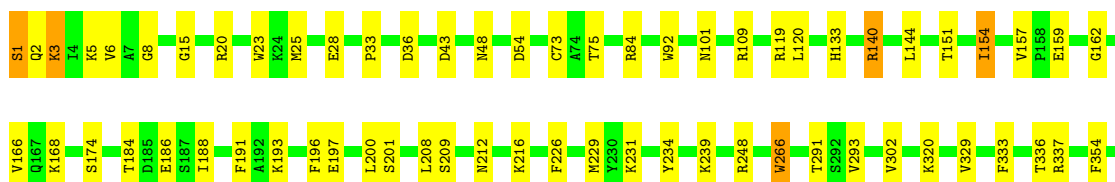
• Molecule 1: Isocitrate dehydrogenase [NADP]

Chain F:  85% 13%



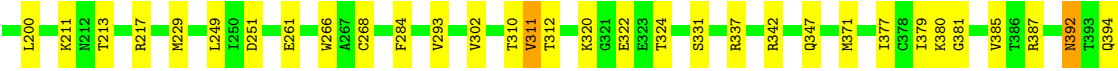
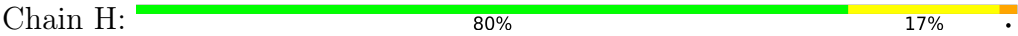
• Molecule 1: Isocitrate dehydrogenase [NADP]

Chain G:  81% 18%





● Molecule 1: Isocitrate dehydrogenase [NADP]



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	123.77Å 123.48Å 127.04Å 90.00° 105.96° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	76.9 (20.00-2.40) 77.0 (20.00-2.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.95 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.202 , 0.283 0.206 , 0.280	Depositor DCC
R_{free} test set	5493 reflections (3.84%)	wwPDB-VP
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 5.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.049 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	26905	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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: NAP, ICT, CA

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	0.94	2/3361 (0.1%)	1.04	2/4531 (0.0%)
1	B	0.94	3/3351 (0.1%)	1.06	8/4517 (0.2%)
1	C	0.90	4/3361 (0.1%)	1.03	4/4531 (0.1%)
1	D	0.91	2/3361 (0.1%)	1.05	6/4531 (0.1%)
1	E	0.98	5/3361 (0.1%)	1.08	8/4531 (0.2%)
1	F	0.85	0/3361	1.00	2/4531 (0.0%)
1	G	0.95	2/3361 (0.1%)	1.07	7/4531 (0.2%)
1	H	0.89	1/3346 (0.0%)	1.06	11/4511 (0.2%)
All	All	0.92	19/26863 (0.1%)	1.05	48/36214 (0.1%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	186	GLU	N-CA	-7.27	1.37	1.46
1	C	266	TRP	C-O	-6.35	1.16	1.24
1	H	15	GLY	C-O	-6.00	1.18	1.23
1	B	265	VAL	C-O	-5.93	1.17	1.24
1	C	403	GLU	C-O	-5.86	1.17	1.24
1	E	157	VAL	CA-C	-5.83	1.48	1.53
1	A	6	VAL	C-O	-5.63	1.18	1.24
1	B	157	VAL	CA-C	-5.62	1.48	1.53
1	A	400	LEU	C-O	-5.57	1.17	1.24
1	D	192	ALA	C-O	-5.54	1.17	1.24
1	E	184	THR	C-O	-5.36	1.17	1.23
1	E	267	ALA	C-O	-5.23	1.17	1.24
1	B	8	GLY	CA-C	-5.20	1.46	1.52
1	E	189	LYS	C-O	-5.18	1.18	1.24
1	G	166	VAL	C-O	-5.18	1.18	1.24
1	G	266	TRP	C-O	-5.17	1.17	1.23
1	D	188	ILE	C-O	-5.11	1.18	1.24
1	C	402	ASP	CA-C	-5.02	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	186	GLU	N-CA	-5.02	1.40	1.46

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	411	SER	N-CA-C	14.34	126.91	111.28
1	G	411	SER	N-CA-C	11.87	124.22	111.28
1	H	411	SER	N-CA-C	11.20	123.05	111.07
1	F	411	SER	N-CA-C	11.13	123.17	111.14
1	D	411	SER	N-CA-C	10.62	122.85	111.28
1	H	4	ILE	N-CA-C	9.80	122.14	109.30
1	G	162	GLY	N-CA-C	-8.97	101.06	112.54
1	G	166	VAL	N-CA-C	8.30	120.43	108.48
1	C	411	SER	N-CA-C	7.75	119.51	111.14
1	A	162	GLY	N-CA-C	-7.55	100.95	112.51
1	H	401	ALA	N-CA-C	7.52	119.11	111.07
1	C	186	GLU	N-CA-CB	-7.33	99.39	110.01
1	B	7	ALA	N-CA-C	7.00	118.70	111.14
1	B	412	LYS	N-CA-C	6.95	118.51	111.07
1	H	15	GLY	N-CA-C	6.90	122.76	112.41
1	D	403	GLU	N-CA-C	6.78	118.75	111.36
1	D	2	GLN	N-CA-C	6.73	118.37	108.14
1	E	31	ILE	CB-CA-C	-6.34	105.42	111.44
1	D	410	ARG	N-CA-C	6.31	118.24	111.36
1	E	412	LYS	N-CA-C	6.29	120.21	111.90
1	B	186	GLU	N-CA-CB	-6.24	100.97	110.01
1	B	166	VAL	N-CA-C	6.22	116.83	107.75
1	H	412	LYS	N-CA-C	6.16	120.87	112.68
1	H	17	GLU	N-CA-C	5.95	117.35	108.31
1	E	166	VAL	N-CA-C	5.93	116.41	108.11
1	H	406	LYS	N-CA-C	-5.78	104.89	111.07
1	H	7	ALA	N-CA-C	5.58	117.44	111.36
1	G	157	VAL	N-CA-C	5.56	113.65	108.15
1	H	69	VAL	N-CA-C	5.54	116.26	108.17
1	G	186	GLU	CB-CA-C	-5.53	102.19	110.88
1	E	7	ALA	CA-C-N	5.49	125.56	120.34
1	E	7	ALA	C-N-CA	5.49	125.56	120.34
1	E	157	VAL	CA-C-N	-5.45	115.12	120.52
1	E	157	VAL	C-N-CA	-5.45	115.12	120.52
1	C	2	GLN	N-CA-C	5.33	116.39	108.60
1	F	137	ASP	CB-CA-C	-5.32	108.89	116.34
1	D	232	ALA	N-CA-C	5.32	117.16	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	407	ALA	N-CA-C	5.29	117.13	111.36
1	C	72	LYS	N-CA-C	5.27	117.00	108.41
1	B	72	LYS	N-CA-C	5.26	116.97	108.34
1	D	329	VAL	N-CA-C	5.25	116.02	110.72
1	E	162	GLY	N-CA-C	-5.25	104.48	112.51
1	H	403	GLU	N-CA-C	-5.21	105.60	111.28
1	B	402	ASP	CA-C-N	5.08	127.08	120.28
1	B	402	ASP	C-N-CA	5.08	127.08	120.28
1	B	380	LYS	N-CA-C	-5.05	103.38	110.35
1	G	395	GLU	N-CA-C	-5.04	105.86	111.36
1	G	8	GLY	N-CA-C	-5.03	106.80	112.33

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3289	0	3264	42	0
1	B	3280	0	3250	44	0
1	C	3289	0	3264	44	0
1	D	3289	0	3264	39	0
1	E	3289	0	3264	43	0
1	F	3289	0	3264	35	0
1	G	3289	0	3264	38	0
1	H	3274	0	3248	51	0
2	A	48	0	25	1	0
2	B	48	0	25	1	0
2	C	48	0	25	1	0
2	D	48	0	25	2	0
2	E	48	0	25	1	0
2	F	48	0	25	1	0
2	G	48	0	25	1	0
2	H	48	0	25	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	13	0	5	3	0
4	B	13	0	5	1	0
4	C	13	0	5	1	0
4	D	13	0	5	1	0
4	E	13	0	5	1	0
4	F	13	0	5	0	0
4	G	13	0	5	0	0
4	H	13	0	5	0	0
5	A	16	0	0	0	0
5	B	24	0	0	0	0
5	C	16	0	0	0	0
5	D	14	0	0	1	0
5	E	14	0	0	0	0
5	F	15	0	0	0	0
5	G	15	0	0	0	0
5	H	7	0	0	1	0
All	All	26905	0	26322	310	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 6.

All (310) 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:1:SER:HB3	1:B:33:PRO:HA	1.32	1.06
1:B:2:GLN:NE2	1:B:36:ASP:OD1	1.88	1.06
1:H:402:ASP:HA	1:H:405:ARG:HG2	1.12	1.06
1:H:402:ASP:CA	1:H:405:ARG:HG2	1.92	1.00
1:F:9:THR:HG23	1:F:67:HIS:ND1	1.77	1.00
1:H:402:ASP:HA	1:H:405:ARG:CG	1.98	0.94
1:H:402:ASP:HB3	1:H:405:ARG:HH11	1.32	0.93
1:F:408:TYR:O	1:F:411:SER:OG	1.85	0.93
4:A:503:ICT:O7	1:B:211:LYS:NZ	2.11	0.84
1:H:402:ASP:HB3	1:H:405:ARG:NH1	1.93	0.82
1:F:2:GLN:HB2	1:F:36:ASP:HB2	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:LYS:HA	1:A:229:MET:HE1	1.64	0.80
1:D:412:LYS:C	1:D:413:ILE:HG13	2.05	0.79
1:H:402:ASP:O	1:H:406:LYS:HG2	1.81	0.79
1:F:9:THR:CG2	1:F:67:HIS:ND1	2.46	0.77
1:F:9:THR:HG21	1:F:67:HIS:CE1	2.21	0.76
1:G:193:LYS:HA	1:G:229:MET:HE1	1.69	0.75
1:A:178:LEU:HD13	1:B:154:ILE:HD11	1.69	0.72
1:B:193:LYS:HA	1:B:229:MET:HE1	1.70	0.72
1:E:258:MET:HE1	1:F:258:MET:HE1	1.70	0.72
1:A:1:SER:O	1:A:32:PHE:O	2.07	0.72
1:A:1:SER:HB2	1:A:33:PRO:HA	1.72	0.71
1:D:1:SER:HB2	1:D:33:PRO:HA	1.74	0.70
1:F:392:ASN:C	1:F:392:ASN:HD22	2.00	0.70
1:B:2:GLN:HB2	1:B:36:ASP:HB2	1.73	0.70
1:F:9:THR:CG2	1:F:67:HIS:CE1	2.75	0.69
1:B:1:SER:CB	1:B:33:PRO:HA	2.19	0.69
1:D:46:MET:HE2	1:D:76:ILE:HB	1.74	0.69
1:A:392:ASN:C	1:A:392:ASN:HD22	2.01	0.68
1:C:193:LYS:HA	1:C:229:MET:HE1	1.77	0.67
1:B:392:ASN:C	1:B:392:ASN:HD22	2.02	0.67
1:B:412:LYS:C	1:B:413:ILE:HG13	2.19	0.67
1:A:2:GLN:HB3	1:A:36:ASP:HB2	1.76	0.67
1:H:402:ASP:CB	1:H:405:ARG:HH11	2.07	0.66
1:D:296:SER:OG	1:D:301:THR:HB	1.95	0.66
1:E:154:ILE:CD1	1:F:178:LEU:HD13	2.26	0.66
1:D:25:MET:HE1	1:D:394:GLN:HA	1.77	0.65
1:B:2:GLN:HE21	1:B:36:ASP:CG	2.02	0.65
1:F:1:SER:O	1:F:2:GLN:HB3	1.97	0.65
1:C:1:SER:O	1:C:2:GLN:HG3	1.96	0.65
1:H:402:ASP:C	1:H:405:ARG:HG2	2.22	0.65
1:H:412:LYS:O	1:H:413:ILE:HB	1.95	0.64
1:E:154:ILE:HD11	1:F:178:LEU:HD13	1.78	0.64
1:H:266:TRP:CD1	1:H:268:CYS:HG	2.17	0.63
1:D:392:ASN:C	1:D:392:ASN:HD22	2.07	0.62
1:C:412:LYS:C	1:C:413:ILE:HG12	2.25	0.62
1:D:29:GLU:OE2	1:D:398:HIS:CD2	2.53	0.62
1:D:29:GLU:OE2	1:D:398:HIS:HD2	1.82	0.61
1:B:25:MET:HE1	1:B:394:GLN:HA	1.84	0.60
1:H:394:GLN:O	1:H:398:HIS:CD2	2.53	0.60
1:D:100:ARG:NH1	4:D:503:ICT:O5	2.32	0.60
1:C:2:GLN:HG2	1:C:36:ASP:OD1	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:179:MET:SD	1:F:181:MET:HE2	2.41	0.60
1:G:2:GLN:HB2	1:G:36:ASP:HB2	1.82	0.60
1:F:393:THR:O	1:F:397:ILE:HD12	2.02	0.60
1:G:25:MET:HE1	1:G:394:GLN:HA	1.84	0.60
1:G:409:GLU:O	1:G:413:ILE:HG12	2.02	0.59
1:B:193:LYS:CA	1:B:229:MET:HE1	2.32	0.59
1:A:20:ARG:NH2	1:A:43:ASP:OD1	2.29	0.58
1:D:324:THR:O	1:D:392:ASN:HB2	2.03	0.58
1:E:229:MET:HE3	1:E:234:TYR:CE2	2.39	0.58
1:G:291:THR:HG21	1:G:337:ARG:NH1	2.18	0.58
1:H:107:VAL:HG23	1:H:134:ALA:HB2	1.84	0.58
1:A:2:GLN:HB3	1:A:36:ASP:CB	2.34	0.58
1:E:120:LEU:HD22	1:F:123:THR:HG23	1.86	0.58
1:A:25:MET:HE1	1:A:394:GLN:HA	1.86	0.57
1:E:381:GLY:O	1:E:385:VAL:HG23	2.04	0.57
1:C:329:VAL:HA	1:C:332:ILE:HD12	1.87	0.57
1:G:354:PHE:CE1	1:G:404:MET:HE2	2.39	0.57
1:E:75:THR:O	2:E:501:NAP:H2N	2.05	0.57
1:A:100:ARG:NH1	4:A:503:ICT:O5	2.38	0.56
1:B:145:VAL:H	1:H:87:ASN:HD21	1.51	0.56
1:E:109:ARG:HA	1:E:291:THR:O	2.06	0.56
1:C:396:PHE:CE2	1:C:400:LEU:HD11	2.40	0.56
1:E:193:LYS:HA	1:E:229:MET:HE1	1.88	0.56
1:D:402:ASP:O	1:D:406:LYS:HG3	2.06	0.56
1:E:1:SER:HB2	1:E:33:PRO:HA	1.87	0.56
1:B:6:VAL:HG13	1:B:36:ASP:O	2.06	0.55
1:H:377:ILE:O	1:H:380:LYS:O	2.23	0.55
1:H:15:GLY:N	1:H:73:CYS:HB3	2.22	0.55
1:H:213:THR:HG23	1:H:249:LEU:HD21	1.88	0.55
1:G:293:VAL:HG13	1:G:302:VAL:HG13	1.89	0.55
1:F:22:ILE:HD11	1:F:326:THR:HB	1.88	0.55
1:C:2:GLN:CB	1:C:36:ASP:HB2	2.38	0.54
1:F:29:GLU:OE2	1:F:398:HIS:HD2	1.90	0.54
1:F:401:ALA:O	1:F:405:ARG:HB2	2.08	0.54
1:F:193:LYS:N	1:F:229:MET:HE1	2.23	0.53
1:C:143:ASP:O	1:C:144:LEU:HD23	2.08	0.53
1:B:22:ILE:HD11	1:B:326:THR:HB	1.89	0.53
1:A:83:VAL:HA	1:A:88:LEU:HD12	1.90	0.53
1:A:5:LYS:HA	1:A:36:ASP:HB3	1.91	0.53
1:A:209:SER:HA	1:A:248:ARG:O	2.09	0.52
1:E:25:MET:HE1	1:E:394:GLN:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1:SER:HB2	1:G:33:PRO:HA	1.91	0.52
1:A:179:MET:SD	1:B:181:MET:HE2	2.50	0.52
1:A:4:ILE:HB	1:A:35:LEU:HD23	1.91	0.52
1:E:396:PHE:CE2	1:E:400:LEU:HD11	2.45	0.52
1:D:109:ARG:HD3	1:D:292:SER:OG	2.10	0.52
1:E:196:PHE:CD2	1:E:229:MET:HE2	2.45	0.52
1:A:296:SER:OG	1:A:301:THR:HB	2.10	0.52
1:D:75:THR:O	2:D:501:NAP:H2N	2.11	0.52
1:E:6:VAL:HG22	1:E:37:VAL:HA	1.92	0.51
1:E:13:LEU:HD23	1:E:44:LEU:HD11	1.92	0.51
1:C:196:PHE:CD2	1:C:229:MET:HE2	2.45	0.51
1:E:324:THR:O	1:E:392:ASN:HB2	2.11	0.51
1:H:40:GLU:OE2	1:H:67:HIS:NE2	2.43	0.51
1:H:211:LYS:NZ	1:H:251:ASP:OD1	2.42	0.51
1:A:258:MET:HE1	1:B:258:MET:HE1	1.93	0.51
1:E:333:PHE:HA	1:E:336:THR:OG1	2.10	0.51
1:A:75:THR:O	2:A:501:NAP:H2N	2.09	0.51
1:B:266:TRP:CD1	1:B:268:CYS:HG	2.29	0.51
1:B:399:LYS:O	1:B:403:GLU:HB2	2.10	0.51
1:F:1:SER:HB3	1:F:33:PRO:HA	1.92	0.51
1:A:6:VAL:HG22	1:A:37:VAL:HA	1.93	0.51
1:B:269:LYS:O	1:B:270:ASN:C	2.54	0.51
1:D:412:LYS:O	1:D:413:ILE:HG13	2.10	0.51
1:H:75:THR:OG1	1:H:95:PRO:HG2	2.10	0.51
1:D:294:LEU:HB3	1:D:303:GLU:HB3	1.93	0.50
1:E:22:ILE:HD11	1:E:326:THR:HB	1.93	0.50
1:C:1:SER:C	1:C:2:GLN:CG	2.84	0.50
1:D:107:VAL:HG23	1:D:134:ALA:HB2	1.93	0.50
1:F:75:THR:O	2:F:501:NAP:H2N	2.11	0.50
1:H:46:MET:HE2	1:H:76:ILE:HB	1.92	0.50
1:A:377:ILE:O	1:A:380:LYS:O	2.28	0.50
1:C:2:GLN:NE2	1:C:2:GLN:N	2.60	0.50
1:G:208:LEU:HD22	1:G:226:PHE:CD1	2.47	0.50
1:A:196:PHE:CD2	1:A:229:MET:HE2	2.47	0.50
1:E:412:LYS:O	1:E:413:ILE:C	2.54	0.50
1:H:392:ASN:HD22	1:H:392:ASN:C	2.19	0.50
1:A:275:VAL:HG13	1:B:254:VAL:HG11	1.93	0.50
1:E:212:ASN:O	1:E:216:LYS:HA	2.12	0.49
1:H:10:VAL:HA	1:H:69:VAL:HG13	1.94	0.49
1:E:25:MET:HE1	1:E:394:GLN:HG3	1.94	0.49
1:H:394:GLN:C	1:H:398:HIS:CD2	2.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:133:HIS:CD2	1:G:191:PHE:HB2	2.48	0.49
1:E:13:LEU:HD11	1:E:64:ILE:HD11	1.95	0.49
1:F:412:LYS:O	1:F:413:ILE:HB	2.12	0.49
1:G:266:TRP:C	1:G:266:TRP:CD1	2.90	0.49
1:H:178:LEU:HD12	1:H:178:LEU:C	2.37	0.49
1:C:129:VAL:HG11	1:C:198:TYR:CE2	2.48	0.48
1:D:2:GLN:HB2	1:D:36:ASP:HB2	1.94	0.48
1:D:10:VAL:HA	1:D:69:VAL:HG13	1.94	0.48
1:H:402:ASP:O	1:H:405:ARG:CG	2.60	0.48
1:B:293:VAL:HG13	1:B:302:VAL:HG13	1.95	0.48
1:C:17:GLU:HB2	1:C:310:THR:HB	1.95	0.48
1:H:111:PRO:HG3	1:H:284:PHE:CD2	2.49	0.48
1:H:402:ASP:O	1:H:405:ARG:HG2	2.14	0.48
1:C:196:PHE:HD2	1:C:229:MET:HE2	1.79	0.48
1:H:75:THR:O	2:H:501:NAP:H2N	2.14	0.47
1:H:380:LYS:HB2	1:H:385:VAL:HG22	1.96	0.47
1:G:377:ILE:O	1:G:380:LYS:O	2.32	0.47
1:C:6:VAL:HG22	1:C:37:VAL:HA	1.96	0.47
1:G:184:THR:O	1:G:188:ILE:HG13	2.14	0.47
1:G:382:MET:HE1	1:H:261:GLU:HG2	1.97	0.47
1:B:29:GLU:OE2	1:B:398:HIS:ND1	2.45	0.47
1:C:406:LYS:O	1:C:410:ARG:HB2	2.15	0.47
1:A:281:ALA:HB2	1:A:290:MET:SD	2.55	0.46
1:B:412:LYS:H	1:B:412:LYS:HG2	1.54	0.46
1:G:54:ASP:HB2	1:G:92:TRP:CE3	2.50	0.46
1:C:157:VAL:HB	1:D:151:THR:HG23	1.96	0.46
1:F:358:LEU:O	1:F:362:VAL:HG23	2.16	0.46
1:H:266:TRP:CD1	1:H:266:TRP:C	2.93	0.46
1:B:20:ARG:NH2	1:B:43:ASP:OD1	2.47	0.46
1:H:3:LYS:HB3	1:H:408:TYR:OH	2.15	0.46
1:A:154:ILE:CD1	1:B:178:LEU:HD13	2.46	0.46
1:H:3:LYS:HG3	1:H:408:TYR:HE2	1.81	0.46
1:G:2:GLN:O	1:G:3:LYS:HB2	2.16	0.46
1:G:154:ILE:HD12	1:H:178:LEU:HD13	1.97	0.46
1:G:229:MET:HE3	1:G:234:TYR:HE2	1.80	0.46
1:H:25:MET:HE1	1:H:394:GLN:HA	1.97	0.46
1:H:396:PHE:CE2	1:H:400:LEU:HD11	2.50	0.46
1:G:5:LYS:HD2	1:G:6:VAL:N	2.30	0.46
1:C:46:MET:HE2	1:C:76:ILE:CG2	2.46	0.46
1:F:25:MET:HE1	1:F:394:GLN:HG3	1.98	0.46
1:H:381:GLY:O	1:H:385:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:LYS:O	1:B:413:ILE:HG13	2.16	0.46
1:E:211:LYS:NZ	1:F:274:ASP:OD1	2.49	0.46
1:G:43:ASP:HB3	1:G:48:ASN:HD22	1.80	0.46
1:A:46:MET:HE2	1:A:76:ILE:CG2	2.46	0.45
1:B:211:LYS:NZ	1:B:251:ASP:OD1	2.44	0.45
1:C:69:VAL:HG21	1:C:338:GLY:O	2.16	0.45
1:D:192:ALA:HA	1:D:226:PHE:CZ	2.51	0.45
1:F:399:LYS:O	1:F:403:GLU:HG2	2.16	0.45
1:H:413:ILE:HD13	1:H:413:ILE:HA	1.73	0.45
4:A:503:ICT:C2	1:B:211:LYS:HZ1	2.22	0.45
1:A:178:LEU:CD1	1:B:154:ILE:HD11	2.40	0.45
1:B:358:LEU:O	1:B:362:VAL:HG23	2.17	0.45
1:G:2:GLN:O	1:G:3:LYS:CB	2.64	0.45
1:G:15:GLY:HA2	1:G:75:THR:HG22	1.96	0.45
1:B:362:VAL:HA	1:B:400:LEU:HD22	1.98	0.45
1:D:295:MET:HE2	1:D:299:GLY:HA2	1.98	0.45
1:E:13:LEU:HD23	1:E:44:LEU:CD1	2.47	0.45
1:G:387:ARG:NE	1:G:387:ARG:O	2.50	0.45
1:H:293:VAL:HG13	1:H:302:VAL:HG13	1.98	0.45
1:B:405:ARG:O	1:B:409:GLU:HB2	2.17	0.45
1:C:1:SER:C	1:C:2:GLN:CD	2.85	0.45
1:E:366:ILE:HA	1:E:370:PHE:O	2.17	0.45
1:G:154:ILE:HD12	1:H:152:PHE:CE2	2.52	0.45
1:D:193:LYS:HA	1:D:229:MET:HE1	1.98	0.45
1:A:154:ILE:HD12	1:B:152:PHE:CE2	2.51	0.44
1:A:399:LYS:O	1:A:403:GLU:HG2	2.17	0.44
2:B:501:NAP:C4N	4:B:503:ICT:H41	2.47	0.44
1:C:2:GLN:HB2	1:C:36:ASP:HB2	1.98	0.44
1:E:365:THR:HG22	1:E:370:PHE:HB2	1.99	0.44
1:A:130:ILE:HD12	1:A:277:SER:HA	1.99	0.44
1:E:152:PHE:HE2	1:F:154:ILE:HG12	1.82	0.44
1:H:17:GLU:OE1	1:H:312:THR:OG1	2.31	0.44
1:C:179:MET:HE2	1:D:181:MET:HG2	1.99	0.44
1:F:178:LEU:C	1:F:178:LEU:HD12	2.42	0.44
1:F:281:ALA:HB2	1:F:290:MET:SD	2.58	0.44
1:C:22:ILE:HG22	1:C:26:ILE:HD11	1.99	0.44
1:C:229:MET:HE3	1:C:234:TYR:HE2	1.81	0.44
1:G:23:TRP:CD2	1:G:73:CYS:HB2	2.52	0.44
1:B:13:LEU:HD23	1:B:44:LEU:HD11	2.00	0.44
1:C:405:ARG:HG2	1:C:405:ARG:HH11	1.82	0.44
1:D:216:LYS:O	1:D:220:GLY:HA3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:MET:HE2	1:E:76:ILE:CG2	2.48	0.44
1:A:80:GLU:OE1	1:A:80:GLU:N	2.50	0.44
1:C:409:GLU:O	1:C:413:ILE:HD13	2.18	0.44
1:D:377:ILE:O	1:D:380:LYS:O	2.35	0.44
1:G:212:ASN:O	1:G:216:LYS:HA	2.17	0.44
1:E:229:MET:HE3	1:E:234:TYR:HE2	1.82	0.44
1:E:154:ILE:HD11	1:F:178:LEU:CD1	2.45	0.44
1:G:329:VAL:HG13	1:G:362:VAL:HG11	1.99	0.44
1:A:399:LYS:NZ	1:A:403:GLU:OE1	2.26	0.43
1:D:185:ASP:O	1:D:189:LYS:HG3	2.18	0.43
1:A:75:THR:OG1	1:A:95:PRO:HG2	2.19	0.43
1:B:2:GLN:CB	1:B:36:ASP:HB2	2.45	0.43
1:C:193:LYS:CA	1:C:229:MET:HE1	2.47	0.43
1:H:310:THR:C	1:H:311:VAL:HG23	2.43	0.43
1:B:209:SER:HA	1:B:248:ARG:O	2.18	0.43
1:C:164:ALA:O	1:C:166:VAL:HG23	2.19	0.43
1:D:293:VAL:HG13	1:D:302:VAL:HG13	2.01	0.43
1:E:255:ALA:O	1:F:282:GLN:HG2	2.19	0.43
1:H:69:VAL:HG11	1:H:342:ARG:HD2	2.01	0.43
1:H:193:LYS:N	1:H:229:MET:HE1	2.34	0.43
1:A:140:ARG:HA	1:A:140:ARG:HD3	1.76	0.43
1:C:357:LEU:O	1:C:361:VAL:HG23	2.18	0.43
1:H:406:LYS:HB3	1:H:406:LYS:HE3	1.64	0.43
1:D:208:LEU:HD22	1:D:226:PHE:CG	2.53	0.43
1:G:2:GLN:CB	1:G:36:ASP:HB2	2.49	0.43
1:H:15:GLY:HA3	1:H:73:CYS:SG	2.59	0.43
1:E:397:ILE:HA	1:E:400:LEU:HD12	2.00	0.43
1:F:9:THR:HG23	1:F:67:HIS:CG	2.51	0.43
1:E:32:PHE:N	1:E:33:PRO:CD	2.82	0.42
1:D:412:LYS:C	1:D:413:ILE:CG1	2.84	0.42
1:C:211:LYS:NZ	1:D:274:ASP:OD1	2.47	0.42
1:C:156:PHE:CZ	1:D:146:VAL:HG13	2.54	0.42
1:G:209:SER:HA	1:G:248:ARG:O	2.19	0.42
1:A:24:LYS:O	1:A:28:GLU:HB2	2.19	0.42
1:C:2:GLN:HB3	1:C:36:ASP:HB2	2.01	0.42
1:H:119:ARG:HD2	5:H:601:HOH:O	2.20	0.42
1:C:189:LYS:HG2	1:C:225:ILE:HG23	2.02	0.42
1:E:366:ILE:HD13	1:E:375:LEU:CD1	2.50	0.42
1:H:371:MET:SD	1:H:379:ILE:HD12	2.59	0.42
1:B:185:ASP:O	1:B:189:LYS:HB2	2.20	0.42
1:C:2:GLN:N	1:C:2:GLN:CD	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:291:THR:HG21	1:E:337:ARG:NH1	2.35	0.42
1:G:75:THR:O	2:G:501:NAP:H2N	2.19	0.42
1:A:275:VAL:CG1	1:B:254:VAL:HG11	2.49	0.42
1:B:154:ILE:CG2	1:B:167:GLN:HB2	2.50	0.42
1:C:46:MET:HE1	1:C:78:PRO:CD	2.50	0.42
1:C:143:ASP:HB2	1:D:218:TYR:HB2	2.02	0.42
1:D:224:ASP:O	1:D:228:GLU:HB2	2.20	0.42
1:C:46:MET:HE1	1:C:78:PRO:CG	2.50	0.42
1:D:152:PHE:CE1	1:D:169:VAL:HG11	2.55	0.42
1:A:23:TRP:CD2	1:A:73:CYS:HB2	2.54	0.41
1:A:109:ARG:HD3	1:A:292:SER:OG	2.20	0.41
1:E:392:ASN:C	1:E:392:ASN:HD22	2.28	0.41
1:G:333:PHE:HA	1:G:336:THR:OG1	2.20	0.41
1:A:154:ILE:O	1:A:166:VAL:HA	2.19	0.41
1:H:402:ASP:HA	1:H:405:ARG:CD	2.49	0.41
1:C:217:ARG:HG2	5:D:613:HOH:O	2.20	0.41
1:E:133:HIS:CD2	1:E:191:PHE:HB2	2.54	0.41
1:B:4:ILE:HB	1:B:35:LEU:HD23	2.03	0.41
1:H:324:THR:O	1:H:392:ASN:HB2	2.20	0.41
1:C:75:THR:O	2:C:501:NAP:H2N	2.21	0.41
1:C:100:ARG:NH1	4:C:503:ICT:O6	2.41	0.41
1:C:296:SER:HB2	1:C:301:THR:HB	2.02	0.41
1:D:377:ILE:HG12	1:D:385:VAL:HG21	2.03	0.41
1:G:20:ARG:NH2	1:G:43:ASP:OD1	2.42	0.41
2:H:501:NAP:O1X	2:H:501:NAP:O3B	2.23	0.41
1:A:1:SER:CB	1:A:33:PRO:HA	2.47	0.41
1:C:80:GLU:OE1	1:C:80:GLU:N	2.52	0.41
1:D:212:ASN:O	1:D:216:LYS:HA	2.20	0.41
1:E:275:VAL:CG1	1:F:254:VAL:HG11	2.51	0.41
1:D:386:THR:O	1:D:387:ARG:C	2.64	0.41
1:F:399:LYS:NZ	1:F:403:GLU:OE1	2.47	0.41
1:G:101:ASN:ND2	1:G:140:ARG:HG3	2.36	0.41
1:G:396:PHE:CE2	1:G:400:LEU:HD11	2.56	0.41
1:A:13:LEU:HD23	1:A:44:LEU:HD11	2.03	0.41
1:B:406:LYS:HE3	1:B:406:LYS:HB3	1.98	0.41
1:E:100:ARG:NH1	4:E:503:ICT:O6	2.54	0.41
1:E:146:VAL:HG13	1:F:156:PHE:CZ	2.56	0.41
1:H:402:ASP:O	1:H:405:ARG:HG3	2.21	0.41
1:B:357:LEU:HD23	1:B:404:MET:HE1	2.03	0.41
1:C:1:SER:C	1:C:2:GLN:HG3	2.44	0.41
1:G:358:LEU:O	1:G:362:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:LYS:NZ	2:D:501:NAP:O2X	2.48	0.40
1:E:20:ARG:NH2	1:E:43:ASP:OD1	2.39	0.40
1:G:15:GLY:HA3	1:G:73:CYS:SG	2.61	0.40
1:G:196:PHE:CD2	1:G:229:MET:HE2	2.56	0.40
1:D:229:MET:HE2	1:D:229:MET:HB3	2.01	0.40
1:G:208:LEU:HD22	1:G:226:PHE:CG	2.56	0.40
1:E:4:ILE:HD13	1:E:4:ILE:HG21	1.88	0.40
1:A:46:MET:HE2	1:A:76:ILE:HB	2.03	0.40
1:B:23:TRP:CD2	1:B:73:CYS:HB2	2.57	0.40
1:F:121:VAL:HG11	1:F:124:TRP:CE2	2.56	0.40
1:A:354:PHE:CD2	1:A:354:PHE:C	3.00	0.40
1:D:22:ILE:HG22	1:D:26:ILE:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	411/413 (100%)	393 (96%)	18 (4%)	0	100	100
1	B	408/413 (99%)	385 (94%)	20 (5%)	3 (1%)	18	28
1	C	411/413 (100%)	390 (95%)	20 (5%)	1 (0%)	43	58
1	D	411/413 (100%)	391 (95%)	18 (4%)	2 (0%)	24	37
1	E	411/413 (100%)	393 (96%)	17 (4%)	1 (0%)	43	58
1	F	411/413 (100%)	385 (94%)	24 (6%)	2 (0%)	24	37
1	G	411/413 (100%)	392 (95%)	18 (4%)	1 (0%)	43	58
1	H	409/413 (99%)	387 (95%)	22 (5%)	0	100	100
All	All	3283/3304 (99%)	3116 (95%)	157 (5%)	10 (0%)	36	50

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	411	SER
1	F	3	LYS
1	G	3	LYS
1	B	3	LYS
1	D	3	LYS
1	E	3	LYS
1	F	2	GLN
1	B	162	GLY
1	C	91	MET
1	D	162	GLY

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	352/352 (100%)	322 (92%)	30 (8%)	10	16
1	B	351/352 (100%)	329 (94%)	22 (6%)	16	29
1	C	352/352 (100%)	329 (94%)	23 (6%)	15	27
1	D	352/352 (100%)	326 (93%)	26 (7%)	13	22
1	E	352/352 (100%)	326 (93%)	26 (7%)	13	22
1	F	352/352 (100%)	328 (93%)	24 (7%)	14	25
1	G	352/352 (100%)	330 (94%)	22 (6%)	16	29
1	H	350/352 (99%)	326 (93%)	24 (7%)	14	24
All	All	2813/2816 (100%)	2616 (93%)	197 (7%)	14	24

All (197) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	2	GLN
1	A	3	LYS
1	A	6	VAL
1	A	19	THR
1	A	28	GLU

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Mol	Chain	Res	Type
1	A	65	LYS
1	A	69	VAL
1	A	90	GLN
1	A	103	LEU
1	A	109	ARG
1	A	119	ARG
1	A	120	LEU
1	A	140	ARG
1	A	144	LEU
1	A	154	ILE
1	A	174	SER
1	A	186	GLU
1	A	189	LYS
1	A	209	SER
1	A	251	ASP
1	A	295	MET
1	A	311	VAL
1	A	337	ARG
1	A	347	GLN
1	A	387	ARG
1	A	392	ASN
1	A	398	HIS
1	A	402	ASP
1	A	410	ARG
1	B	2	GLN
1	B	6	VAL
1	B	28	GLU
1	B	69	VAL
1	B	75	THR
1	B	84	ARG
1	B	87	ASN
1	B	103	LEU
1	B	109	ARG
1	B	119	ARG
1	B	151	THR
1	B	174	SER
1	B	200	LEU
1	B	217	ARG
1	B	231	LYS
1	B	295	MET
1	B	311	VAL
1	B	337	ARG

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Mol	Chain	Res	Type
1	B	392	ASN
1	B	402	ASP
1	B	409	GLU
1	B	413	ILE
1	C	1	SER
1	C	2	GLN
1	C	5	LYS
1	C	6	VAL
1	C	28	GLU
1	C	37	VAL
1	C	109	ARG
1	C	119	ARG
1	C	151	THR
1	C	154	ILE
1	C	159	GLU
1	C	174	SER
1	C	179	MET
1	C	186	GLU
1	C	200	LEU
1	C	311	VAL
1	C	337	ARG
1	C	347	GLN
1	C	360	LYS
1	C	364	SER
1	C	387	ARG
1	C	392	ASN
1	C	413	ILE
1	D	3	LYS
1	D	6	VAL
1	D	37	VAL
1	D	55	GLN
1	D	84	ARG
1	D	90	GLN
1	D	103	LEU
1	D	109	ARG
1	D	115	LYS
1	D	120	LEU
1	D	151	THR
1	D	154	ILE
1	D	159	GLU
1	D	194	SER
1	D	200	LEU

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Mol	Chain	Res	Type
1	D	203	LYS
1	D	231	LYS
1	D	295	MET
1	D	320	LYS
1	D	337	ARG
1	D	386	THR
1	D	387	ARG
1	D	392	ASN
1	D	409	GLU
1	D	412	LYS
1	D	413	ILE
1	E	1	SER
1	E	3	LYS
1	E	6	VAL
1	E	69	VAL
1	E	109	ARG
1	E	119	ARG
1	E	144	LEU
1	E	152	PHE
1	E	154	ILE
1	E	181	MET
1	E	193	LYS
1	E	200	LEU
1	E	201	SER
1	E	231	LYS
1	E	240	LYS
1	E	296	SER
1	E	311	VAL
1	E	320	LYS
1	E	322	GLU
1	E	336	THR
1	E	337	ARG
1	E	347	GLN
1	E	350	LYS
1	E	387	ARG
1	E	392	ASN
1	E	409	GLU
1	F	6	VAL
1	F	9	THR
1	F	19	THR
1	F	28	GLU
1	F	44	LEU

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Mol	Chain	Res	Type
1	F	69	VAL
1	F	109	ARG
1	F	119	ARG
1	F	123	THR
1	F	151	THR
1	F	154	ILE
1	F	160	SER
1	F	174	SER
1	F	186	GLU
1	F	200	LEU
1	F	217	ARG
1	F	311	VAL
1	F	337	ARG
1	F	347	GLN
1	F	392	ASN
1	F	405	ARG
1	F	409	GLU
1	F	410	ARG
1	F	412	LYS
1	G	1	SER
1	G	28	GLU
1	G	84	ARG
1	G	109	ARG
1	G	119	ARG
1	G	120	LEU
1	G	140	ARG
1	G	144	LEU
1	G	151	THR
1	G	154	ILE
1	G	159	GLU
1	G	168	LYS
1	G	174	SER
1	G	197	GLU
1	G	200	LEU
1	G	201	SER
1	G	231	LYS
1	G	239	LYS
1	G	320	LYS
1	G	387	ARG
1	G	392	ASN
1	G	412	LYS
1	H	3	LYS

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Mol	Chain	Res	Type
1	H	6	VAL
1	H	28	GLU
1	H	47	GLU
1	H	90	GLN
1	H	103	LEU
1	H	119	ARG
1	H	151	THR
1	H	154	ILE
1	H	159	GLU
1	H	173	LYS
1	H	200	LEU
1	H	217	ARG
1	H	311	VAL
1	H	320	LYS
1	H	322	GLU
1	H	331	SER
1	H	337	ARG
1	H	347	GLN
1	H	387	ARG
1	H	392	ASN
1	H	409	GLU
1	H	410	ARG
1	H	412	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	HIS
1	A	155	HIS
1	A	353	GLN
1	A	392	ASN
1	B	282	GLN
1	B	348	ASN
1	B	353	GLN
1	B	392	ASN
1	C	2	GLN
1	D	101	ASN
1	D	212	ASN
1	D	276	GLN
1	D	341	HIS
1	D	392	ASN
1	D	398	HIS

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Mol	Chain	Res	Type
1	E	55	GLN
1	E	101	ASN
1	E	318	HIS
1	E	353	GLN
1	E	383	ASN
1	E	392	ASN
1	E	398	HIS
1	F	62	HIS
1	F	212	ASN
1	F	392	ASN
1	F	398	HIS
1	G	48	ASN
1	G	90	GLN
1	G	147	ASN
1	G	347	GLN
1	G	353	GLN
1	G	383	ASN
1	G	392	ASN
1	H	87	ASN
1	H	167	GLN
1	H	319	GLN
1	H	353	GLN
1	H	392	ASN
1	H	398	HIS

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 [i](#)

Of 24 ligands modelled in this entry, 8 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$
4	ICT	C	503	3	12,12,12	1.16	0	13,16,16	1.48	3 (23%)
2	NAP	D	501	-	50,52,52	1.41	8 (16%)	71,80,80	1.48	12 (16%)
4	ICT	A	503	3	12,12,12	0.96	0	13,16,16	2.55	6 (46%)
4	ICT	D	503	3	12,12,12	1.33	1 (8%)	13,16,16	2.29	6 (46%)
4	ICT	F	503	3	12,12,12	1.18	0	13,16,16	0.92	0
2	NAP	A	501	-	50,52,52	1.36	7 (14%)	71,80,80	1.56	11 (15%)
2	NAP	H	501	-	50,52,52	1.13	4 (8%)	71,80,80	1.61	14 (19%)
2	NAP	C	501	-	50,52,52	1.19	5 (10%)	71,80,80	1.66	12 (16%)
2	NAP	B	501	-	50,52,52	1.40	7 (14%)	71,80,80	1.48	12 (16%)
2	NAP	F	501	-	50,52,52	1.12	4 (8%)	71,80,80	1.65	15 (21%)
4	ICT	B	503	3	12,12,12	0.97	0	13,16,16	1.93	5 (38%)
4	ICT	G	503	3	12,12,12	1.14	0	13,16,16	1.31	2 (15%)
4	ICT	E	503	3	12,12,12	1.20	0	13,16,16	1.88	3 (23%)
2	NAP	G	501	-	50,52,52	1.28	5 (10%)	71,80,80	1.67	11 (15%)
4	ICT	H	503	3	12,12,12	1.14	0	13,16,16	1.60	2 (15%)
2	NAP	E	501	-	50,52,52	1.39	7 (14%)	71,80,80	1.65	12 (16%)

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	ICT	C	503	3	-	8/16/16/16	-
2	NAP	D	501	-	-	10/35/67/67	0/5/5/5
4	ICT	A	503	3	-	5/16/16/16	-
4	ICT	D	503	3	-	6/16/16/16	-
4	ICT	F	503	3	-	8/16/16/16	-
2	NAP	A	501	-	-	9/35/67/67	0/5/5/5
2	NAP	H	501	-	-	12/35/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	C	501	-	-	8/35/67/67	0/5/5/5
2	NAP	B	501	-	-	9/35/67/67	0/5/5/5
2	NAP	F	501	-	-	9/35/67/67	0/5/5/5
4	ICT	B	503	3	-	8/16/16/16	-
4	ICT	G	503	3	-	6/16/16/16	-
4	ICT	E	503	3	-	6/16/16/16	-
2	NAP	G	501	-	-	7/35/67/67	0/5/5/5
4	ICT	H	503	3	-	4/16/16/16	-
2	NAP	E	501	-	-	7/35/67/67	0/5/5/5

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAP	C5A-C4A	5.20	1.48	1.39
2	D	501	NAP	C5A-C4A	4.85	1.47	1.39
2	H	501	NAP	C5A-C4A	4.83	1.47	1.39
2	F	501	NAP	C5A-C4A	4.55	1.47	1.39
2	E	501	NAP	C5A-C4A	4.47	1.47	1.39
2	G	501	NAP	C5A-C4A	4.26	1.46	1.39
2	C	501	NAP	C5A-C4A	4.22	1.46	1.39
2	B	501	NAP	PA-O3	4.08	1.63	1.59
2	D	501	NAP	C5A-N7A	-4.00	1.31	1.39
2	A	501	NAP	PA-O3	3.95	1.63	1.59
2	E	501	NAP	C5A-N7A	-3.92	1.31	1.39
2	A	501	NAP	C5A-C4A	3.84	1.45	1.39
2	G	501	NAP	C5A-N7A	-3.69	1.32	1.39
2	G	501	NAP	PA-O3	3.69	1.63	1.59
2	D	501	NAP	PA-O3	3.58	1.63	1.59
2	E	501	NAP	O4D-C1D	3.55	1.45	1.40
2	C	501	NAP	PA-O3	3.33	1.63	1.59
2	H	501	NAP	C5A-N7A	-3.02	1.33	1.39
2	B	501	NAP	C5A-N7A	-2.96	1.33	1.39
2	A	501	NAP	C4A-N9A	-2.92	1.31	1.37
2	A	501	NAP	C5A-N7A	-2.88	1.33	1.39
2	A	501	NAP	P2B-O2B	2.82	1.64	1.59
2	E	501	NAP	PA-O3	2.77	1.62	1.59
2	F	501	NAP	C4A-N9A	-2.76	1.31	1.37
2	B	501	NAP	C4A-N9A	-2.75	1.32	1.37
2	C	501	NAP	C5A-N7A	-2.72	1.34	1.39
2	B	501	NAP	O4D-C1D	2.71	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	NAP	PN-O3	2.68	1.62	1.59
2	D	501	NAP	O4D-C1D	2.55	1.44	1.40
2	B	501	NAP	C5A-C6A	2.52	1.48	1.41
2	E	501	NAP	PN-O3	2.48	1.62	1.59
2	D	501	NAP	C4A-N9A	-2.46	1.32	1.37
2	C	501	NAP	C8A-N7A	2.45	1.36	1.31
2	E	501	NAP	C4A-N9A	-2.44	1.32	1.37
2	F	501	NAP	C5A-C6A	2.44	1.47	1.41
2	A	501	NAP	O4D-C1D	2.43	1.44	1.40
2	H	501	NAP	C4A-N9A	-2.39	1.32	1.37
4	D	503	ICT	C4-C3	2.39	1.57	1.53
2	H	501	NAP	C5A-C6A	2.36	1.47	1.41
2	F	501	NAP	C5A-N7A	-2.32	1.34	1.39
2	B	501	NAP	PN-O3	2.29	1.62	1.59
2	E	501	NAP	C5A-C6A	2.23	1.47	1.41
2	D	501	NAP	C5A-C6A	2.21	1.47	1.41
2	A	501	NAP	C5A-C6A	2.19	1.47	1.41
2	G	501	NAP	C4A-N9A	-2.16	1.33	1.37
2	C	501	NAP	O4D-C1D	2.09	1.43	1.40
2	D	501	NAP	C8A-N9A	-2.01	1.34	1.37
2	G	501	NAP	C5A-C6A	2.00	1.46	1.41

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	501	NAP	C5A-C4A-N3A	-6.48	117.79	126.72
2	E	501	NAP	C5A-C4A-N3A	-5.66	118.93	126.72
4	A	503	ICT	O7-C2-C3	-5.47	98.29	110.63
2	C	501	NAP	C5A-C4A-N3A	-5.46	119.20	126.72
2	G	501	NAP	N3A-C4A-N9A	5.19	136.00	127.17
2	H	501	NAP	C5A-C4A-N3A	-5.16	119.61	126.72
2	A	501	NAP	C5A-C4A-N3A	-5.07	119.73	126.72
2	H	501	NAP	N3A-C4A-N9A	5.01	135.68	127.17
2	D	501	NAP	C5A-C4A-N3A	-4.58	120.41	126.72
2	E	501	NAP	N3A-C4A-N9A	4.51	134.84	127.17
2	C	501	NAP	N3A-C4A-N9A	4.49	134.81	127.17
4	A	503	ICT	O2-C1-C2	4.39	125.52	113.31
2	C	501	NAP	C3N-C7N-N7N	4.31	123.04	117.74
4	E	503	ICT	O7-C2-C1	-4.27	101.57	110.69
2	B	501	NAP	C5A-C4A-N3A	-4.20	120.93	126.72
2	A	501	NAP	N3A-C2A-N1A	-4.16	122.29	128.58
2	A	501	NAP	N3A-C4A-N9A	4.11	134.15	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	NAP	C4A-C5A-N7A	-4.05	105.95	110.58
2	C	501	NAP	N3A-C2A-N1A	-4.03	122.48	128.58
2	G	501	NAP	C2A-N3A-C4A	4.01	121.62	111.83
2	F	501	NAP	N3A-C4A-N9A	3.97	133.92	127.17
2	F	501	NAP	C4A-N9A-C8A	3.95	109.89	105.74
2	B	501	NAP	N3A-C4A-N9A	3.85	133.71	127.17
2	C	501	NAP	C2A-N3A-C4A	3.84	121.22	111.83
2	G	501	NAP	N3A-C2A-N1A	-3.84	122.78	128.58
2	F	501	NAP	C5A-C4A-N3A	-3.79	121.50	126.72
2	A	501	NAP	C2A-N3A-C4A	3.70	120.87	111.83
4	B	503	ICT	O2-C1-C2	3.66	123.48	113.31
2	F	501	NAP	N3A-C2A-N1A	-3.61	123.12	128.58
2	E	501	NAP	C2A-N3A-C4A	3.59	120.60	111.83
2	G	501	NAP	O2B-P2B-O1X	-3.59	96.54	109.33
2	E	501	NAP	N3A-C2A-N1A	-3.50	123.29	128.58
2	F	501	NAP	O3-PN-O1N	-3.49	100.19	110.70
2	F	501	NAP	C3N-C7N-N7N	3.48	122.03	117.74
2	D	501	NAP	N3A-C4A-N9A	3.48	133.08	127.17
2	H	501	NAP	C3N-C7N-N7N	3.40	121.92	117.74
4	D	503	ICT	O2-C1-C2	3.31	122.50	113.31
2	H	501	NAP	N3A-C2A-N1A	-3.24	123.67	128.58
4	E	503	ICT	O2-C1-C2	3.23	122.27	113.31
2	D	501	NAP	C5A-N7A-C8A	3.22	108.50	103.45
2	H	501	NAP	O7N-C7N-N7N	-3.19	118.00	122.62
2	H	501	NAP	C2A-N3A-C4A	3.17	119.58	111.83
2	E	501	NAP	C4A-C5A-N7A	-3.12	107.01	110.58
2	H	501	NAP	N6A-C6A-N1A	3.09	125.27	118.38
4	D	503	ICT	O6-C6-C3	3.09	121.94	113.93
2	E	501	NAP	O7N-C7N-N7N	-3.07	118.17	122.62
2	D	501	NAP	C2A-N1A-C6A	3.00	123.66	118.73
2	G	501	NAP	C4A-C5A-N7A	-3.00	107.15	110.58
2	C	501	NAP	O7N-C7N-N7N	-2.98	118.31	122.62
4	D	503	ICT	C4-C3-C6	2.97	115.97	111.25
2	A	501	NAP	C4A-N9A-C8A	2.96	108.85	105.74
2	E	501	NAP	O2B-P2B-O1X	-2.96	98.79	109.33
2	F	501	NAP	C2A-N3A-C4A	2.95	119.02	111.83
4	A	503	ICT	O1-C1-C2	-2.93	113.82	121.62
2	H	501	NAP	C4A-N9A-C8A	2.89	108.78	105.74
4	H	503	ICT	O5-C6-C3	-2.86	116.26	123.01
4	D	503	ICT	O4-C5-C4	2.85	122.85	114.00
2	E	501	NAP	C6N-N1N-C2N	-2.84	119.46	121.88
2	H	501	NAP	O3X-P2B-O2X	2.84	118.43	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	NAP	N3A-C2A-N1A	-2.83	124.30	128.58
2	B	501	NAP	C2A-N3A-C4A	2.79	118.64	111.83
4	H	503	ICT	O6-C6-C3	2.77	121.13	113.93
2	G	501	NAP	O3X-P2B-O1X	2.77	121.64	110.83
2	D	501	NAP	C2A-N3A-C4A	2.73	118.49	111.83
4	D	503	ICT	C3-C4-C5	2.72	119.04	113.95
4	A	503	ICT	O5-C6-C3	-2.72	116.59	123.01
2	B	501	NAP	O2A-PA-O3	-2.70	99.98	107.27
4	B	503	ICT	O6-C6-C3	2.69	120.91	113.93
4	A	503	ICT	C4-C3-C6	2.69	115.51	111.25
2	A	501	NAP	C4A-C5A-N7A	-2.66	107.54	110.58
4	C	503	ICT	C4-C3-C6	2.66	115.47	111.25
2	B	501	NAP	C4A-N9A-C8A	2.62	108.49	105.74
2	F	501	NAP	N6A-C6A-N1A	2.60	124.16	118.38
4	B	503	ICT	O5-C6-C3	-2.59	116.90	123.01
2	B	501	NAP	N3A-C2A-N1A	-2.57	124.69	128.58
4	C	503	ICT	O6-C6-C3	2.55	120.54	113.93
4	D	503	ICT	O4-C5-O3	-2.55	116.78	123.33
4	B	503	ICT	O4-C5-C4	2.54	121.89	114.00
2	G	501	NAP	N6A-C6A-N1A	2.53	124.02	118.38
2	B	501	NAP	N6A-C6A-N1A	2.53	124.01	118.38
2	B	501	NAP	C3N-C7N-N7N	2.53	120.85	117.74
2	C	501	NAP	O2A-PA-O3	-2.53	100.44	107.27
2	E	501	NAP	C5A-N7A-C8A	2.50	107.38	103.45
2	D	501	NAP	C3N-C7N-N7N	2.48	120.80	117.74
2	B	501	NAP	O3X-P2B-O1X	2.48	120.50	110.83
2	F	501	NAP	C2A-N1A-C6A	2.46	122.78	118.73
4	B	503	ICT	O1-C1-C2	-2.46	115.07	121.62
2	G	501	NAP	C5A-N7A-C8A	2.42	107.25	103.45
4	A	503	ICT	O6-C6-C3	2.40	120.17	113.93
2	H	501	NAP	O3-PN-O1N	-2.39	103.52	110.70
2	C	501	NAP	C2A-N1A-C6A	2.37	122.62	118.73
2	A	501	NAP	C6N-N1N-C2N	-2.37	119.86	121.88
2	A	501	NAP	N9A-C8A-N7A	-2.36	110.58	113.94
2	E	501	NAP	N6A-C6A-N1A	2.36	123.63	118.38
2	A	501	NAP	O7N-C7N-N7N	-2.35	119.22	122.62
2	F	501	NAP	O2B-C2B-C1B	-2.35	101.81	110.05
2	C	501	NAP	O3B-C3B-C2B	2.33	117.70	111.19
2	G	501	NAP	O5B-C5B-C4B	2.32	116.91	108.99
2	D	501	NAP	O7N-C7N-N7N	-2.32	119.26	122.62
2	B	501	NAP	O2N-PN-O1N	2.32	123.23	112.44
2	E	501	NAP	O3X-P2B-O1X	2.28	119.72	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	503	ICT	O7-C2-C1	-2.28	105.82	110.69
4	G	503	ICT	O6-C6-C3	2.21	119.67	113.93
2	F	501	NAP	C2D-C3D-C4D	2.21	106.87	102.61
2	B	501	NAP	C6N-N1N-C2N	-2.19	120.01	121.88
2	A	501	NAP	C5A-N7A-C8A	2.19	106.89	103.45
2	H	501	NAP	C2A-N1A-C6A	2.18	122.31	118.73
2	D	501	NAP	C6A-C5A-N7A	2.18	136.29	132.09
2	F	501	NAP	O2N-PN-O1N	2.16	122.48	112.44
2	C	501	NAP	C4A-N9A-C8A	2.16	108.00	105.74
2	C	501	NAP	C4A-C5A-N7A	-2.13	108.14	110.58
2	C	501	NAP	O3X-P2B-O2X	2.12	115.77	107.80
2	H	501	NAP	C5A-C6A-N6A	-2.12	118.03	123.29
2	H	501	NAP	O2N-PN-O1N	2.11	122.26	112.44
2	D	501	NAP	C2D-C3D-C4D	2.11	106.68	102.61
2	B	501	NAP	C4A-C5A-N7A	-2.10	108.18	110.58
2	G	501	NAP	C5A-C6A-N6A	-2.10	118.09	123.29
2	A	501	NAP	C3B-C2B-C1B	-2.07	98.84	102.81
2	F	501	NAP	C4A-C5A-N7A	-2.06	108.22	110.58
2	E	501	NAP	C2A-N1A-C6A	2.06	122.11	118.73
4	E	503	ICT	O1-C1-C2	-2.06	116.14	121.62
2	F	501	NAP	C2B-C1B-N9A	-2.05	110.38	113.75
2	D	501	NAP	C4A-N9A-C8A	2.04	107.88	105.74
4	C	503	ICT	O5-C6-C3	-2.03	118.22	123.01
2	F	501	NAP	O3X-P2B-O1X	2.02	118.71	110.83
2	H	501	NAP	O2A-PA-O1A	2.00	121.77	112.44

There are no chirality outliers.

All (122) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NAP	O4D-C1D-N1N-C2N
2	A	501	NAP	O4D-C1D-N1N-C6N
2	A	501	NAP	C2D-C1D-N1N-C2N
2	A	501	NAP	C2D-C1D-N1N-C6N
2	B	501	NAP	C5B-O5B-PA-O1A
2	B	501	NAP	C5B-O5B-PA-O2A
2	B	501	NAP	C5D-O5D-PN-O3
2	B	501	NAP	C5D-O5D-PN-O1N
2	B	501	NAP	C5D-O5D-PN-O2N
2	B	501	NAP	O4D-C1D-N1N-C2N
2	B	501	NAP	O4D-C1D-N1N-C6N
2	B	501	NAP	C2D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
2	C	501	NAP	C5B-O5B-PA-O3
2	C	501	NAP	C5D-O5D-PN-O3
2	C	501	NAP	C5D-O5D-PN-O1N
2	C	501	NAP	C5D-O5D-PN-O2N
2	C	501	NAP	O4D-C1D-N1N-C2N
2	C	501	NAP	O4D-C1D-N1N-C6N
2	D	501	NAP	C5B-O5B-PA-O2A
2	D	501	NAP	C5D-O5D-PN-O3
2	D	501	NAP	C5D-O5D-PN-O1N
2	D	501	NAP	C5D-O5D-PN-O2N
2	D	501	NAP	O4D-C1D-N1N-C2N
2	D	501	NAP	O4D-C1D-N1N-C6N
2	D	501	NAP	C2D-C1D-N1N-C2N
2	D	501	NAP	C2D-C1D-N1N-C6N
2	E	501	NAP	O4D-C1D-N1N-C2N
2	E	501	NAP	O4D-C1D-N1N-C6N
2	E	501	NAP	C2D-C1D-N1N-C2N
2	E	501	NAP	C2D-C1D-N1N-C6N
2	F	501	NAP	C5D-O5D-PN-O3
2	F	501	NAP	C5D-O5D-PN-O1N
2	F	501	NAP	C5D-O5D-PN-O2N
2	F	501	NAP	O4D-C1D-N1N-C2N
2	F	501	NAP	O4D-C1D-N1N-C6N
2	F	501	NAP	C2D-C1D-N1N-C2N
2	G	501	NAP	C5D-O5D-PN-O3
2	G	501	NAP	C5D-O5D-PN-O1N
2	G	501	NAP	C5D-O5D-PN-O2N
2	G	501	NAP	O4D-C1D-N1N-C2N
2	G	501	NAP	O4D-C1D-N1N-C6N
2	G	501	NAP	C2D-C1D-N1N-C2N
2	G	501	NAP	C2D-C1D-N1N-C6N
2	H	501	NAP	C5B-O5B-PA-O1A
2	H	501	NAP	C5B-O5B-PA-O2A
2	H	501	NAP	C5B-O5B-PA-O3
2	H	501	NAP	C5D-O5D-PN-O3
2	H	501	NAP	C5D-O5D-PN-O1N
2	H	501	NAP	C5D-O5D-PN-O2N
2	H	501	NAP	O4D-C1D-N1N-C2N
2	H	501	NAP	O4D-C1D-N1N-C6N
4	B	503	ICT	O1-C1-C2-O7
4	E	503	ICT	O1-C1-C2-C3
4	E	503	ICT	O2-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	F	503	ICT	O1-C1-C2-C3
4	F	503	ICT	O2-C1-C2-C3
4	G	503	ICT	O1-C1-C2-O7
4	G	503	ICT	O2-C1-C2-O7
4	H	503	ICT	O2-C1-C2-O7
4	B	503	ICT	O2-C1-C2-O7
4	E	503	ICT	O1-C1-C2-O7
4	E	503	ICT	O2-C1-C2-O7
4	H	503	ICT	O1-C1-C2-O7
4	B	503	ICT	O1-C1-C2-C3
4	B	503	ICT	O2-C1-C2-C3
4	G	503	ICT	O1-C1-C2-C3
4	G	503	ICT	O2-C1-C2-C3
4	D	503	ICT	O2-C1-C2-O7
4	C	503	ICT	O1-C1-C2-O7
4	C	503	ICT	O2-C1-C2-O7
4	D	503	ICT	O1-C1-C2-O7
4	F	503	ICT	O1-C1-C2-O7
4	F	503	ICT	O2-C1-C2-O7
2	A	501	NAP	O4D-C4D-C5D-O5D
2	A	501	NAP	C3D-C4D-C5D-O5D
2	F	501	NAP	O4B-C4B-C5B-O5B
4	B	503	ICT	C4-C3-C6-O6
2	C	501	NAP	C1B-C2B-O2B-P2B
2	E	501	NAP	PN-O3-PA-O5B
2	H	501	NAP	PA-O3-PN-O5D
2	F	501	NAP	C3B-C4B-C5B-O5B
4	A	503	ICT	O2-C1-C2-C3
4	A	503	ICT	O1-C1-C2-C3
4	D	503	ICT	O1-C1-C2-C3
2	A	501	NAP	C5B-O5B-PA-O3
2	A	501	NAP	C5D-O5D-PN-O1N
2	B	501	NAP	C5B-O5B-PA-O3
2	D	501	NAP	C5B-O5B-PA-O1A
2	D	501	NAP	C5B-O5B-PA-O3
4	A	503	ICT	C3-C4-C5-O3
4	C	503	ICT	C2-C3-C6-O5
4	C	503	ICT	C2-C3-C6-O6
4	F	503	ICT	C2-C3-C6-O5
4	F	503	ICT	C2-C3-C6-O6
4	A	503	ICT	C3-C4-C5-O4
4	B	503	ICT	C3-C4-C5-O3

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Mol	Chain	Res	Type	Atoms
4	B	503	ICT	C3-C4-C5-O4
4	H	503	ICT	C3-C4-C5-O3
4	H	503	ICT	C3-C4-C5-O4
4	B	503	ICT	C4-C3-C6-O5
4	D	503	ICT	C3-C4-C5-O4
4	G	503	ICT	C3-C4-C5-O4
2	C	501	NAP	C3B-C2B-O2B-P2B
2	F	501	NAP	C1B-C2B-O2B-P2B
2	H	501	NAP	O4D-C4D-C5D-O5D
4	D	503	ICT	O7-C2-C3-C6
4	E	503	ICT	C3-C4-C5-O4
2	E	501	NAP	C3B-C4B-C5B-O5B
4	E	503	ICT	C3-C4-C5-O3
2	A	501	NAP	O4B-C4B-C5B-O5B
4	C	503	ICT	C3-C4-C5-O4
4	D	503	ICT	C3-C4-C5-O3
4	F	503	ICT	C3-C4-C5-O3
4	F	503	ICT	C3-C4-C5-O4
2	H	501	NAP	PN-O3-PA-O1A
4	G	503	ICT	C3-C4-C5-O3
4	C	503	ICT	C4-C3-C6-O5
4	C	503	ICT	C4-C3-C6-O6
2	E	501	NAP	O4B-C4B-C5B-O5B
4	C	503	ICT	C3-C4-C5-O3
4	A	503	ICT	C1-C2-C3-C6
2	H	501	NAP	PN-O3-PA-O2A

There are no ring outliers.

13 monomers are involved in 16 short contacts:

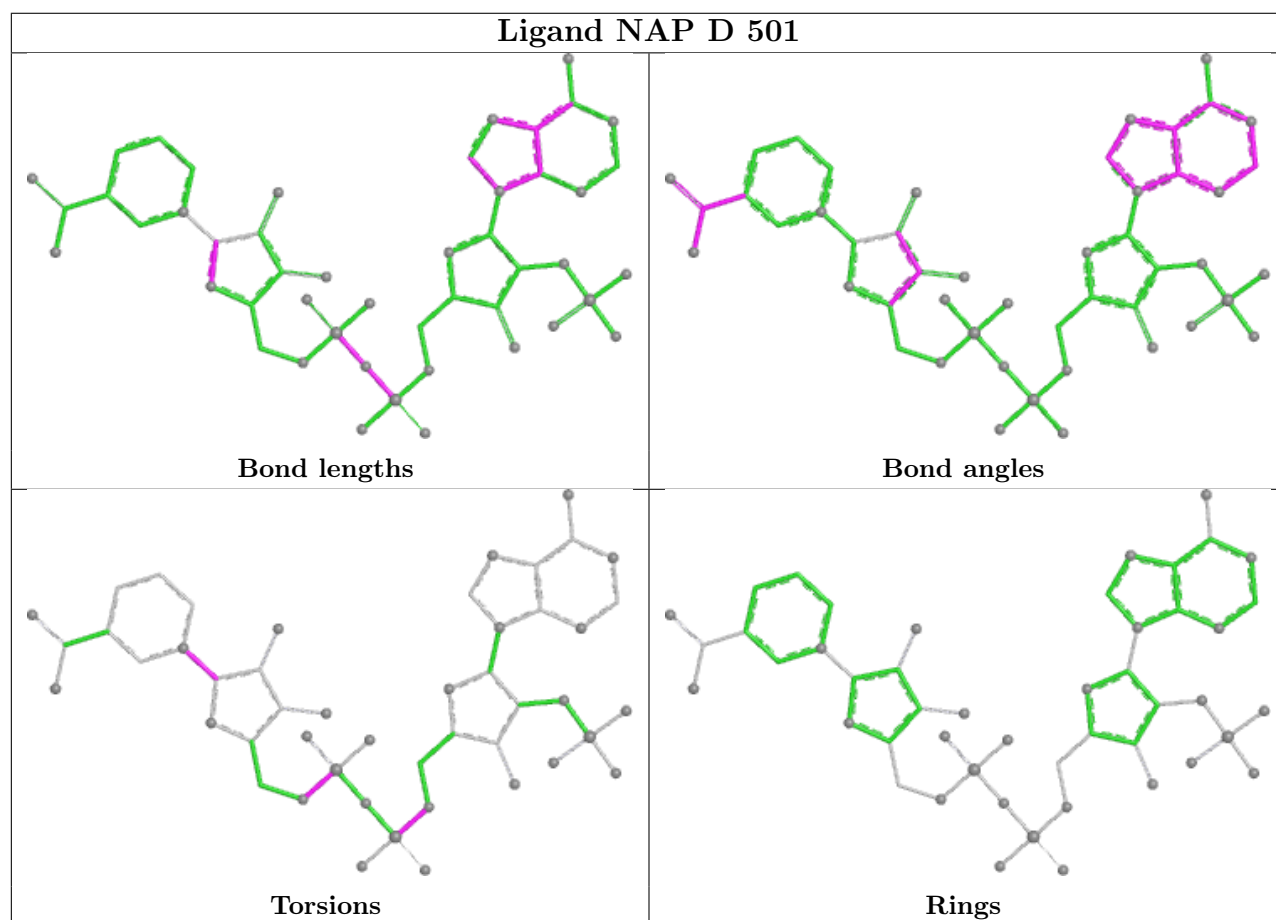
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	503	ICT	1	0
2	D	501	NAP	2	0
4	A	503	ICT	3	0
4	D	503	ICT	1	0
2	A	501	NAP	1	0
2	H	501	NAP	2	0
2	C	501	NAP	1	0
2	B	501	NAP	1	0
2	F	501	NAP	1	0
4	B	503	ICT	1	0
4	E	503	ICT	1	0

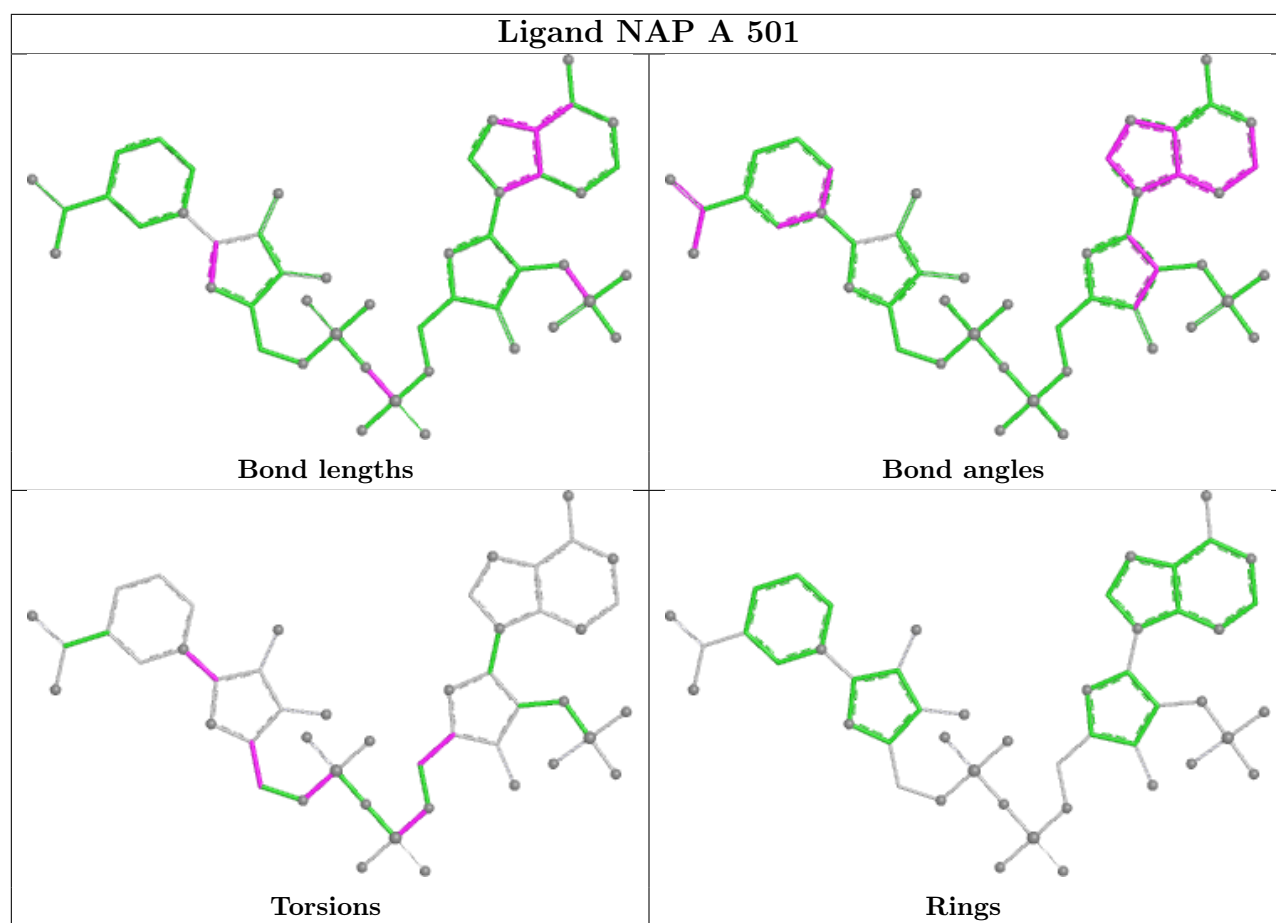
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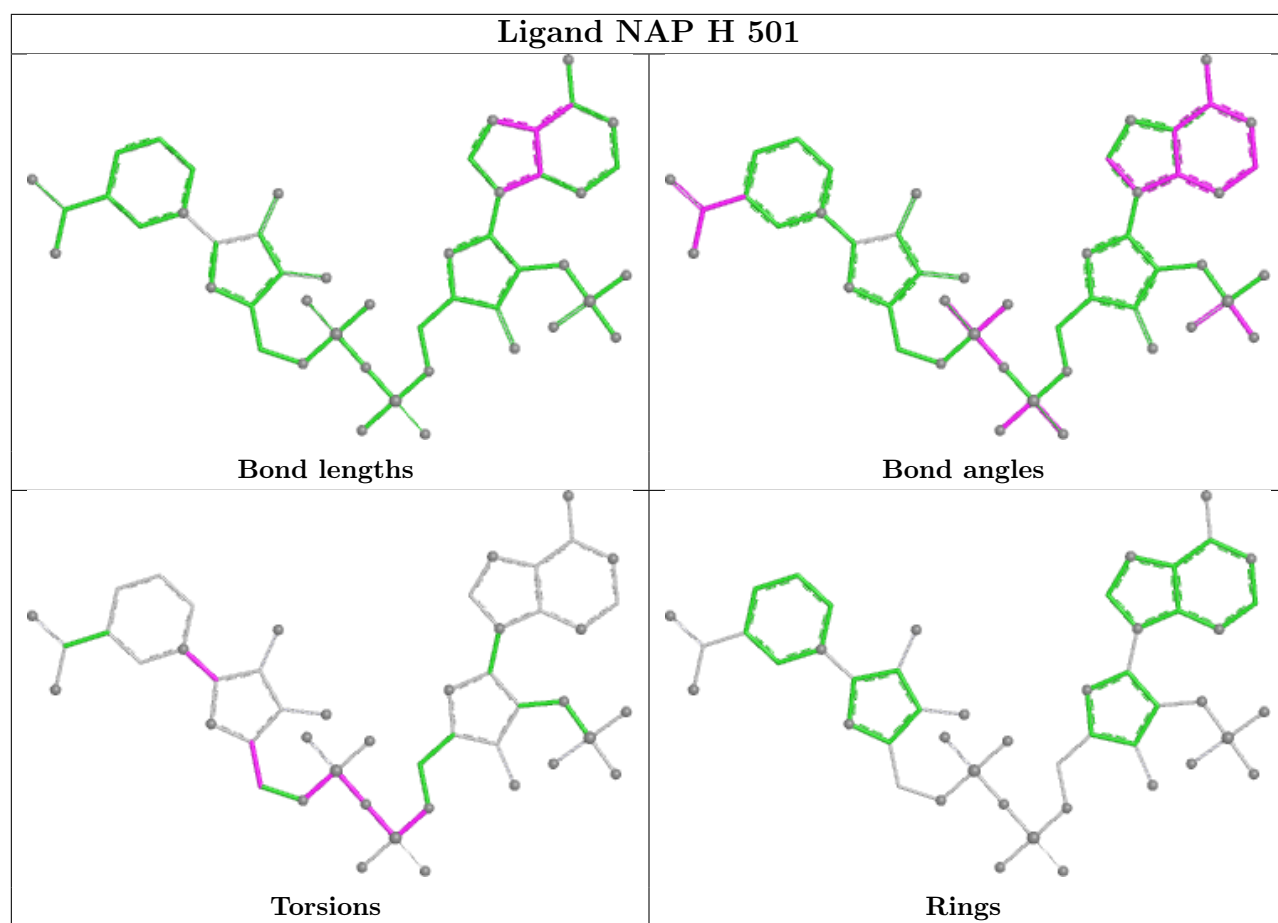
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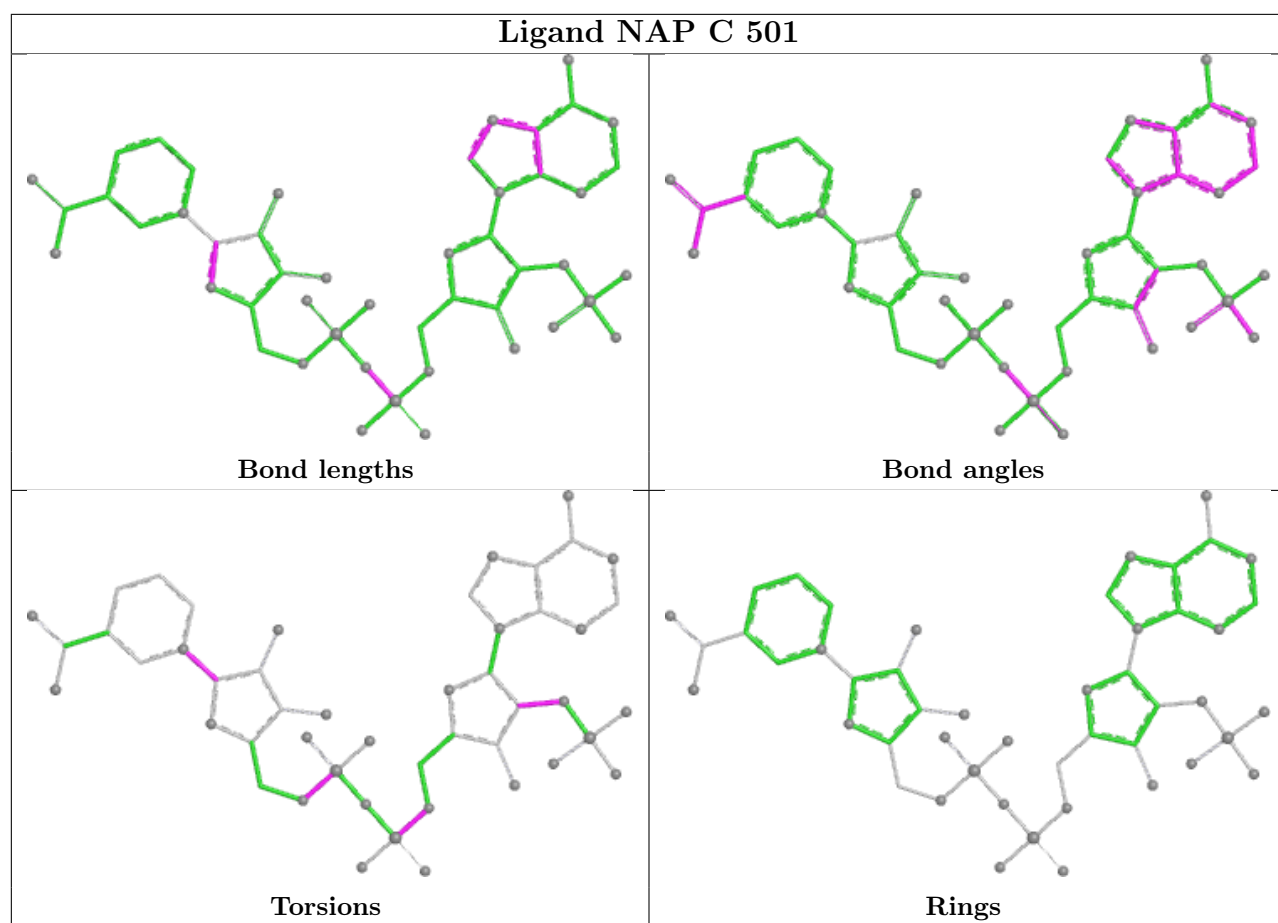
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	501	NAP	1	0
2	E	501	NAP	1	0

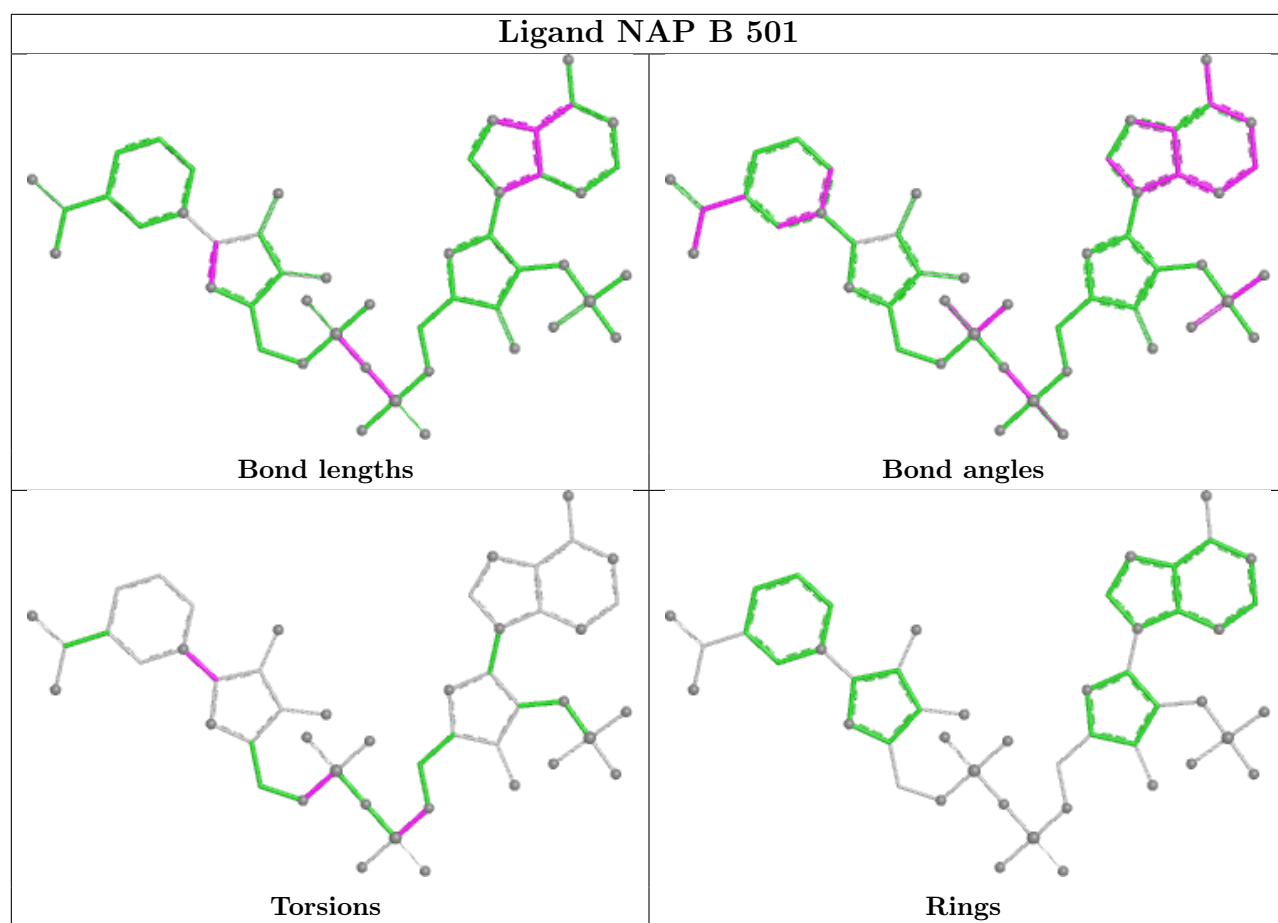
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

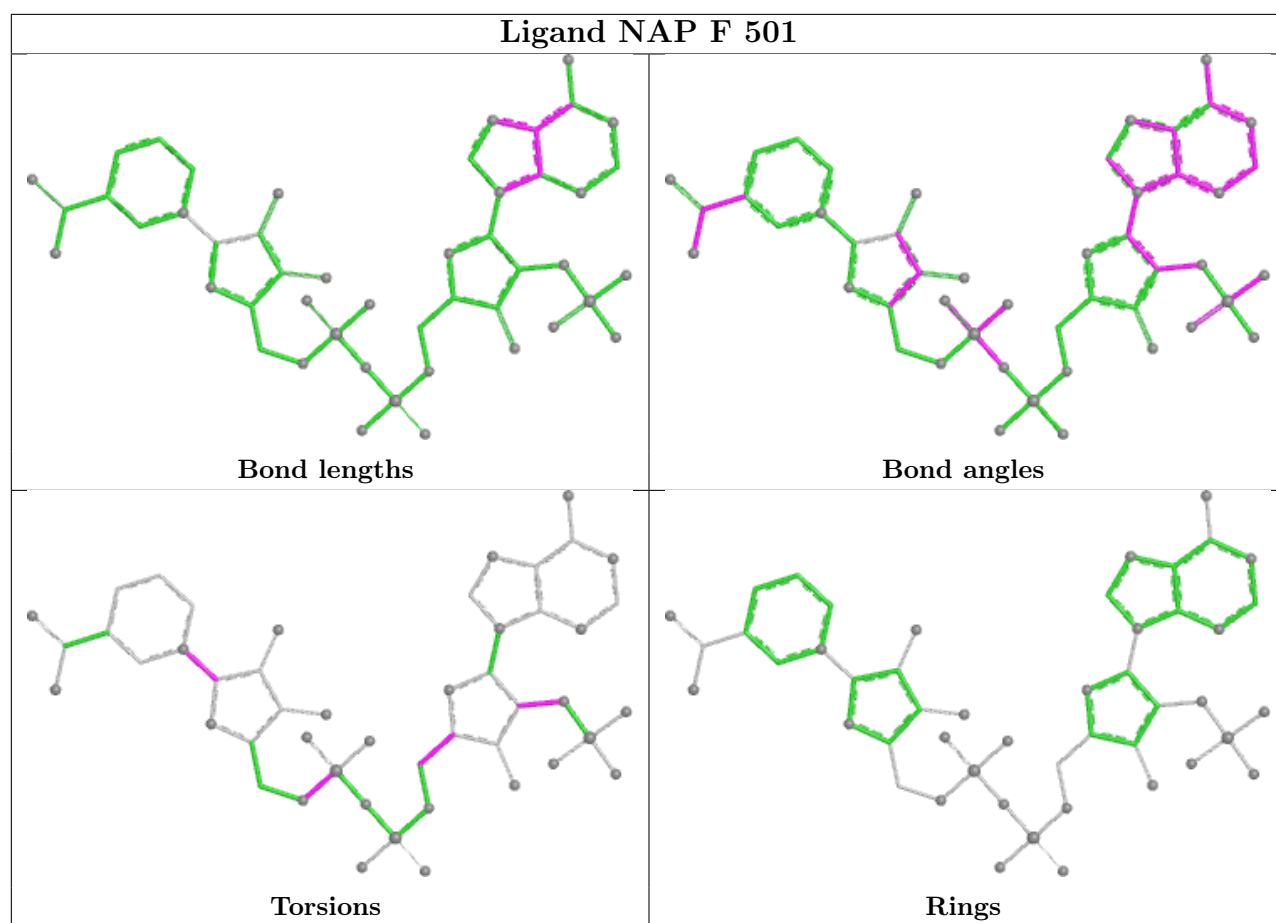


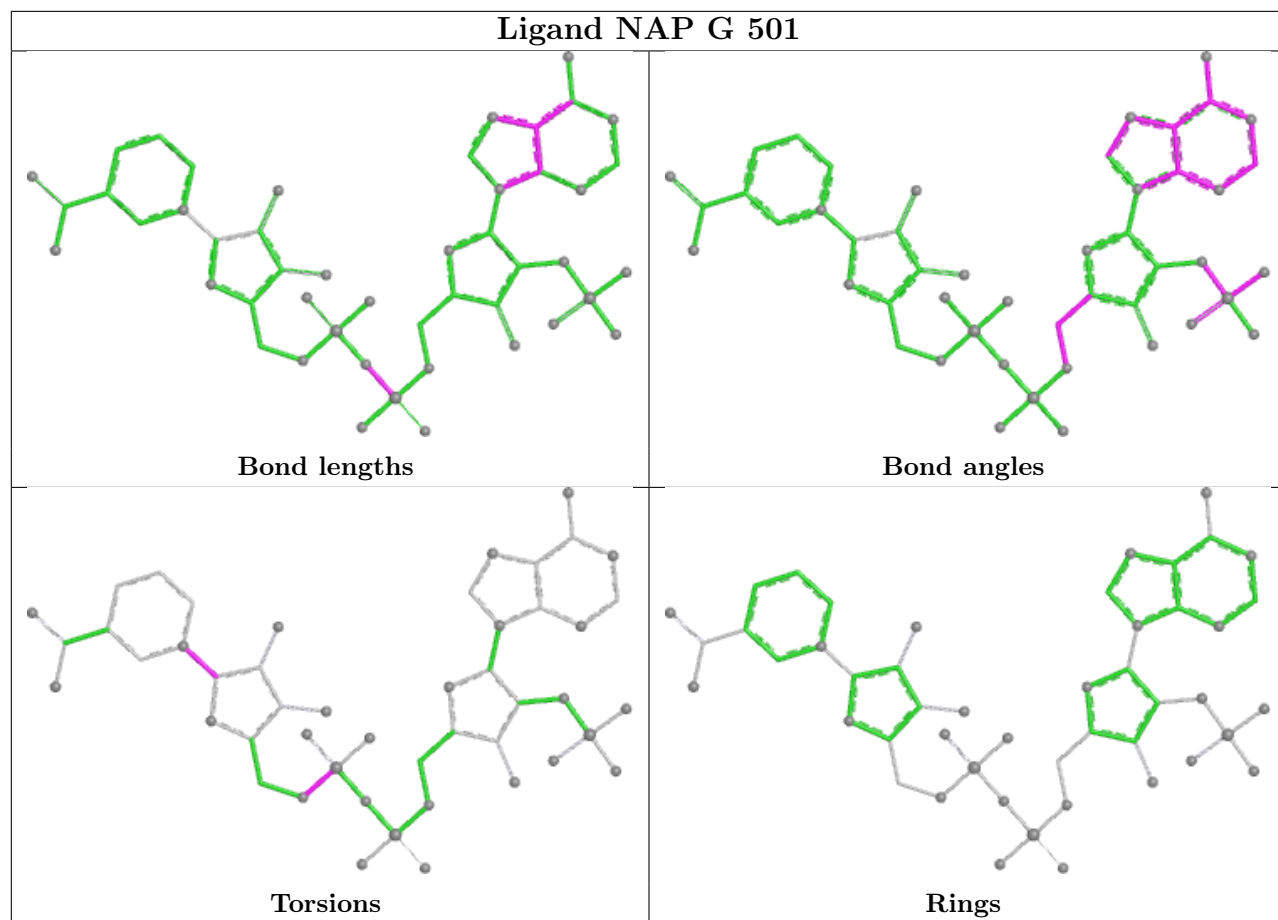


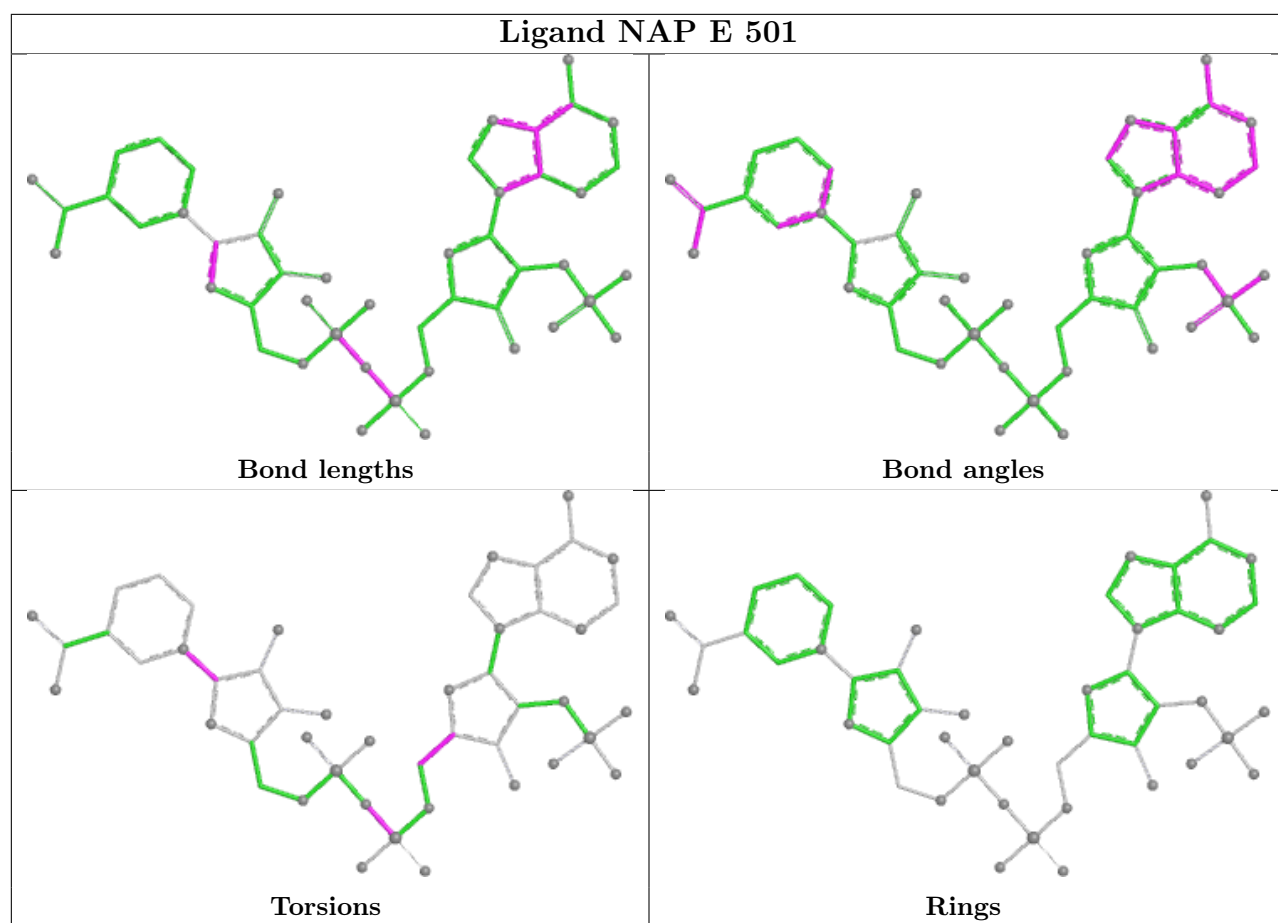












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	413/413 (100%)	-1.71	0 100 100	23, 35, 54, 104	0
1	B	412/413 (99%)	-1.69	0 100 100	23, 36, 59, 84	0
1	C	413/413 (100%)	-1.70	0 100 100	24, 36, 62, 101	0
1	D	413/413 (100%)	-1.72	0 100 100	22, 34, 55, 102	0
1	E	413/413 (100%)	-1.71	0 100 100	21, 33, 55, 81	0
1	F	413/413 (100%)	-1.68	0 100 100	23, 38, 63, 104	0
1	G	413/413 (100%)	-1.69	0 100 100	22, 36, 57, 116	0
1	H	411/413 (99%)	-1.67	0 100 100	26, 42, 68, 142	0
All	All	3301/3304 (99%)	-1.70	0 100 100	21, 36, 60, 142	0

There are no RSRZ outliers to report.

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](#)

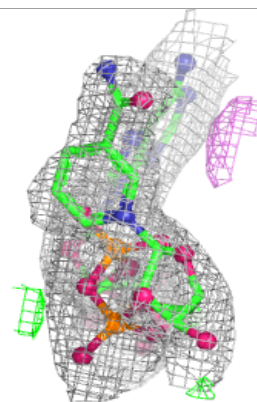
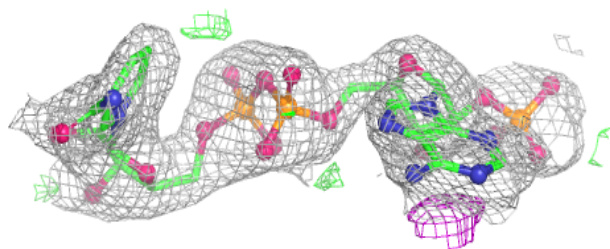
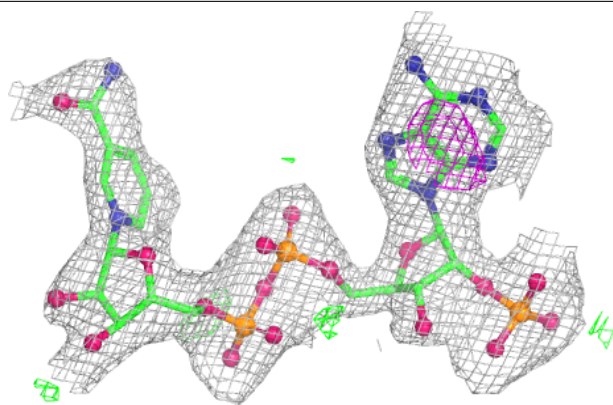
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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
4	ICT	B	503	13/13	0.99	0.03	44,52,56,57	0
4	ICT	D	503	13/13	0.99	0.03	36,44,49,50	0
4	ICT	E	503	13/13	0.99	0.02	32,37,42,45	0
4	ICT	F	503	13/13	0.99	0.03	52,60,65,65	0
4	ICT	G	503	13/13	0.99	0.04	39,44,48,49	0
4	ICT	H	503	13/13	0.99	0.03	39,49,54,60	0
2	NAP	G	501	48/48	1.00	0.02	31,35,40,43	0
2	NAP	H	501	48/48	1.00	0.02	31,41,48,54	0
3	CA	A	502	1/1	1.00	0.01	43,43,43,43	0
3	CA	B	502	1/1	1.00	0.01	36,36,36,36	0
3	CA	C	502	1/1	1.00	0.01	39,39,39,39	0
3	CA	D	502	1/1	1.00	0.01	35,35,35,35	0
3	CA	E	502	1/1	1.00	0.02	40,40,40,40	0
3	CA	F	502	1/1	1.00	0.02	42,42,42,42	0
3	CA	G	502	1/1	1.00	0.02	36,36,36,36	0
3	CA	H	502	1/1	1.00	0.01	44,44,44,44	0
4	ICT	A	503	13/13	1.00	0.02	33,40,49,49	0
2	NAP	A	501	48/48	1.00	0.02	25,29,36,42	0
4	ICT	C	503	13/13	1.00	0.03	34,40,55,58	0
2	NAP	B	501	48/48	1.00	0.02	27,32,45,48	0
2	NAP	C	501	48/48	1.00	0.02	30,36,47,50	0
2	NAP	D	501	48/48	1.00	0.02	21,27,33,33	0
2	NAP	E	501	48/48	1.00	0.02	25,32,38,42	0
2	NAP	F	501	48/48	1.00	0.02	27,32,37,40	0

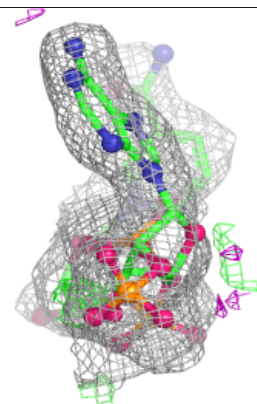
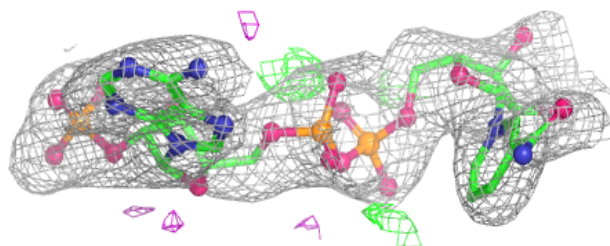
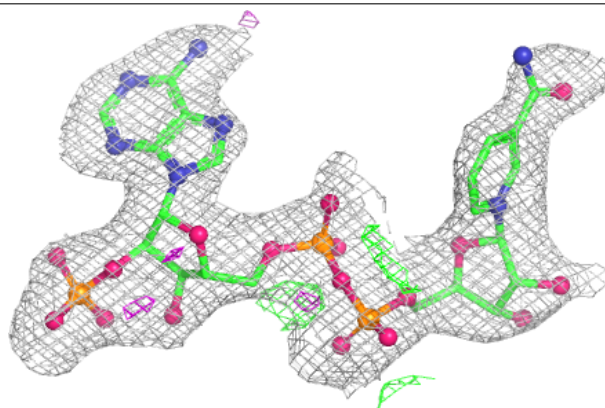
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP G 501:

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

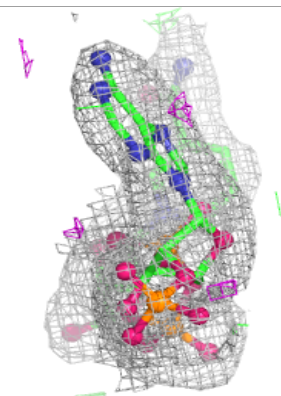
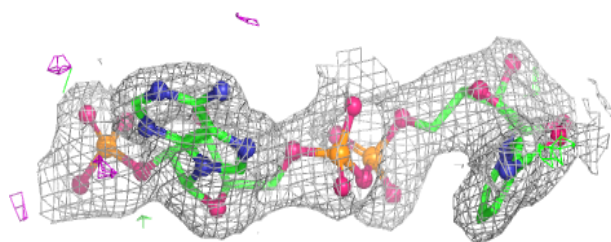
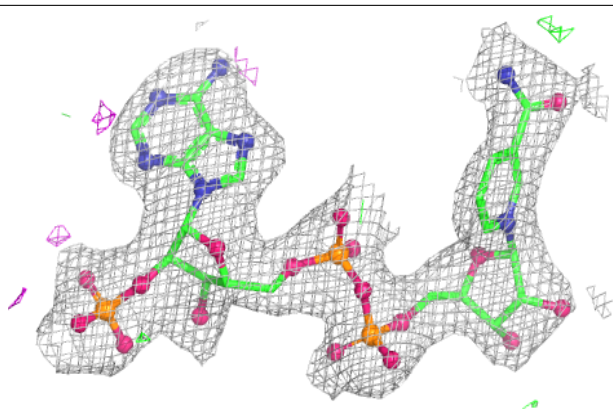
**Electron density around NAP H 501:**

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

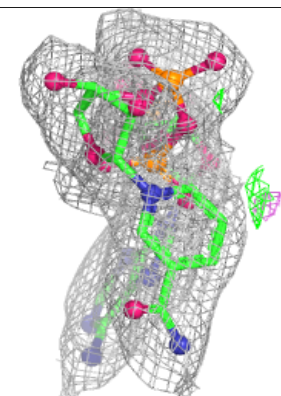
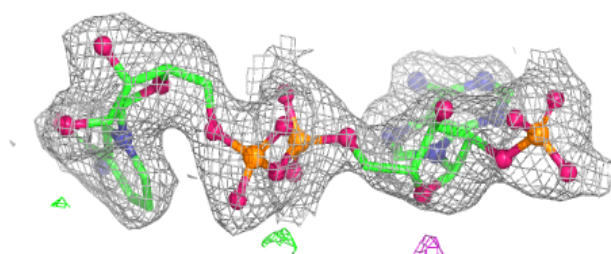
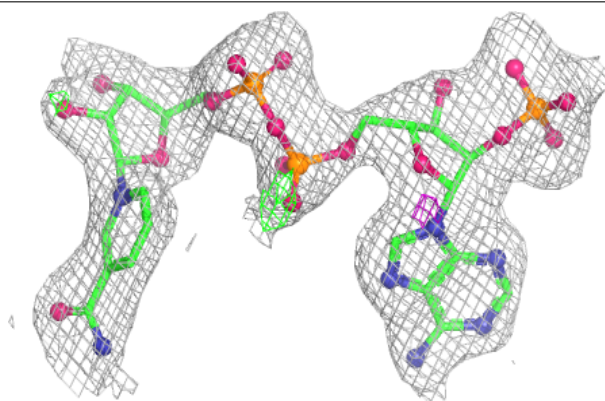


Electron density around NAP A 501:

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

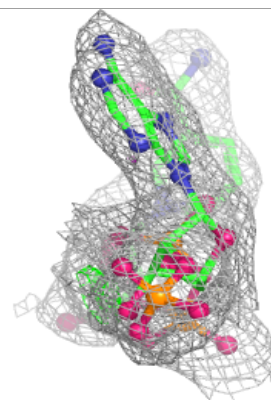
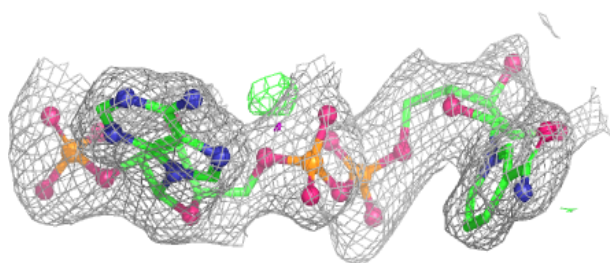
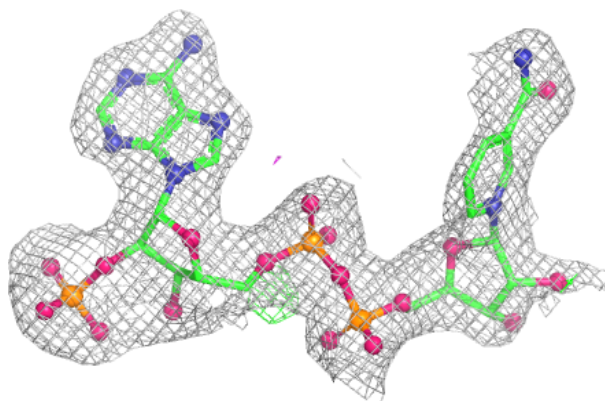
**Electron density around NAP B 501:**

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

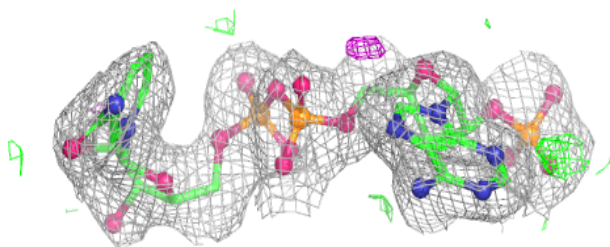
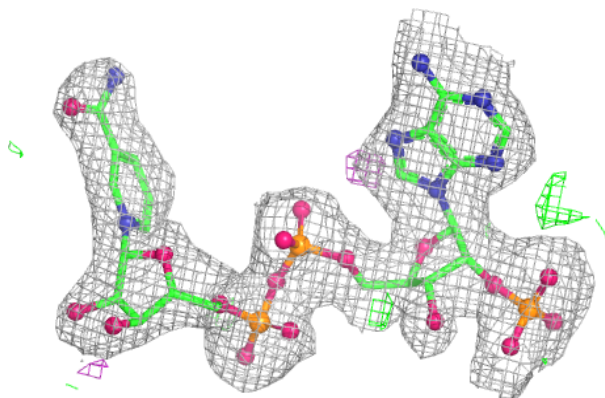


Electron density around NAP C 501:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

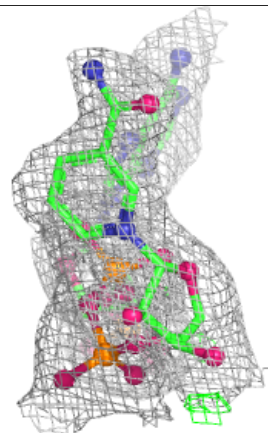
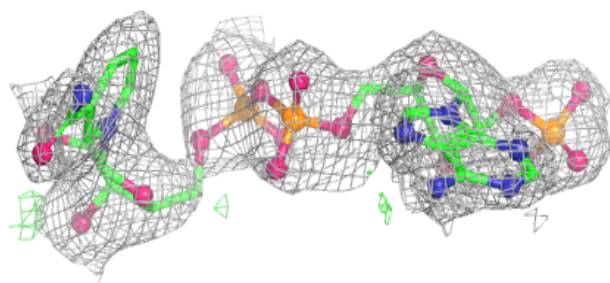
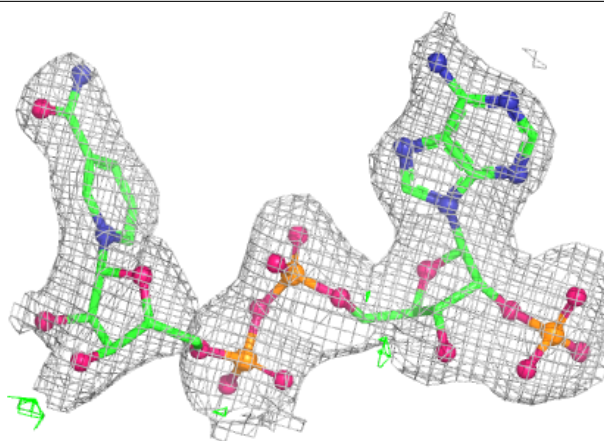
**Electron density around NAP D 501:**

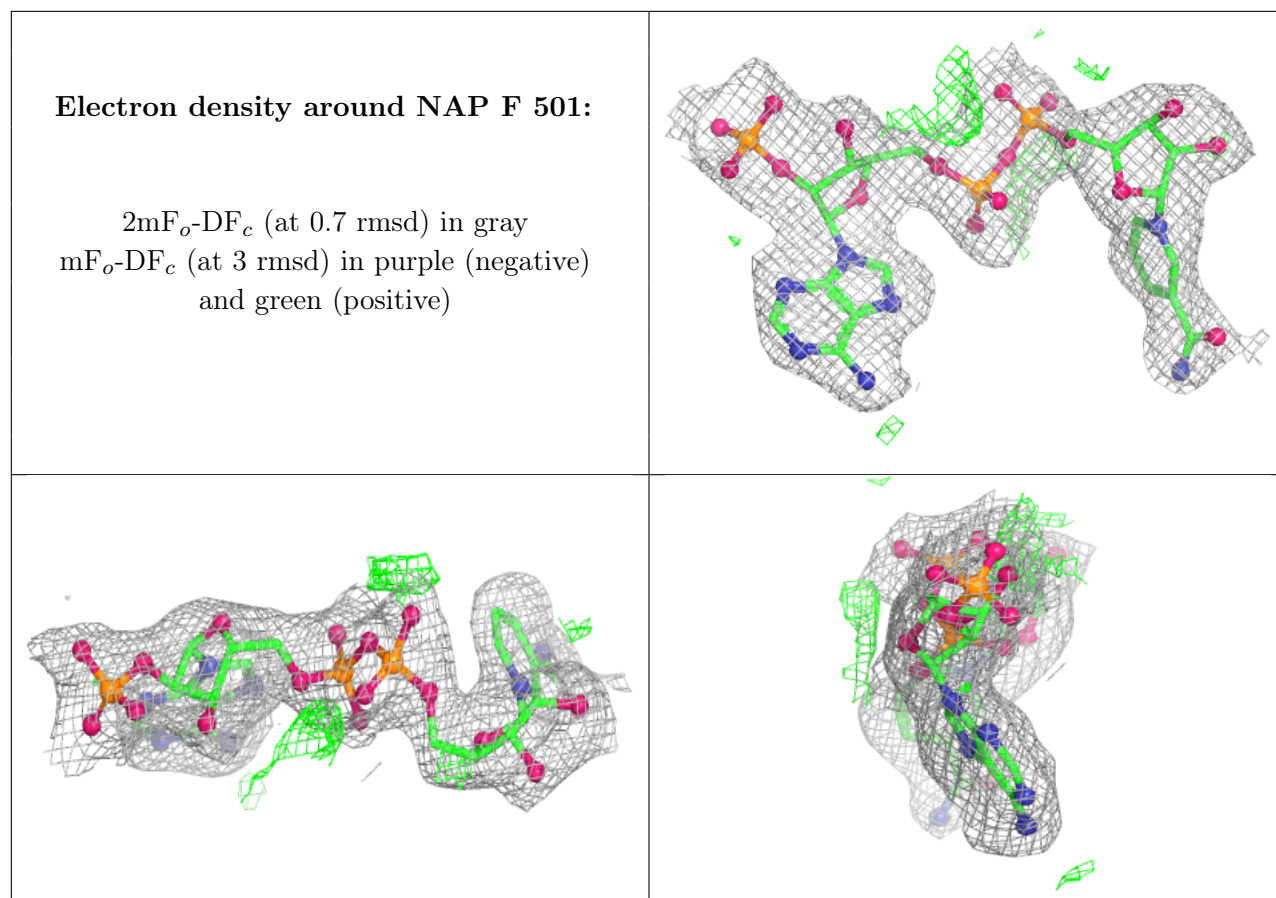
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NAP E 501:

$2mF_o-DF_c$ (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.