



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 11:56 PM UTC

PDB ID : 5IJZ / pdb_00005ijz
Title : Crystal structure of glutamate dehydrogenase(GDH) from Corynebacterium glutamicum
Authors : Son, H.-F.; Kim, K.-J.
Deposited on : 2016-03-03
Resolution : 2.29 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

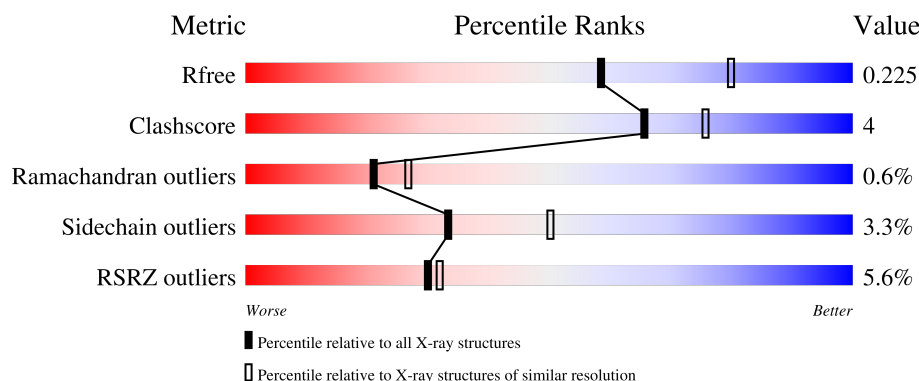
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	447	90% 10%
1	B	447	89% 11%
1	C	447	90% 9% .
1	D	447	% 89% 9% .
1	E	447	91% 9%

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Mol	Chain	Length	Quality of chain
1	F	447	
1	G	447	
1	H	447	
1	I	447	
1	J	447	
1	K	447	
1	L	447	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	AKG	A	502	-	X	-	-
3	AKG	B	502	-	X	-	-
3	AKG	C	502	-	X	-	-
3	AKG	E	502	-	X	-	-
3	AKG	F	502	-	X	-	-
3	AKG	H	502	-	X	-	-
3	AKG	J	502	-	X	-	-

2 Entry composition [i](#)

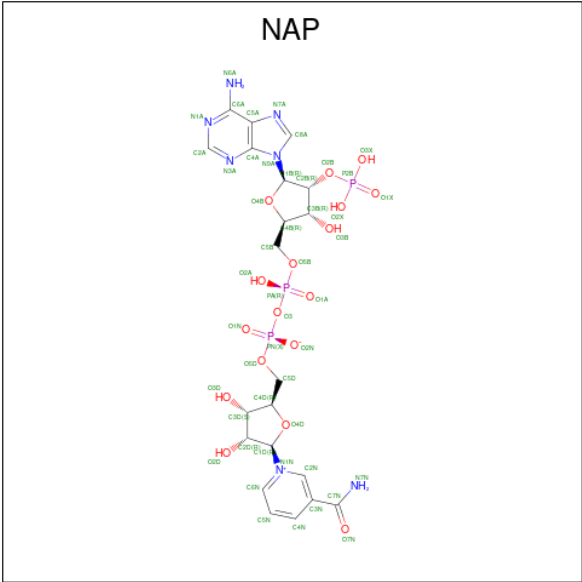
There are 4 unique types of molecules in this entry. The entry contains 42426 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NADP-specific glutamate dehydrogenase.

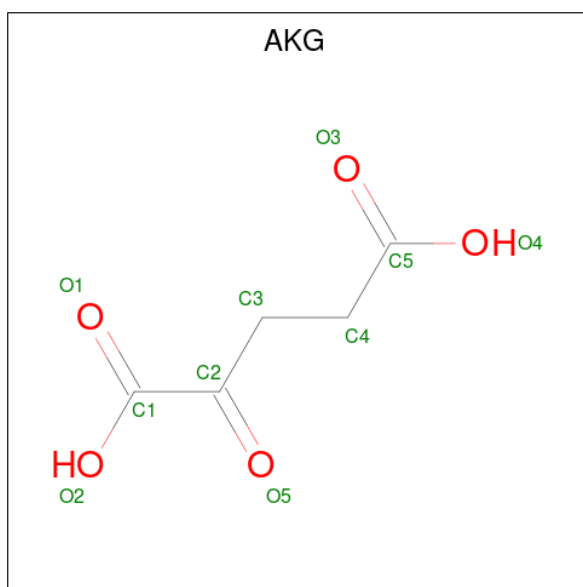
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	0	0	0
			3447	2166	605	659	17			
1	B	447	Total	C	N	O	S	0	0	0
			3447	2166	605	659	17			
1	C	447	Total	C	N	O	S	0	0	0
			3447	2166	605	659	17			
1	D	447	Total	C	N	O	S	0	0	0
			3447	2166	605	659	17			
1	E	447	Total	C	N	O	S	0	0	0
			3447	2166	605	659	17			
1	F	447	Total	C	N	O	S	0	0	0
			3447	2166	605	659	17			
1	G	447	Total	C	N	O	S	0	0	0
			3447	2166	605	659	17			
1	H	447	Total	C	N	O	S	0	0	0
			3447	2166	605	659	17			
1	I	447	Total	C	N	O	S	0	0	0
			3447	2166	605	659	17			
1	J	447	Total	C	N	O	S	0	0	0
			3447	2166	605	659	17			
1	K	304	Total	C	N	O	S	0	0	0
			2358	1495	413	437	13			
1	L	447	Total	C	N	O	S	0	0	0
			3447	2166	605	659	17			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
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		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	J	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: C₅H₆O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	5	5		
3	B	1	Total	C	O	0	0
			10	5	5		
3	C	1	Total	C	O	0	0
			10	5	5		
3	D	1	Total	C	O	0	0
			10	5	5		
3	E	1	Total	C	O	0	0
			10	5	5		
3	F	1	Total	C	O	0	0
			10	5	5		
3	G	1	Total	C	O	0	0
			10	5	5		
3	H	1	Total	C	O	0	0
			10	5	5		
3	J	1	Total	C	O	0	0
			10	5	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	169	Total	O	0	0
			169	169		
4	B	172	Total	O	0	0
			172	172		
4	C	161	Total	O	0	0
			161	161		

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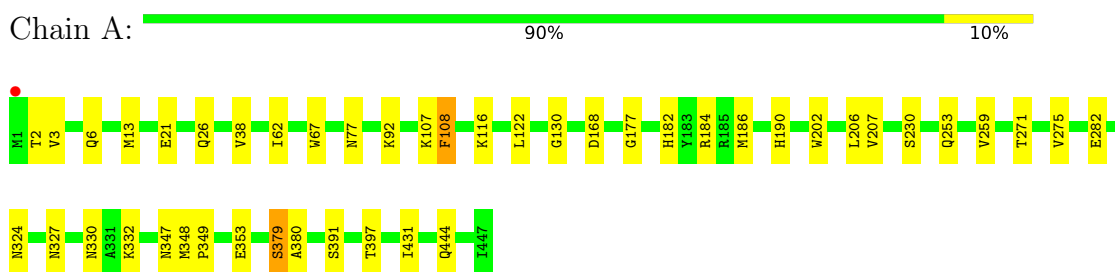
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	172	Total 172	O 172	0	0
4	E	160	Total 160	O 160	0	0
4	F	162	Total 162	O 162	0	0
4	G	149	Total 149	O 149	0	0
4	H	111	Total 111	O 111	0	0
4	I	107	Total 107	O 107	0	0
4	J	68	Total 68	O 68	0	0
4	K	66	Total 66	O 66	0	0
4	L	132	Total 132	O 132	0	0

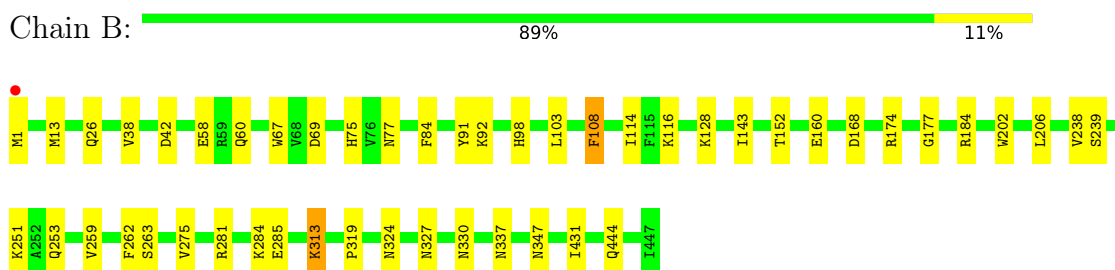
3 Residue-property plots

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.

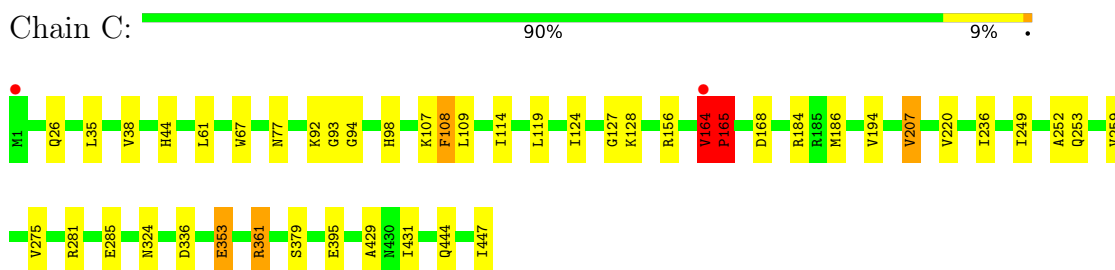
- Molecule 1: NADP-specific glutamate dehydrogenase



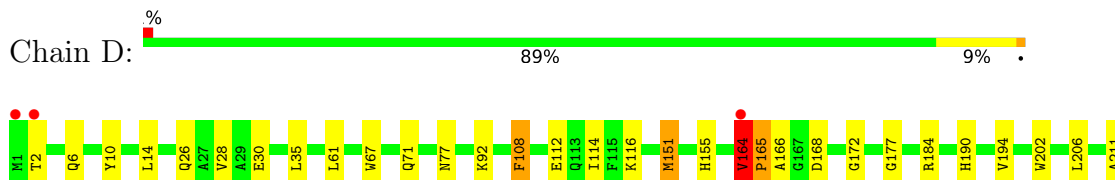
- Molecule 1: NADP-specific glutamate dehydrogenase



- Molecule 1: NADP-specific glutamate dehydrogenase



- Molecule 1: NADP-specific glutamate dehydrogenase

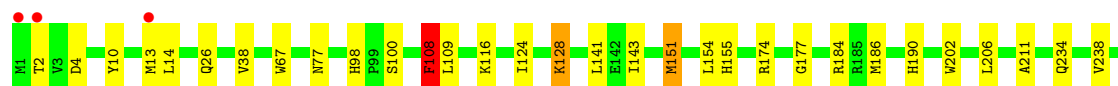
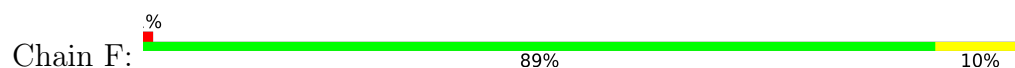




- Molecule 1: NADP-specific glutamate dehydrogenase



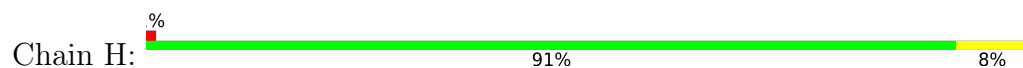
- Molecule 1: NADP-specific glutamate dehydrogenase



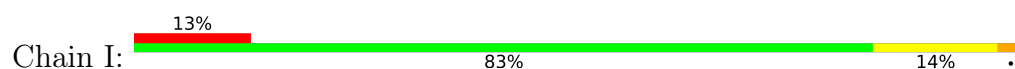
- Molecule 1: NADP-specific glutamate dehydrogenase

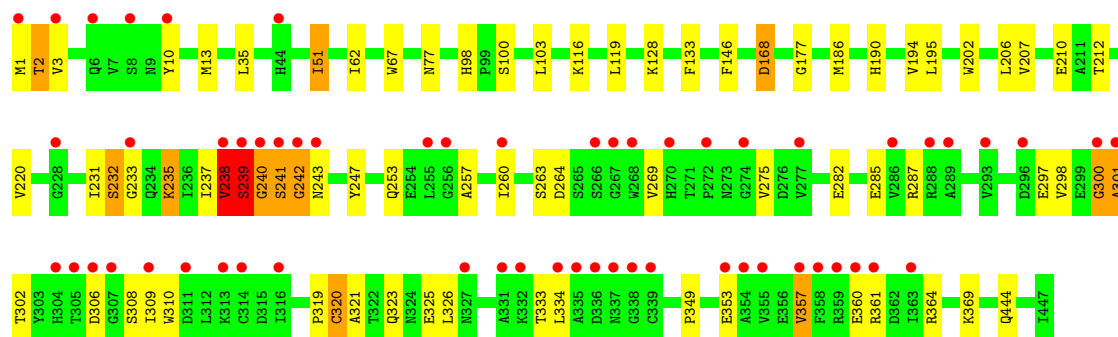


- Molecule 1: NADP-specific glutamate dehydrogenase

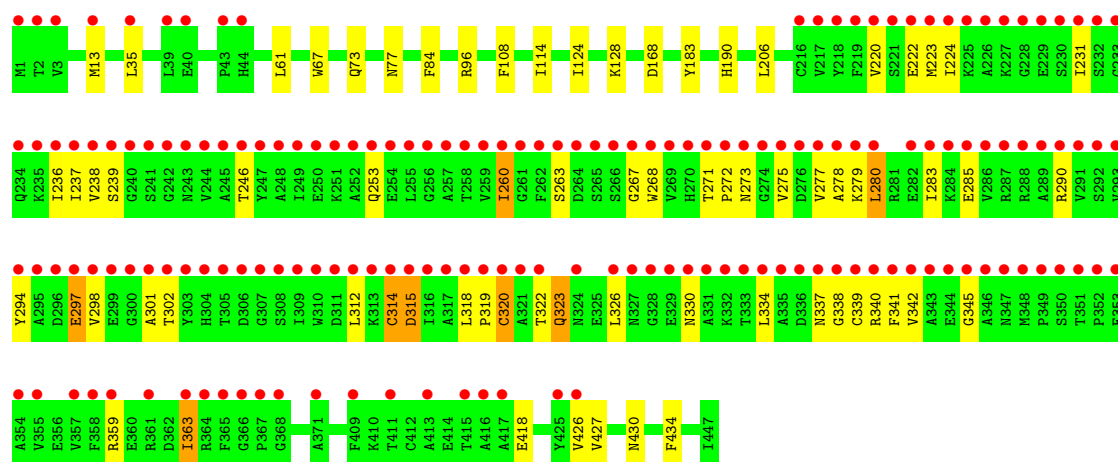
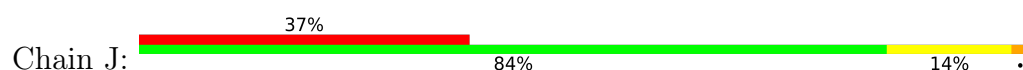


- Molecule 1: NADP-specific glutamate dehydrogenase

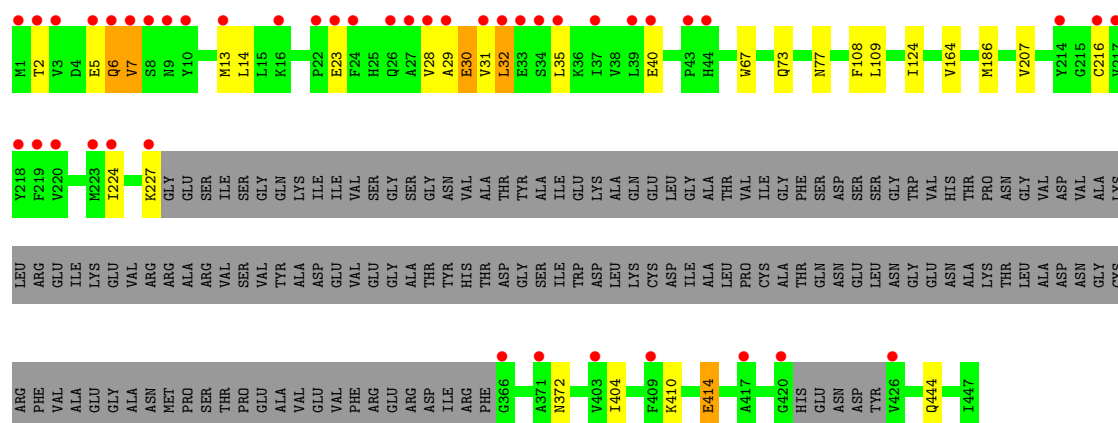




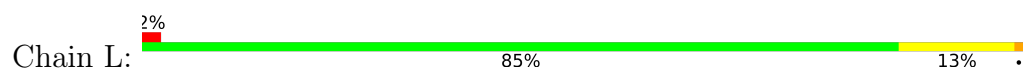
• Molecule 1: NADP-specific glutamate dehydrogenase

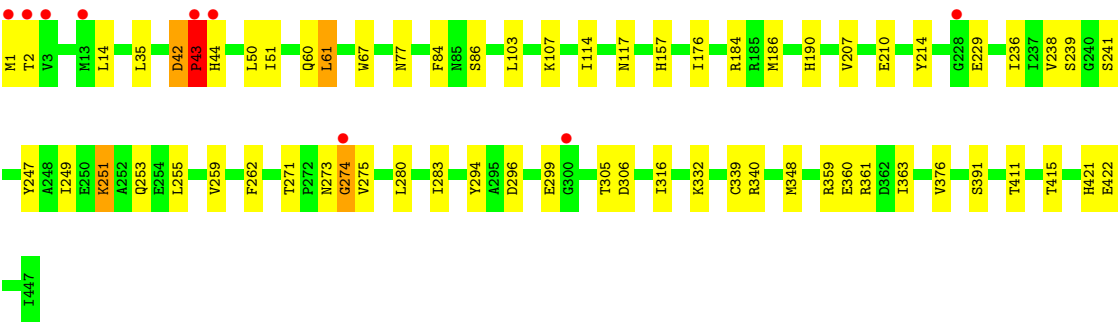


• Molecule 1: NADP-specific glutamate dehydrogenase



• Molecule 1: NADP-specific glutamate dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	171.22Å 93.03Å 187.88Å 90.00° 108.16° 90.00°	Depositor
Resolution (Å)	34.37 – 2.29 34.37 – 2.29	Depositor EDS
% Data completeness (in resolution range)	97.7 (34.37-2.29) 97.7 (34.37-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.20 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.165 , 0.222 0.173 , 0.225	Depositor DCC
R_{free} test set	12145 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 34.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	42426	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, AKG

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	1.09	2/3517 (0.1%)	1.07	1/4748 (0.0%)
1	B	1.07	0/3517	1.10	4/4748 (0.1%)
1	C	1.09	3/3517 (0.1%)	1.09	7/4748 (0.1%)
1	D	1.10	5/3517 (0.1%)	1.11	11/4748 (0.2%)
1	E	1.06	0/3517	1.07	7/4748 (0.1%)
1	F	1.07	3/3517 (0.1%)	1.08	6/4748 (0.1%)
1	G	1.04	2/3517 (0.1%)	1.08	2/4748 (0.0%)
1	H	1.03	1/3517 (0.0%)	1.08	1/4748 (0.0%)
1	I	1.06	3/3517 (0.1%)	1.14	7/4748 (0.1%)
1	J	1.06	1/3517 (0.0%)	1.12	6/4748 (0.1%)
1	K	0.99	0/2407	1.07	2/3239 (0.1%)
1	L	1.01	1/3517 (0.0%)	1.11	10/4748 (0.2%)
All	All	1.06	21/41094 (0.1%)	1.09	64/55467 (0.1%)

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	C	0	2
1	D	0	1
1	I	0	2
1	J	0	1
1	L	0	2
All	All	0	8

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	206	LEU	C-O	9.94	1.35	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	164	VAL	CA-C	8.56	1.61	1.52
1	G	348	MET	C-O	-7.41	1.20	1.23
1	I	242	GLY	N-CA	-6.62	1.38	1.45
1	C	164	VAL	CA-C	6.60	1.59	1.52
1	F	151	MET	SD-CE	-6.45	1.63	1.79
1	D	151	MET	SD-CE	-6.04	1.64	1.79
1	L	274	GLY	N-CA	5.81	1.52	1.45
1	D	356	GLU	C-O	-5.71	1.17	1.24
1	A	271	THR	CA-CB	5.65	1.60	1.53
1	F	206	LEU	C-O	5.61	1.30	1.24
1	D	172	GLY	N-CA	5.54	1.48	1.44
1	F	271	THR	CA-CB	5.52	1.59	1.53
1	C	353	GLU	CD-OE1	5.51	1.35	1.25
1	I	232	SER	CA-C	5.45	1.60	1.52
1	I	212	THR	CA-C	5.45	1.59	1.52
1	C	186	MET	C-O	-5.42	1.17	1.24
1	J	271	THR	CA-C	5.39	1.58	1.52
1	H	446	VAL	C-O	5.20	1.29	1.23
1	G	152	THR	C-O	-5.13	1.18	1.24
1	A	130	GLY	N-CA	-5.11	1.40	1.45

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	164	VAL	CB-CA-C	12.18	133.53	111.36
1	F	206	LEU	N-CA-C	9.85	123.24	111.33
1	H	206	LEU	N-CA-C	9.25	123.59	111.75
1	I	235	LYS	N-CA-C	8.81	122.46	109.07
1	D	164	VAL	O-C-N	-8.70	111.18	121.10
1	C	164	VAL	CA-C-N	8.64	130.64	119.84
1	C	164	VAL	C-N-CA	8.64	130.64	119.84
1	B	206	LEU	N-CA-C	8.51	121.33	111.11
1	B	284	LYS	N-CA-C	8.41	120.53	111.36
1	D	164	VAL	C-N-CD	-8.15	102.67	120.60
1	E	206	LEU	N-CA-C	7.60	120.23	111.11
1	I	232	SER	N-CA-C	7.32	126.39	110.80
1	L	422	GLU	N-CA-C	7.29	121.43	112.54
1	L	42	ASP	CA-C-N	7.04	128.64	119.84
1	L	42	ASP	C-N-CA	7.04	128.64	119.84
1	D	206	LEU	N-CA-C	6.95	118.85	111.28
1	I	206	LEU	N-CA-C	6.78	119.53	111.33
1	D	306	ASP	N-CA-C	-6.70	97.67	109.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	211	ALA	N-CA-C	6.57	118.23	111.14
1	J	206	LEU	CA-C-N	-6.46	112.47	122.09
1	J	206	LEU	C-N-CA	-6.46	112.47	122.09
1	I	320	CYS	N-CA-C	6.35	120.64	112.26
1	L	274	GLY	CA-C-N	6.33	133.09	121.70
1	L	274	GLY	C-N-CA	6.33	133.09	121.70
1	C	165	PRO	N-CA-C	6.24	125.33	112.47
1	C	164	VAL	N-CA-C	6.17	122.20	108.88
1	A	206	LEU	N-CA-C	6.13	121.48	111.37
1	D	164	VAL	CA-C-N	5.91	141.19	127.00
1	D	164	VAL	C-N-CA	5.91	141.19	127.00
1	F	211	ALA	N-CA-C	5.91	117.81	111.36
1	J	271	THR	N-CA-C	5.91	117.80	108.23
1	J	206	LEU	N-CA-C	5.88	118.64	111.82
1	C	114	ILE	CB-CA-C	-5.88	104.36	111.88
1	F	128	LYS	CB-CA-C	-5.84	100.59	109.99
1	C	107	LYS	N-CA-C	5.80	117.60	111.28
1	I	357	VAL	CB-CA-C	-5.74	104.54	111.88
1	D	164	VAL	CA-C-O	-5.67	112.36	119.95
1	E	208	ARG	N-CA-C	5.66	117.45	111.28
1	E	38	VAL	CB-CA-C	-5.64	104.53	112.14
1	E	160	GLU	N-CA-C	5.60	118.11	111.33
1	L	241	SER	CA-C-N	-5.60	112.83	121.45
1	L	241	SER	C-N-CA	-5.60	112.83	121.45
1	L	43	PRO	N-CA-C	5.57	123.95	112.47
1	E	94	GLY	N-CA-C	5.53	121.61	112.66
1	J	267	GLY	N-CA-C	5.51	119.71	110.56
1	E	32	LEU	N-CA-C	5.44	117.20	111.28
1	L	2	THR	N-CA-C	5.35	117.77	110.55
1	I	301	ALA	N-CA-C	5.35	115.19	108.45
1	K	164	VAL	CA-C-N	-5.34	115.27	120.98
1	K	164	VAL	C-N-CA	-5.34	115.27	120.98
1	F	10	TYR	CA-CB-CG	-5.33	104.30	113.90
1	I	239	SER	N-CA-C	5.33	119.65	113.20
1	J	263	SER	N-CA-C	5.29	116.69	109.18
1	D	322	THR	CB-CA-C	-5.27	101.06	111.91
1	B	160	GLU	N-CA-C	5.26	117.70	111.33
1	C	164	VAL	C-N-CD	-5.22	103.60	125.00
1	B	263	SER	N-CA-C	5.20	116.19	108.60
1	L	239	SER	N-CA-C	-5.19	103.18	110.50
1	F	108	PHE	N-CA-C	-5.11	105.60	111.07
1	E	128	LYS	CB-CA-C	-5.08	101.16	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	277	VAL	N-CA-C	5.08	115.81	110.62
1	D	114	ILE	CB-CA-C	-5.08	105.38	111.88
1	F	141	LEU	N-CA-C	5.06	116.80	111.28
1	G	263	SER	N-CA-C	5.01	116.45	108.79

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	164	VAL	Peptide,Mainchain
1	D	306	ASP	Peptide
1	I	238	VAL	Peptide
1	I	301	ALA	Peptide
1	J	314	CYS	Peptide
1	L	273	ASN	Peptide
1	L	421	HIS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3447	0	3356	27	0
1	B	3447	0	3356	27	0
1	C	3447	0	3356	29	0
1	D	3447	0	3356	38	0
1	E	3447	0	3356	18	0
1	F	3447	0	3356	32	0
1	G	3447	0	3356	16	0
1	H	3447	0	3356	23	0
1	I	3447	0	3356	39	0
1	J	3447	0	3356	28	0
1	K	2358	0	2313	15	0
1	L	3447	0	3356	33	0
2	A	48	0	25	0	0
2	B	48	0	25	0	0
2	C	48	0	25	0	0
2	D	48	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	48	0	25	0	0
2	F	48	0	25	0	0
2	G	48	0	25	2	0
2	H	48	0	25	0	0
2	J	48	0	25	0	0
3	A	10	0	4	0	0
3	B	10	0	4	2	0
3	C	10	0	4	1	0
3	D	10	0	4	0	0
3	E	10	0	4	1	0
3	F	10	0	4	0	0
3	G	10	0	4	0	0
3	H	10	0	4	0	0
3	J	10	0	4	1	0
4	A	169	0	0	1	0
4	B	172	0	0	1	0
4	C	161	0	0	7	0
4	D	172	0	0	6	0
4	E	160	0	0	1	0
4	F	162	0	0	2	0
4	G	149	0	0	1	0
4	H	111	0	0	0	0
4	I	107	0	0	1	0
4	J	68	0	0	0	0
4	K	66	0	0	0	0
4	L	132	0	0	1	0
All	All	42426	0	39490	304	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 4.

All (304) 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:164:VAL:O	1:C:194:VAL:O	1.65	1.11
1:D:165:PRO:HA	4:D:601:HOH:O	1.52	1.09
1:D:164:VAL:CA	4:D:601:HOH:O	2.18	0.90
1:C:164:VAL:C	4:C:601:HOH:O	2.18	0.86
1:C:165:PRO:N	4:C:601:HOH:O	2.08	0.86
1:D:165:PRO:CA	4:D:601:HOH:O	2.17	0.83
1:H:269:VAL:HG23	1:H:291:VAL:CG1	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:297:GLU:HB3	1:J:298:VAL:HA	1.60	0.81
1:I:239:SER:OG	1:I:320:CYS:C	2.24	0.81
1:D:253:GLN:HE22	1:D:275:VAL:H	1.31	0.77
1:B:26:GLN:HE22	1:B:324:ASN:HD21	1.32	0.77
1:G:253:GLN:HE22	1:G:275:VAL:H	1.30	0.76
1:G:327:ASN:H	1:G:330:ASN:HD22	1.32	0.75
1:F:151:MET:HE2	1:F:155:HIS:CA	2.18	0.74
1:C:164:VAL:CA	4:C:601:HOH:O	2.35	0.74
1:F:67:TRP:HE1	1:F:77:ASN:HD22	1.36	0.74
1:G:395:GLU:HG2	4:G:709:HOH:O	1.87	0.74
1:G:67:TRP:HE1	1:G:77:ASN:HD22	1.35	0.73
1:F:253:GLN:HE22	1:F:275:VAL:H	1.34	0.73
1:I:353:GLU:O	1:I:357:VAL:HG23	1.89	0.72
1:J:96:ARG:HH12	1:J:323:GLN:HE22	1.34	0.72
1:F:26:GLN:HE22	1:F:324:ASN:HD21	1.36	0.70
1:E:253:GLN:HE22	1:E:275:VAL:H	1.39	0.70
1:D:26:GLN:HE22	1:D:324:ASN:HD21	1.39	0.69
1:E:26:GLN:HE22	1:E:324:ASN:HD21	1.39	0.69
1:F:151:MET:HE2	1:F:155:HIS:N	2.07	0.69
1:F:151:MET:CE	1:F:155:HIS:N	2.55	0.69
1:D:164:VAL:C	4:D:601:HOH:O	2.32	0.69
1:G:26:GLN:HE22	1:G:324:ASN:HD21	1.40	0.68
1:C:253:GLN:HE22	1:C:275:VAL:H	1.41	0.68
1:C:165:PRO:CA	4:C:601:HOH:O	2.40	0.68
1:I:67:TRP:HE1	1:I:77:ASN:HD22	1.42	0.68
1:C:165:PRO:HA	4:C:601:HOH:O	1.94	0.68
1:B:253:GLN:HE22	1:B:275:VAL:H	1.41	0.68
1:I:242:GLY:HA2	1:I:243:ASN:C	2.18	0.67
1:K:410:LYS:O	1:K:414:GLU:HG2	1.94	0.67
1:E:253:GLN:HE21	1:E:259:VAL:H	1.43	0.66
1:H:69:ASP:OD2	1:H:75:HIS:HE1	1.79	0.66
1:H:67:TRP:HE1	1:H:77:ASN:HD22	1.41	0.66
1:L:271:THR:HG21	1:L:275:VAL:HG22	1.77	0.66
1:L:271:THR:OG1	1:L:274:GLY:HA3	1.96	0.66
1:I:238:VAL:HG21	1:I:325:GLU:OE1	1.96	0.66
1:A:67:TRP:HE1	1:A:77:ASN:HD22	1.42	0.65
1:A:253:GLN:HE21	1:A:259:VAL:H	1.43	0.65
1:L:67:TRP:HE1	1:L:77:ASN:HD22	1.44	0.65
1:A:253:GLN:HE22	1:A:275:VAL:H	1.44	0.64
1:E:67:TRP:HE1	1:E:77:ASN:HD22	1.47	0.62
1:I:238:VAL:HG22	1:I:319:PRO:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:GLN:HE22	1:C:324:ASN:HD21	1.47	0.62
1:B:253:GLN:HE21	1:B:259:VAL:H	1.48	0.62
1:D:151:MET:HE1	1:D:155:HIS:HA	1.81	0.61
1:G:253:GLN:HE21	1:G:259:VAL:H	1.48	0.61
1:A:26:GLN:HE22	1:A:324:ASN:HD21	1.48	0.61
1:F:151:MET:HE3	1:F:151:MET:HA	1.83	0.61
1:H:269:VAL:HG23	1:H:291:VAL:HG12	1.83	0.60
1:H:26:GLN:HE22	1:H:324:ASN:HD21	1.50	0.60
1:J:298:VAL:O	1:J:298:VAL:HG13	2.02	0.60
1:B:327:ASN:H	1:B:330:ASN:HD22	1.49	0.60
1:D:190:HIS:HE1	4:D:640:HOH:O	1.84	0.59
1:L:253:GLN:HE22	1:L:275:VAL:H	1.50	0.59
1:A:327:ASN:H	1:A:330:ASN:HD22	1.48	0.59
1:L:190:HIS:HE1	4:L:506:HOH:O	1.86	0.59
1:B:128:LYS:NZ	3:B:502:AKG:O5	2.33	0.59
1:J:67:TRP:HE1	1:J:77:ASN:HD22	1.52	0.58
1:J:320:CYS:SG	1:J:345:GLY:HA3	2.43	0.58
1:K:23:GLU:O	1:K:108:PHE:CD1	2.56	0.58
1:D:151:MET:CE	1:D:155:HIS:CA	2.81	0.58
1:I:98:HIS:HD2	1:I:100:SER:H	1.51	0.58
1:C:67:TRP:HE1	1:C:77:ASN:HD22	1.52	0.58
1:K:28:VAL:O	1:K:32:LEU:HB2	2.03	0.57
1:B:67:TRP:HE1	1:B:77:ASN:HD22	1.53	0.57
1:F:253:GLN:HE21	1:F:259:VAL:H	1.51	0.57
1:C:253:GLN:HE21	1:C:259:VAL:H	1.53	0.57
1:I:10:TYR:O	1:I:13:MET:HB3	2.04	0.57
1:I:241:SER:OG	1:I:242:GLY:N	2.34	0.56
1:B:92:LYS:NZ	3:B:502:AKG:O3	2.36	0.55
1:J:236:ILE:HB	1:J:318:LEU:HD23	1.88	0.55
1:H:253:GLN:HE22	1:H:275:VAL:H	1.53	0.55
1:I:239:SER:O	1:I:240:GLY:C	2.48	0.55
1:D:30:GLU:OE2	1:D:112:GLU:OE2	2.24	0.55
1:L:253:GLN:HE22	1:L:275:VAL:N	2.04	0.55
1:A:184:ARG:HE	1:H:444:GLN:HE22	1.55	0.55
1:K:67:TRP:HE1	1:K:77:ASN:HD22	1.54	0.54
1:J:298:VAL:HG12	1:J:301:ALA:HB2	1.89	0.54
1:H:269:VAL:HG23	1:H:291:VAL:HG13	1.88	0.54
1:B:60:GLN:HE21	1:B:103:LEU:HD11	1.73	0.54
1:K:224:ILE:HA	1:K:227:LYS:HE2	1.89	0.54
1:I:190:HIS:HE1	4:I:501:HOH:O	1.91	0.54
1:J:277:VAL:O	1:J:278:ALA:C	2.49	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:7:VAL:HG13	1:K:32:LEU:HD23	1.89	0.54
1:I:238:VAL:HG13	1:I:310:TRP:CH2	2.43	0.53
1:F:151:MET:HE2	1:F:155:HIS:HA	1.91	0.53
1:I:239:SER:HG	1:I:320:CYS:HB2	1.74	0.53
1:I:239:SER:HB3	1:I:321:ALA:HA	1.90	0.53
1:L:42:ASP:O	1:L:44:HIS:N	2.42	0.53
1:I:35:LEU:HD22	1:I:51:ILE:HG21	1.91	0.53
1:L:411:THR:O	1:L:415:THR:HG23	2.09	0.53
1:K:186:MET:HA	1:K:186:MET:HE2	1.91	0.52
1:H:269:VAL:CG2	1:H:291:VAL:HG13	2.39	0.52
1:L:359:ARG:O	1:L:361:ARG:O	2.28	0.52
1:C:336:ASP:OD1	1:C:361:ARG:NH2	2.34	0.52
1:I:231:ILE:O	1:I:233:GLY:N	2.43	0.52
1:L:61:LEU:HD21	1:L:157:HIS:NE2	2.25	0.52
1:D:67:TRP:HE1	1:D:77:ASN:HD22	1.57	0.51
1:D:92:LYS:HD2	1:D:164:VAL:HB	1.93	0.51
1:L:271:THR:HG21	1:L:275:VAL:CG2	2.40	0.51
1:F:327:ASN:H	1:F:330:ASN:HD22	1.59	0.51
1:E:109:LEU:HB3	1:E:128:LYS:HG3	1.93	0.51
1:L:35:LEU:HD13	1:L:51:ILE:HD11	1.92	0.51
1:E:327:ASN:H	1:E:330:ASN:HD22	1.59	0.51
1:I:287:ARG:NH2	1:I:297:GLU:OE2	2.32	0.50
1:J:297:GLU:N	1:J:297:GLU:OE2	2.44	0.50
1:D:151:MET:HE2	1:D:155:HIS:HB3	1.93	0.50
1:E:184:ARG:HE	1:F:444:GLN:HE22	1.59	0.50
3:J:502:AKG:O2	3:J:502:AKG:H41	2.11	0.50
1:D:116:LYS:NZ	1:D:347:ASN:HD21	2.09	0.50
1:L:271:THR:HG23	1:L:271:THR:O	2.10	0.50
1:I:239:SER:HB3	1:I:321:ALA:CA	2.41	0.50
1:I:128:LYS:NZ	1:I:168:ASP:OD2	2.45	0.50
1:I:207:VAL:O	1:I:207:VAL:HG12	2.12	0.50
1:I:238:VAL:HG12	1:I:309:ILE:HG21	1.93	0.50
1:A:62:ILE:HB	1:L:60:GLN:HB2	1.94	0.49
1:A:67:TRP:HE1	1:A:77:ASN:ND2	2.08	0.49
1:A:182:HIS:CE1	1:A:186:MET:HE3	2.47	0.49
1:I:238:VAL:O	1:I:263:SER:N	2.45	0.49
1:J:246:THR:HG23	1:J:280:LEU:HD12	1.93	0.49
1:F:184:ARG:HH21	1:I:444:GLN:NE2	2.10	0.49
1:L:60:GLN:NE2	1:L:107:LYS:HD2	2.28	0.49
1:D:151:MET:HE3	1:D:155:HIS:N	2.28	0.49
1:J:35:LEU:HD21	1:J:434:PHE:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:238:VAL:O	1:L:262:PHE:HA	2.11	0.49
1:A:444:GLN:NE2	1:G:184:ARG:HH21	2.11	0.49
1:D:151:MET:CE	1:D:155:HIS:HA	2.41	0.49
1:D:151:MET:CE	1:D:155:HIS:N	2.76	0.49
1:H:14:LEU:HD22	1:H:28:VAL:HG11	1.92	0.49
1:D:238:VAL:O	1:D:262:PHE:HA	2.13	0.49
1:I:235:LYS:NZ	1:I:257:ALA:HB1	2.27	0.49
1:B:58:GLU:OE2	1:B:91:TYR:OH	2.27	0.48
1:I:323:GLN:HA	1:I:349:PRO:HA	1.95	0.48
1:D:151:MET:CE	1:D:155:HIS:HB3	2.44	0.48
1:D:253:GLN:HE21	1:D:259:VAL:H	1.62	0.48
1:K:224:ILE:HA	1:K:227:LYS:CE	2.43	0.48
1:B:69:ASP:OD2	1:B:75:HIS:HE1	1.96	0.48
1:F:151:MET:HE3	1:F:154:LEU:HB3	1.94	0.48
1:B:38:VAL:HG23	1:B:431:ILE:HG12	1.96	0.48
1:C:281:ARG:HD2	1:C:285:GLU:OE2	2.14	0.48
1:F:190:HIS:HE1	4:F:616:HOH:O	1.97	0.48
1:K:32:LEU:HD12	1:K:35:LEU:HD22	1.95	0.48
1:J:190:HIS:CD2	1:L:86:SER:O	2.67	0.47
1:C:38:VAL:HG23	1:C:431:ILE:HG12	1.96	0.47
1:F:238:VAL:O	1:F:262:PHE:HA	2.15	0.47
1:A:190:HIS:CD2	1:H:86:SER:O	2.68	0.47
1:A:207:VAL:HG12	1:A:207:VAL:O	2.14	0.47
1:B:313:LYS:HG3	1:B:337:ASN:HB3	1.97	0.47
1:B:444:GLN:HE22	1:D:184:ARG:HE	1.62	0.47
1:B:98:HIS:HE1	4:B:609:HOH:O	1.98	0.47
1:D:151:MET:HE1	1:D:155:HIS:CA	2.44	0.47
1:K:5:GLU:O	1:K:6:GLN:C	2.58	0.47
1:J:84:PHE:CD1	1:J:114:ILE:HD11	2.50	0.46
1:D:151:MET:HE3	1:D:151:MET:O	2.15	0.46
1:J:297:GLU:CB	1:J:298:VAL:HA	2.37	0.46
1:J:238:VAL:HA	1:J:318:LEU:O	2.15	0.46
1:H:238:VAL:O	1:H:262:PHE:HA	2.16	0.46
1:L:42:ASP:N	1:L:43:PRO:CD	2.79	0.46
1:E:184:ARG:HE	1:F:444:GLN:NE2	2.14	0.46
1:E:184:ARG:HH21	1:F:444:GLN:NE2	2.14	0.46
1:G:283:ILE:HG23	1:G:289:ALA:HB3	1.96	0.46
1:K:108:PHE:CD2	1:K:109:LEU:HD23	2.50	0.46
1:L:61:LEU:HD21	1:L:157:HIS:CD2	2.51	0.46
1:B:152:THR:HG23	1:I:186:MET:HE1	1.97	0.46
1:G:152:THR:HG23	1:L:186:MET:HE1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:194:VAL:HG13	1:I:195:LEU:HG	1.98	0.46
1:A:182:HIS:NE2	1:A:186:MET:HE3	2.31	0.46
1:B:108:PHE:CD1	1:B:108:PHE:C	2.93	0.46
1:B:143:ILE:HD13	1:B:174:ARG:NH2	2.31	0.46
1:L:253:GLN:HE21	1:L:259:VAL:H	1.64	0.46
1:H:236:ILE:HD12	1:H:252:ALA:HB1	1.98	0.45
1:A:177:GLY:HA2	1:A:202:TRP:CH2	2.51	0.45
1:E:116:LYS:HZ2	3:E:502:AKG:C1	2.29	0.45
1:J:314:CYS:HB3	1:J:315:ASP:HA	1.97	0.45
1:C:119:LEU:HD11	1:C:429:ALA:HB1	1.97	0.45
1:D:10:TYR:CZ	1:D:14:LEU:HD13	2.51	0.45
1:D:164:VAL:O	1:D:194:VAL:O	2.34	0.45
1:I:133:PHE:HB2	1:I:146:PHE:CZ	2.51	0.45
1:B:60:GLN:HB2	1:E:62:ILE:HB	1.99	0.45
1:D:14:LEU:HD23	1:D:28:VAL:HG11	1.99	0.45
1:L:339:CYS:O	1:L:363:ILE:HD12	2.17	0.45
1:J:298:VAL:HG12	1:J:301:ALA:CB	2.47	0.45
1:K:28:VAL:O	1:K:32:LEU:HD13	2.17	0.45
1:A:21:GLU:CD	1:A:107:LYS:HZ3	2.25	0.45
1:B:444:GLN:NE2	1:D:184:ARG:HH21	2.15	0.45
1:C:92:LYS:HD2	1:C:164:VAL:HB	1.99	0.45
1:H:177:GLY:HA2	1:H:202:TRP:CH2	2.52	0.45
1:L:117:ASN:OD1	1:L:376:VAL:HG21	2.17	0.45
1:L:229:GLU:OE2	1:L:340:ARG:NH1	2.50	0.45
1:A:38:VAL:HG23	1:A:431:ILE:HG12	1.98	0.44
1:F:177:GLY:HA2	1:F:202:TRP:CH2	2.52	0.44
1:I:238:VAL:CG1	1:I:310:TRP:CZ2	3.00	0.44
1:A:92:LYS:HE3	1:A:379:SER:HB3	1.99	0.44
1:D:164:VAL:CB	4:D:601:HOH:O	2.58	0.44
1:D:327:ASN:H	1:D:330:ASN:HD22	1.64	0.44
1:I:298:VAL:O	1:I:300:GLY:N	2.50	0.44
1:I:2:THR:OG1	1:I:3:VAL:N	2.51	0.44
1:E:400:ARG:NH1	4:E:607:HOH:O	2.49	0.44
1:A:444:GLN:HE22	1:G:184:ARG:HE	1.66	0.44
1:J:220:VAL:HG22	1:J:223:MET:HE2	1.99	0.44
1:C:184:ARG:HE	1:D:444:GLN:HE22	1.65	0.44
1:F:151:MET:HE2	1:F:155:HIS:HB3	2.00	0.44
1:J:323:GLN:H	1:J:323:GLN:HE21	1.63	0.44
1:J:330:ASN:O	1:J:334:LEU:N	2.51	0.44
1:C:98:HIS:HE1	4:C:668:HOH:O	2.00	0.44
1:A:190:HIS:HD2	1:H:86:SER:O	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:61:LEU:HD22	1:E:157:HIS:CD2	2.53	0.43
1:F:108:PHE:CD1	1:F:108:PHE:C	2.95	0.43
1:G:242:GLY:HA3	2:G:501:NAP:O5B	2.18	0.43
1:I:237:ILE:O	1:I:238:VAL:C	2.60	0.43
1:D:151:MET:HE2	1:D:155:HIS:CB	2.48	0.43
1:F:151:MET:HE2	1:F:155:HIS:CB	2.47	0.43
1:I:253:GLN:HE22	1:I:275:VAL:H	1.66	0.43
1:E:183:TYR:CD1	1:E:183:TYR:C	2.97	0.43
1:F:98:HIS:HE1	4:F:641:HOH:O	2.00	0.43
1:F:151:MET:CE	1:F:155:HIS:CA	2.94	0.43
1:G:38:VAL:HG23	1:G:431:ILE:HG12	2.00	0.43
1:I:210:GLU:HG3	1:I:247:TYR:CD1	2.53	0.43
1:K:444:GLN:NE2	1:L:184:ARG:HE	2.16	0.43
1:B:84:PHE:CD1	1:B:114:ILE:HD11	2.54	0.43
1:E:30:GLU:OE2	1:E:112:GLU:OE2	2.37	0.43
1:E:108:PHE:CD1	1:E:108:PHE:C	2.96	0.43
1:A:207:VAL:HG23	1:A:397:THR:HB	2.00	0.43
1:D:151:MET:CE	1:D:155:HIS:CB	2.96	0.43
1:F:38:VAL:HG23	1:F:431:ILE:HG12	2.00	0.43
1:C:184:ARG:HE	1:D:444:GLN:NE2	2.17	0.43
1:G:177:GLY:HA2	1:G:202:TRP:CH2	2.54	0.43
1:H:269:VAL:CG2	1:H:291:VAL:CG1	2.87	0.43
1:G:108:PHE:CD1	1:G:108:PHE:C	2.97	0.43
1:H:407:ASN:O	1:H:411:THR:HG23	2.19	0.43
1:J:268:TRP:CZ3	1:J:312:LEU:HD11	2.54	0.43
1:L:84:PHE:CD1	1:L:114:ILE:HD11	2.54	0.43
1:H:108:PHE:CD1	1:H:108:PHE:C	2.96	0.42
1:H:116:LYS:NZ	1:H:347:ASN:HD21	2.17	0.42
1:L:60:GLN:HE21	1:L:103:LEU:HD11	1.84	0.42
1:D:177:GLY:HA2	1:D:202:TRP:CH2	2.54	0.42
1:F:98:HIS:HD2	1:F:100:SER:H	1.67	0.42
1:H:239:SER:OG	1:H:319:PRO:HA	2.20	0.42
1:C:207:VAL:HG12	1:C:207:VAL:O	2.20	0.42
1:E:238:VAL:O	1:E:262:PHE:HA	2.19	0.42
1:A:184:ARG:HE	1:H:444:GLN:NE2	2.16	0.42
1:C:156:ARG:NH2	1:F:186:MET:O	2.52	0.42
1:F:143:ILE:HD13	1:F:174:ARG:NH2	2.34	0.42
1:F:283:ILE:CD1	1:F:294:TYR:HA	2.49	0.42
1:L:249:ILE:HG12	1:L:259:VAL:HG11	2.02	0.42
1:B:281:ARG:HD2	1:B:285:GLU:OE2	2.20	0.42
2:G:501:NAP:O2A	2:G:501:NAP:O1N	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:177:GLY:HA2	1:I:202:TRP:CH2	2.55	0.42
1:L:214:TYR:CD1	1:L:251:LYS:HB2	2.55	0.42
1:D:108:PHE:CD1	1:D:108:PHE:C	2.97	0.42
1:E:86:SER:HB3	1:E:91:TYR:CE1	2.55	0.42
1:J:224:ILE:HG23	1:J:341:PHE:CE2	2.55	0.42
1:B:177:GLY:HA2	1:B:202:TRP:CH2	2.55	0.42
1:C:94:GLY:O	1:C:128:LYS:HD3	2.20	0.42
1:C:236:ILE:HD12	1:C:252:ALA:HB1	2.02	0.42
1:J:183:TYR:CD2	1:J:183:TYR:C	2.97	0.42
1:J:314:CYS:CB	1:J:315:ASP:HA	2.50	0.42
1:J:426:VAL:O	1:J:430:ASN:HB2	2.20	0.42
1:D:71:GLN:N	1:D:71:GLN:CD	2.78	0.42
1:A:190:HIS:HE1	4:A:611:HOH:O	2.01	0.42
1:B:67:TRP:HE1	1:B:77:ASN:ND2	2.16	0.42
1:F:109:LEU:HB3	1:F:128:LYS:HG3	2.02	0.42
1:J:340:ARG:O	1:J:363:ILE:HG23	2.20	0.42
1:L:262:PHE:CE2	1:L:280:LEU:HD13	2.55	0.42
1:B:239:SER:OG	1:B:319:PRO:HA	2.20	0.41
1:C:379:SER:OG	3:C:502:AKG:O4	2.35	0.41
1:C:447:ILE:C	4:C:700:HOH:O	2.62	0.41
1:I:116:LYS:HG3	1:I:369:LYS:O	2.19	0.41
1:H:86:SER:HB3	1:H:91:TYR:CE1	2.56	0.41
1:K:14:LEU:HD13	1:K:28:VAL:HG11	2.02	0.41
1:L:236:ILE:HG12	1:L:316:ILE:HB	2.02	0.41
1:A:116:LYS:NZ	1:A:347:ASN:HD21	2.19	0.41
1:J:314:CYS:HB3	1:J:315:ASP:CA	2.51	0.41
1:C:93:GLY:HA3	1:C:127:GLY:O	2.20	0.41
1:K:29:ALA:O	1:K:30:GLU:C	2.63	0.41
1:C:109:LEU:HB3	1:C:128:LYS:HG3	2.03	0.41
1:D:165:PRO:HB2	1:D:166:ALA:H	1.64	0.41
1:F:2:THR:HG22	1:F:4:ASP:N	2.36	0.41
1:B:238:VAL:O	1:B:262:PHE:HA	2.21	0.41
1:D:348:MET:N	1:D:349:PRO:CD	2.84	0.41
1:I:239:SER:HB3	1:I:321:ALA:HB2	2.03	0.41
1:A:122:LEU:HD13	1:A:380:ALA:HB3	2.03	0.41
1:A:348:MET:N	1:A:349:PRO:CD	2.84	0.41
1:B:116:LYS:NZ	1:B:347:ASN:HD21	2.19	0.41
1:B:184:ARG:HH21	1:C:444:GLN:NE2	2.19	0.41
1:C:249:ILE:HG12	1:C:259:VAL:HG11	2.03	0.41
1:A:108:PHE:CD1	1:A:108:PHE:C	2.98	0.41
1:J:237:ILE:HG22	1:J:260:ILE:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:VAL:CG2	1:A:431:ILE:HG12	2.51	0.40
1:G:86:SER:O	1:H:190:HIS:CD2	2.75	0.40
1:C:108:PHE:CD1	1:C:108:PHE:C	2.99	0.40
1:F:151:MET:CE	1:F:155:HIS:HA	2.51	0.40
1:I:62:ILE:HD11	1:I:103:LEU:HD22	2.03	0.40
1:F:116:LYS:NZ	1:F:347:ASN:HD21	2.19	0.40
1:I:238:VAL:HG11	1:I:310:TRP:CZ2	2.56	0.40
1:L:283:ILE:HD13	1:L:294:TYR:HA	2.04	0.40
1:G:315:ASP:C	1:G:316:ILE:HG13	2.47	0.40
1:L:210:GLU:HG3	1:L:247:TYR:CD1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	445/447 (100%)	435 (98%)	8 (2%)	2 (0%)	30	38
1	B	445/447 (100%)	434 (98%)	10 (2%)	1 (0%)	43	55
1	C	445/447 (100%)	433 (97%)	9 (2%)	3 (1%)	18	23
1	D	445/447 (100%)	435 (98%)	7 (2%)	3 (1%)	18	23
1	E	445/447 (100%)	436 (98%)	8 (2%)	1 (0%)	43	55
1	F	445/447 (100%)	434 (98%)	11 (2%)	0	100	100
1	G	445/447 (100%)	435 (98%)	8 (2%)	2 (0%)	30	38
1	H	445/447 (100%)	437 (98%)	7 (2%)	1 (0%)	43	55
1	I	445/447 (100%)	420 (94%)	19 (4%)	6 (1%)	9	10
1	J	445/447 (100%)	390 (88%)	45 (10%)	10 (2%)	5	4
1	K	298/447 (67%)	283 (95%)	13 (4%)	2 (1%)	18	23
1	L	445/447 (100%)	429 (96%)	14 (3%)	2 (0%)	30	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5193/5364 (97%)	5001 (96%)	159 (3%)	33 (1%)	21	27

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	165	PRO
1	C	207	VAL
1	D	164	VAL
1	D	165	PRO
1	G	207	VAL
1	I	232	SER
1	J	272	PRO
1	J	319	PRO
1	J	337	ASN
1	K	207	VAL
1	L	43	PRO
1	L	207	VAL
1	G	168	ASP
1	I	240	GLY
1	I	300	GLY
1	J	253	GLN
1	E	168	ASP
1	H	168	ASP
1	I	241	SER
1	J	320	CYS
1	K	6	GLN
1	A	168	ASP
1	B	168	ASP
1	J	297	GLU
1	J	338	GLY
1	J	418	GLU
1	C	168	ASP
1	D	168	ASP
1	I	168	ASP
1	J	168	ASP
1	A	3	VAL
1	I	238	VAL
1	J	231	ILE

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	358/358 (100%)	348 (97%)	10 (3%)	38	56
1	B	358/358 (100%)	352 (98%)	6 (2%)	53	72
1	C	358/358 (100%)	349 (98%)	9 (2%)	42	60
1	D	358/358 (100%)	351 (98%)	7 (2%)	48	67
1	E	358/358 (100%)	349 (98%)	9 (2%)	42	60
1	F	358/358 (100%)	350 (98%)	8 (2%)	45	65
1	G	358/358 (100%)	353 (99%)	5 (1%)	59	76
1	H	358/358 (100%)	348 (97%)	10 (3%)	38	56
1	I	358/358 (100%)	337 (94%)	21 (6%)	18	26
1	J	358/358 (100%)	331 (92%)	27 (8%)	12	17
1	K	243/358 (68%)	230 (95%)	13 (5%)	20	30
1	L	358/358 (100%)	343 (96%)	15 (4%)	26	40
All	All	4181/4296 (97%)	4041 (97%)	140 (3%)	33	50

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	6	GLN
1	A	13	MET
1	A	108	PHE
1	A	230	SER
1	A	282	GLU
1	A	332	LYS
1	A	353	GLU
1	A	379	SER
1	A	391	SER
1	B	1	MET
1	B	13	MET
1	B	42	ASP
1	B	108	PHE

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Mol	Chain	Res	Type
1	B	251	LYS
1	B	313	LYS
1	C	35	LEU
1	C	44	HIS
1	C	61	LEU
1	C	108	PHE
1	C	124	ILE
1	C	220	VAL
1	C	353	GLU
1	C	361	ARG
1	C	395	GLU
1	D	2	THR
1	D	6	GLN
1	D	35	LEU
1	D	61	LEU
1	D	108	PHE
1	D	306	ASP
1	D	329	GLU
1	E	2	THR
1	E	13	MET
1	E	14	LEU
1	E	40	GLU
1	E	108	PHE
1	E	234	GLN
1	E	235	LYS
1	E	359	ARG
1	E	399	GLU
1	F	13	MET
1	F	14	LEU
1	F	108	PHE
1	F	124	ILE
1	F	234	GLN
1	F	391	SER
1	F	395	GLU
1	F	410	LYS
1	G	50	LEU
1	G	108	PHE
1	G	124	ILE
1	G	391	SER
1	G	410	LYS
1	H	14	LEU
1	H	38	VAL

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Mol	Chain	Res	Type
1	H	40	GLU
1	H	108	PHE
1	H	124	ILE
1	H	230	SER
1	H	333	THR
1	H	353	GLU
1	H	391	SER
1	H	411	THR
1	I	1	MET
1	I	2	THR
1	I	51	ILE
1	I	119	LEU
1	I	220	VAL
1	I	238	VAL
1	I	239	SER
1	I	260	ILE
1	I	264	ASP
1	I	269	VAL
1	I	282	GLU
1	I	285	GLU
1	I	302	THR
1	I	306	ASP
1	I	308	SER
1	I	326	LEU
1	I	333	THR
1	I	334	LEU
1	I	360	GLU
1	I	361	ARG
1	I	364	ARG
1	J	13	MET
1	J	61	LEU
1	J	73	GLN
1	J	108	PHE
1	J	124	ILE
1	J	128	LYS
1	J	222	GLU
1	J	239	SER
1	J	260	ILE
1	J	273	ASN
1	J	275	VAL
1	J	279	LYS
1	J	280	LEU

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Mol	Chain	Res	Type
1	J	283	ILE
1	J	285	GLU
1	J	290	ARG
1	J	294	TYR
1	J	302	THR
1	J	315	ASP
1	J	322	THR
1	J	323	GLN
1	J	326	LEU
1	J	339	CYS
1	J	342	VAL
1	J	359	ARG
1	J	363	ILE
1	J	427	VAL
1	K	2	THR
1	K	7	VAL
1	K	13	MET
1	K	30	GLU
1	K	31	VAL
1	K	32	LEU
1	K	40	GLU
1	K	73	GLN
1	K	124	ILE
1	K	216	CYS
1	K	372	ASN
1	K	404	ILE
1	K	414	GLU
1	L	1	MET
1	L	14	LEU
1	L	50	LEU
1	L	61	LEU
1	L	176	ILE
1	L	251	LYS
1	L	255	LEU
1	L	296	ASP
1	L	299	GLU
1	L	305	THR
1	L	306	ASP
1	L	332	LYS
1	L	348	MET
1	L	360	GLU
1	L	391	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (129) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	75	HIS
1	A	77	ASN
1	A	188	ASN
1	A	190	HIS
1	A	234	GLN
1	A	243	ASN
1	A	253	GLN
1	A	324	ASN
1	A	330	ASN
1	A	347	ASN
1	A	384	GLN
1	A	423	ASN
1	A	444	GLN
1	B	60	GLN
1	B	75	HIS
1	B	77	ASN
1	B	98	HIS
1	B	155	HIS
1	B	190	HIS
1	B	234	GLN
1	B	253	GLN
1	B	324	ASN
1	B	330	ASN
1	B	347	ASN
1	B	423	ASN
1	B	444	GLN
1	C	75	HIS
1	C	77	ASN
1	C	98	HIS
1	C	190	HIS
1	C	243	ASN
1	C	253	GLN
1	C	324	ASN
1	C	330	ASN
1	C	347	ASN
1	C	384	GLN
1	C	444	GLN
1	D	60	GLN
1	D	75	HIS
1	D	77	ASN

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Mol	Chain	Res	Type
1	D	98	HIS
1	D	155	HIS
1	D	190	HIS
1	D	253	GLN
1	D	324	ASN
1	D	347	ASN
1	D	423	ASN
1	D	444	GLN
1	E	75	HIS
1	E	77	ASN
1	E	98	HIS
1	E	190	HIS
1	E	253	GLN
1	E	324	ASN
1	E	330	ASN
1	E	347	ASN
1	E	423	ASN
1	E	444	GLN
1	F	75	HIS
1	F	77	ASN
1	F	98	HIS
1	F	155	HIS
1	F	190	HIS
1	F	253	GLN
1	F	270	HIS
1	F	324	ASN
1	F	330	ASN
1	F	347	ASN
1	F	444	GLN
1	G	26	GLN
1	G	75	HIS
1	G	77	ASN
1	G	98	HIS
1	G	243	ASN
1	G	253	GLN
1	G	330	ASN
1	G	347	ASN
1	G	384	GLN
1	G	444	GLN
1	H	25	HIS
1	H	75	HIS
1	H	77	ASN

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Mol	Chain	Res	Type
1	H	98	HIS
1	H	155	HIS
1	H	188	ASN
1	H	190	HIS
1	H	253	GLN
1	H	324	ASN
1	H	330	ASN
1	H	347	ASN
1	H	444	GLN
1	I	60	GLN
1	I	75	HIS
1	I	77	ASN
1	I	98	HIS
1	I	188	ASN
1	I	190	HIS
1	I	253	GLN
1	I	384	GLN
1	I	444	GLN
1	J	75	HIS
1	J	77	ASN
1	J	98	HIS
1	J	155	HIS
1	J	190	HIS
1	J	243	ASN
1	J	270	HIS
1	J	323	GLN
1	J	324	ASN
1	J	423	ASN
1	J	444	GLN
1	K	60	GLN
1	K	75	HIS
1	K	77	ASN
1	K	98	HIS
1	K	190	HIS
1	K	407	ASN
1	K	444	GLN
1	L	60	GLN
1	L	75	HIS
1	L	77	ASN
1	L	98	HIS
1	L	190	HIS
1	L	243	ASN

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Mol	Chain	Res	Type
1	L	253	GLN
1	L	384	GLN
1	L	402	GLN
1	L	444	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

18 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	501	-	50,52,52	1.68	7 (14%)	71,80,80	2.07	15 (21%)
2	NAP	C	501	-	50,52,52	1.80	7 (14%)	71,80,80	2.28	18 (25%)
2	NAP	B	501	-	50,52,52	1.89	10 (20%)	71,80,80	1.81	11 (15%)
2	NAP	G	501	-	50,52,52	2.91	7 (14%)	71,80,80	2.93	22 (30%)
3	AKG	D	502	-	9,9,9	1.70	1 (11%)	11,11,11	2.31	4 (36%)
2	NAP	E	501	-	50,52,52	2.06	8 (16%)	71,80,80	2.06	17 (23%)
3	AKG	B	502	-	9,9,9	2.24	4 (44%)	11,11,11	2.03	4 (36%)
3	AKG	C	502	-	9,9,9	1.94	2 (22%)	11,11,11	2.27	3 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AKG	G	502	-	9,9,9	2.36	2 (22%)	11,11,11	1.84	3 (27%)
3	AKG	E	502	-	9,9,9	2.17	2 (22%)	11,11,11	2.55	6 (54%)
2	NAP	F	501	-	50,52,52	1.96	8 (16%)	71,80,80	1.88	14 (19%)
2	NAP	D	501	-	50,52,52	2.03	11 (22%)	71,80,80	2.13	16 (22%)
3	AKG	F	502	-	9,9,9	1.62	1 (11%)	11,11,11	3.22	7 (63%)
2	NAP	J	501	-	50,52,52	2.19	11 (22%)	71,80,80	2.10	11 (15%)
2	NAP	H	501	-	50,52,52	2.01	9 (18%)	71,80,80	2.22	22 (30%)
3	AKG	A	502	-	9,9,9	2.19	2 (22%)	11,11,11	3.37	5 (45%)
3	AKG	H	502	-	9,9,9	2.21	1 (11%)	11,11,11	3.47	7 (63%)
3	AKG	J	502	-	9,9,9	1.63	2 (22%)	11,11,11	2.03	5 (45%)

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	501	-	-	4/35/67/67	0/5/5/5
2	NAP	C	501	-	-	3/35/67/67	0/5/5/5
2	NAP	B	501	-	-	6/35/67/67	0/5/5/5
2	NAP	G	501	-	-	8/35/67/67	0/5/5/5
3	AKG	D	502	-	-	2/9/9/9	-
2	NAP	E	501	-	-	5/35/67/67	0/5/5/5
3	AKG	B	502	-	-	4/9/9/9	-
3	AKG	C	502	-	-	7/9/9/9	-
3	AKG	G	502	-	-	6/9/9/9	-
3	AKG	E	502	-	-	6/9/9/9	-
2	NAP	F	501	-	-	6/35/67/67	0/5/5/5
2	NAP	D	501	-	-	3/35/67/67	0/5/5/5
3	AKG	F	502	-	-	8/9/9/9	-
2	NAP	J	501	-	-	10/35/67/67	0/5/5/5
2	NAP	H	501	-	-	4/35/67/67	0/5/5/5
3	AKG	A	502	-	-	6/9/9/9	-
3	AKG	H	502	-	-	4/9/9/9	-
3	AKG	J	502	-	-	7/9/9/9	-

All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	501	NAP	PA-O3	15.17	1.75	1.59
2	E	501	NAP	C4N-C3N	9.71	1.54	1.39
2	F	501	NAP	C4N-C3N	8.90	1.52	1.39
2	H	501	NAP	C4N-C3N	8.64	1.52	1.39
2	J	501	NAP	C4N-C3N	8.64	1.52	1.39
2	B	501	NAP	C4N-C3N	8.48	1.52	1.39
2	D	501	NAP	C4N-C3N	8.42	1.52	1.39
2	G	501	NAP	C4N-C3N	8.10	1.51	1.39
2	C	501	NAP	C4N-C3N	7.81	1.51	1.39
2	A	501	NAP	C4N-C3N	7.58	1.50	1.39
3	G	502	AKG	C2-C1	-6.11	1.44	1.53
3	H	502	AKG	C2-C1	-5.74	1.44	1.53
2	J	501	NAP	C5A-C4A	5.51	1.48	1.39
2	J	501	NAP	PA-O3	5.49	1.65	1.59
3	E	502	AKG	C2-C1	-5.42	1.45	1.53
3	A	502	AKG	C2-C1	-5.32	1.45	1.53
2	F	501	NAP	C5A-C4A	4.99	1.48	1.39
2	J	501	NAP	PN-O3	4.93	1.64	1.59
3	B	502	AKG	C2-C1	-4.79	1.46	1.53
2	G	501	NAP	C5A-C4A	4.54	1.47	1.39
2	E	501	NAP	C5A-C4A	4.48	1.47	1.39
2	H	501	NAP	C5N-C4N	4.47	1.46	1.38
2	G	501	NAP	C5N-C4N	4.40	1.46	1.38
2	C	501	NAP	C5A-C4A	4.39	1.46	1.39
2	D	501	NAP	PN-O3	4.39	1.64	1.59
2	H	501	NAP	C5A-C4A	4.37	1.46	1.39
2	C	501	NAP	C5N-C4N	4.37	1.46	1.38
3	D	502	AKG	C2-C1	-4.36	1.46	1.53
2	B	501	NAP	C5A-C4A	4.35	1.46	1.39
2	G	501	NAP	O4D-C1D	4.34	1.46	1.40
2	J	501	NAP	C5N-C4N	4.29	1.46	1.38
3	C	502	AKG	C2-C1	-4.27	1.47	1.53
2	D	501	NAP	PA-O3	4.21	1.64	1.59
2	H	501	NAP	PN-O3	4.12	1.63	1.59
2	E	501	NAP	C5N-C4N	4.08	1.45	1.38
2	B	501	NAP	C4A-N9A	-4.05	1.29	1.37
2	D	501	NAP	C5N-C4N	4.01	1.45	1.38
2	A	501	NAP	C5N-C4N	3.88	1.45	1.38
2	H	501	NAP	PA-O3	3.71	1.63	1.59
2	G	501	NAP	PN-O3	-3.70	1.55	1.59
2	A	501	NAP	C5A-C4A	3.59	1.45	1.39
2	D	501	NAP	C8A-N7A	3.57	1.38	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	501	NAP	C5A-C6A	3.57	1.50	1.41
2	F	501	NAP	C4A-N9A	-3.56	1.30	1.37
2	B	501	NAP	C5N-C4N	3.54	1.45	1.38
2	H	501	NAP	C5A-C6A	3.50	1.50	1.41
2	F	501	NAP	C5N-C4N	3.49	1.44	1.38
3	F	502	AKG	C2-C1	-3.47	1.48	1.53
2	D	501	NAP	P2B-O2B	3.45	1.65	1.59
2	E	501	NAP	C8A-N7A	3.27	1.38	1.31
2	D	501	NAP	C5A-C4A	3.25	1.44	1.39
2	B	501	NAP	PN-O3	3.16	1.62	1.59
2	C	501	NAP	C2A-N1A	3.02	1.39	1.33
2	E	501	NAP	C5A-C6A	2.98	1.49	1.41
3	J	502	AKG	C2-C1	-2.98	1.49	1.53
2	F	501	NAP	O4D-C1D	2.96	1.44	1.40
2	F	501	NAP	C8A-N7A	2.96	1.37	1.31
2	H	501	NAP	C4A-N3A	2.86	1.39	1.34
2	J	501	NAP	C8A-N7A	2.82	1.37	1.31
2	E	501	NAP	P2B-O2B	2.80	1.64	1.59
2	F	501	NAP	PA-O3	2.79	1.62	1.59
3	A	502	AKG	C3-C2	-2.73	1.48	1.51
2	E	501	NAP	C5A-N7A	-2.71	1.34	1.39
2	E	501	NAP	C4A-N9A	-2.62	1.32	1.37
2	D	501	NAP	C4A-N3A	2.59	1.39	1.34
2	H	501	NAP	C8A-N7A	2.56	1.36	1.31
2	B	501	NAP	C2N-N1N	-2.54	1.32	1.35
2	A	501	NAP	PA-O3	2.44	1.62	1.59
3	G	502	AKG	O4-C5	-2.41	1.22	1.30
2	C	501	NAP	PA-O3	2.41	1.62	1.59
2	A	501	NAP	C4A-N9A	-2.40	1.32	1.37
3	C	502	AKG	O1-C1	2.39	1.28	1.22
2	F	501	NAP	C2N-N1N	-2.39	1.32	1.35
3	B	502	AKG	O1-C1	2.38	1.28	1.22
2	J	501	NAP	O4D-C1D	2.35	1.44	1.40
2	B	501	NAP	PA-O3	2.34	1.62	1.59
2	C	501	NAP	C4A-N9A	-2.30	1.32	1.37
2	B	501	NAP	C5A-N7A	-2.30	1.34	1.39
2	D	501	NAP	C5A-C6A	2.30	1.47	1.41
2	J	501	NAP	P2B-O2B	2.29	1.63	1.59
3	B	502	AKG	O4-C5	-2.28	1.23	1.30
3	B	502	AKG	C4-C5	-2.26	1.45	1.50
2	G	501	NAP	C8A-N7A	2.24	1.36	1.31
2	C	501	NAP	C2A-N3A	2.22	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	NAP	O4D-C1D	2.17	1.43	1.40
2	A	501	NAP	C5A-N7A	-2.16	1.35	1.39
2	H	501	NAP	C2A-N1A	2.13	1.37	1.33
3	J	502	AKG	O4-C5	-2.12	1.23	1.30
2	B	501	NAP	O4D-C1D	2.10	1.43	1.40
2	A	501	NAP	C3N-C7N	-2.07	1.47	1.50
2	B	501	NAP	C8A-N7A	2.06	1.35	1.31
2	J	501	NAP	C1B-N9A	2.05	1.52	1.46
2	D	501	NAP	C2N-N1N	-2.05	1.32	1.35
3	E	502	AKG	C3-C2	-2.03	1.48	1.51
2	J	501	NAP	C4A-N3A	2.01	1.38	1.34

All (190) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	501	NAP	O3-PN-O1N	-10.84	78.10	110.70
2	G	501	NAP	O2A-PA-O3	8.95	131.47	107.27
2	B	501	NAP	C5N-C4N-C3N	-8.89	111.63	120.36
2	J	501	NAP	C5N-C4N-C3N	-8.66	111.85	120.36
2	F	501	NAP	C5N-C4N-C3N	-8.54	111.97	120.36
3	A	502	AKG	O1-C1-C2	-8.45	111.30	121.81
2	C	501	NAP	C5N-C4N-C3N	-8.35	112.15	120.36
3	H	502	AKG	O1-C1-C2	-8.00	111.86	121.81
2	G	501	NAP	C5N-C4N-C3N	-7.76	112.73	120.36
2	D	501	NAP	C5N-C4N-C3N	-7.28	113.21	120.36
2	E	501	NAP	C5N-C4N-C3N	-7.17	113.31	120.36
2	A	501	NAP	C5N-C4N-C3N	-7.05	113.43	120.36
2	H	501	NAP	C5N-C4N-C3N	-6.80	113.68	120.36
3	F	502	AKG	O1-C1-C2	-6.49	113.74	121.81
2	J	501	NAP	C5A-C4A-N3A	-6.41	117.89	126.72
2	D	501	NAP	N3A-C2A-N1A	-6.39	118.91	128.58
2	H	501	NAP	C4A-N9A-C8A	6.23	112.28	105.74
2	G	501	NAP	N3A-C4A-N9A	6.17	137.66	127.17
2	C	501	NAP	N3A-C4A-N9A	6.00	137.38	127.17
2	C	501	NAP	N6A-C6A-N1A	5.83	131.37	118.38
2	J	501	NAP	O4B-C1B-N9A	5.76	119.16	108.09
2	C	501	NAP	C4A-N9A-C8A	5.72	111.74	105.74
2	E	501	NAP	O4B-C1B-N9A	5.66	118.96	108.09
3	H	502	AKG	C3-C4-C5	-5.51	99.05	113.67
2	G	501	NAP	C5A-C4A-N3A	-5.40	119.29	126.72
2	A	501	NAP	N3A-C4A-N9A	5.31	136.19	127.17
2	G	501	NAP	N3A-C2A-N1A	-5.22	120.69	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	NAP	C5A-C4A-N3A	-5.15	119.63	126.72
2	G	501	NAP	O2N-PN-O3	5.06	120.96	107.27
2	H	501	NAP	N3A-C2A-N1A	-5.05	120.93	128.58
2	A	501	NAP	C5A-C4A-N3A	-5.01	119.82	126.72
2	C	501	NAP	N3A-C2A-N1A	-4.95	121.09	128.58
2	A	501	NAP	C4D-O4D-C1D	-4.91	105.42	109.92
2	D	501	NAP	C4A-N9A-C1B	-4.85	115.28	126.63
3	D	502	AKG	O1-C1-C2	-4.82	115.81	121.81
2	J	501	NAP	N3A-C4A-N9A	4.76	135.27	127.17
2	C	501	NAP	C5A-C6A-N6A	-4.74	111.54	123.29
2	C	501	NAP	C5A-C4A-N9A	-4.70	100.69	105.81
3	F	502	AKG	C4-C3-C2	-4.67	104.14	112.91
2	G	501	NAP	N6A-C6A-N1A	4.65	128.74	118.38
2	C	501	NAP	O2A-PA-O3	4.64	119.83	107.27
2	G	501	NAP	O3-PA-O1A	-4.62	96.82	110.70
2	F	501	NAP	N3A-C2A-N1A	-4.57	121.67	128.58
2	D	501	NAP	C2A-N3A-C4A	4.55	122.95	111.83
2	A	501	NAP	C3N-C7N-N7N	4.55	123.35	117.74
2	F	501	NAP	C3N-C7N-N7N	4.51	123.30	117.74
2	A	501	NAP	N3A-C2A-N1A	-4.50	121.77	128.58
2	J	501	NAP	C2A-N3A-C4A	4.50	122.81	111.83
3	C	502	AKG	O5-C2-C1	4.42	125.98	119.67
3	A	502	AKG	C3-C4-C5	-4.42	101.94	113.67
2	B	501	NAP	N3A-C2A-N1A	-4.40	121.92	128.58
3	D	502	AKG	C3-C2-C1	4.35	123.26	115.86
2	H	501	NAP	N9A-C8A-N7A	-4.31	107.82	113.94
2	G	501	NAP	C2A-N3A-C4A	4.28	122.29	111.83
2	G	501	NAP	C5A-C6A-N6A	-4.27	112.71	123.29
2	A	501	NAP	N6A-C6A-N1A	4.27	127.88	118.38
3	C	502	AKG	C3-C4-C5	-4.23	102.44	113.67
2	H	501	NAP	C4A-N9A-C1B	-4.22	116.75	126.63
2	E	501	NAP	N3A-C2A-N1A	-4.21	122.20	128.58
2	J	501	NAP	N3A-C2A-N1A	-4.21	122.22	128.58
3	J	502	AKG	C3-C2-C1	4.17	122.95	115.86
2	E	501	NAP	C2A-N3A-C4A	4.17	122.01	111.83
2	D	501	NAP	C4A-N9A-C8A	4.13	110.08	105.74
2	G	501	NAP	C4A-N9A-C8A	4.08	110.03	105.74
3	B	502	AKG	C4-C3-C2	-4.05	105.31	112.91
2	H	501	NAP	N3A-C4A-N9A	4.04	134.04	127.17
2	E	501	NAP	C3N-C7N-N7N	4.04	122.72	117.74
2	E	501	NAP	O7N-C7N-N7N	-4.04	116.78	122.62
2	B	501	NAP	N3A-C4A-N9A	4.03	134.02	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	501	NAP	C4A-C5A-N7A	-3.95	106.07	110.58
2	G	501	NAP	C3N-C7N-N7N	3.93	122.58	117.74
2	H	501	NAP	C3N-C7N-N7N	3.92	122.57	117.74
2	A	501	NAP	C2A-N3A-C4A	3.89	121.34	111.83
2	H	501	NAP	C2A-N3A-C4A	3.82	121.15	111.83
2	G	501	NAP	O5D-PN-O1N	-3.78	93.97	108.94
2	B	501	NAP	N6A-C6A-N1A	3.76	126.74	118.38
2	E	501	NAP	N3A-C4A-N9A	3.74	133.52	127.17
3	E	502	AKG	O3-C5-C4	-3.74	111.24	123.09
2	B	501	NAP	C5A-C4A-N3A	-3.68	121.65	126.72
2	D	501	NAP	C5A-C4A-N3A	-3.65	121.69	126.72
3	E	502	AKG	C3-C4-C5	-3.62	104.07	113.67
2	H	501	NAP	C5A-C4A-N3A	-3.57	121.80	126.72
2	D	501	NAP	N3A-C4A-N9A	3.55	133.21	127.17
3	A	502	AKG	O2-C1-C2	3.50	123.28	113.59
2	C	501	NAP	C5A-C4A-N3A	-3.48	121.92	126.72
3	F	502	AKG	O5-C2-C1	3.46	124.61	119.67
2	A	501	NAP	C5A-C6A-N6A	-3.45	114.75	123.29
2	B	501	NAP	C2N-C3N-C4N	3.44	122.26	118.26
2	A	501	NAP	C4A-N9A-C8A	3.42	109.33	105.74
2	D	501	NAP	C1B-N9A-C8A	3.40	134.64	127.09
2	B	501	NAP	C5A-C6A-N6A	-3.40	114.87	123.29
2	H	501	NAP	C6A-C5A-N7A	3.38	138.61	132.09
3	F	502	AKG	O2-C1-C2	3.36	122.91	113.59
2	E	501	NAP	C4A-C5A-N7A	-3.35	106.75	110.58
2	F	501	NAP	C2A-N1A-C6A	3.25	124.08	118.73
2	B	501	NAP	C2A-N3A-C4A	3.25	119.78	111.83
2	D	501	NAP	O4B-C1B-N9A	3.24	114.31	108.09
3	E	502	AKG	O5-C2-C1	3.22	124.26	119.67
2	H	501	NAP	C5A-N7A-C8A	3.18	108.45	103.45
2	A	501	NAP	O7N-C7N-C3N	-3.18	115.71	119.60
2	D	501	NAP	C6A-C5A-C4A	-3.17	112.85	117.18
3	H	502	AKG	O2-C1-C2	3.16	122.35	113.59
2	D	501	NAP	O7N-C7N-C3N	3.15	123.45	119.60
2	E	501	NAP	C4A-N9A-C8A	3.15	109.04	105.74
2	D	501	NAP	O7N-C7N-N7N	-3.12	118.11	122.62
2	F	501	NAP	N6A-C6A-N1A	3.12	125.33	118.38
2	D	501	NAP	C5A-C6A-N6A	-3.12	115.56	123.29
2	F	501	NAP	C2B-C1B-N9A	-3.12	108.62	113.75
2	J	501	NAP	O4B-C1B-C2B	-3.11	101.24	106.59
3	J	502	AKG	C4-C3-C2	3.05	118.64	112.91
2	D	501	NAP	C6A-C5A-N7A	3.03	137.93	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	502	AKG	O5-C2-C1	3.00	123.95	119.67
2	C	501	NAP	C2A-N3A-C4A	3.00	119.16	111.83
3	E	502	AKG	O1-C1-C2	-2.98	118.11	121.81
3	E	502	AKG	C3-C2-C1	-2.97	110.82	115.86
2	E	501	NAP	N9A-C8A-N7A	-2.95	109.75	113.94
2	F	501	NAP	O7N-C7N-C3N	-2.94	116.00	119.60
2	A	501	NAP	O2A-PA-O3	2.93	115.20	107.27
2	B	501	NAP	C4A-N9A-C8A	2.92	108.81	105.74
2	J	501	NAP	C5A-N7A-C8A	2.92	108.04	103.45
3	E	502	AKG	O4-C5-O3	2.90	130.80	123.33
2	J	501	NAP	C6A-C5A-N7A	2.89	137.66	132.09
3	G	502	AKG	O1-C1-C2	-2.89	118.22	121.81
2	H	501	NAP	C4A-C5A-N7A	-2.88	107.29	110.58
2	E	501	NAP	C6A-C5A-N7A	2.86	137.60	132.09
2	H	501	NAP	O3-PA-O1A	-2.85	102.12	110.70
2	G	501	NAP	O7N-C7N-C3N	-2.85	116.11	119.60
2	F	501	NAP	C2A-N3A-C4A	2.82	118.72	111.83
2	F	501	NAP	C4A-N9A-C8A	2.78	108.66	105.74
2	F	501	NAP	C4D-O4D-C1D	-2.76	107.39	109.92
2	E	501	NAP	O4B-C1B-C2B	-2.75	101.85	106.59
2	C	501	NAP	C2A-N1A-C6A	2.74	123.23	118.73
2	F	501	NAP	N3A-C4A-N9A	2.73	131.81	127.17
3	G	502	AKG	O3-C5-C4	-2.72	114.47	123.09
3	B	502	AKG	O3-C5-C4	-2.72	114.47	123.09
2	F	501	NAP	C5A-C4A-N3A	-2.72	122.97	126.72
2	J	501	NAP	C2N-C3N-C4N	2.70	121.40	118.26
3	C	502	AKG	C3-C2-C1	-2.68	111.30	115.86
2	D	501	NAP	N9A-C8A-N7A	-2.68	110.13	113.94
3	F	502	AKG	O5-C2-C3	-2.68	115.42	121.17
2	G	501	NAP	O3X-P2B-O2X	2.66	117.76	107.80
2	E	501	NAP	C5A-N7A-C8A	2.64	107.61	103.45
3	F	502	AKG	O3-C5-C4	-2.63	114.76	123.09
3	H	502	AKG	O3-C5-C4	-2.61	114.81	123.09
2	H	501	NAP	O3X-P2B-O2X	2.60	117.57	107.80
2	A	501	NAP	O2N-PN-O1N	2.56	124.34	112.44
3	A	502	AKG	O5-C2-C1	2.54	123.30	119.67
2	G	501	NAP	C5A-C4A-N9A	-2.54	103.05	105.81
2	C	501	NAP	O7N-C7N-C3N	2.52	122.69	119.60
2	C	501	NAP	O3X-P2B-O2X	2.51	117.22	107.80
2	G	501	NAP	O2B-P2B-O1X	-2.50	100.44	109.33
2	E	501	NAP	O2X-P2B-O2B	-2.49	96.16	105.85
2	H	501	NAP	O2A-PA-O3	2.48	113.99	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	501	NAP	C2A-N1A-C6A	2.48	122.80	118.73
3	A	502	AKG	O3-C5-C4	-2.45	115.31	123.09
3	D	502	AKG	O2-C1-C2	2.45	120.39	113.59
2	A	501	NAP	C2B-C1B-N9A	-2.45	109.72	113.75
2	G	501	NAP	O2N-PN-O1N	-2.43	101.15	112.44
2	G	501	NAP	P2B-O2B-C2B	-2.41	116.98	123.43
3	D	502	AKG	O5-C2-C1	-2.41	116.23	119.67
3	F	502	AKG	C3-C2-C1	2.41	119.95	115.86
3	J	502	AKG	O2-C1-C2	2.37	120.17	113.59
3	B	502	AKG	C3-C4-C5	-2.37	107.39	113.67
2	D	501	NAP	C2B-C1B-N9A	2.37	117.64	113.75
3	B	502	AKG	O4-C5-C4	2.35	121.42	114.00
2	C	501	NAP	C2N-C3N-C4N	2.33	120.97	118.26
2	C	501	NAP	O7N-C7N-N7N	-2.31	119.28	122.62
2	C	501	NAP	C4D-O4D-C1D	-2.29	107.83	109.92
2	G	501	NAP	C5N-C6N-N1N	2.28	123.50	120.38
2	H	501	NAP	C6A-C5A-C4A	-2.26	114.09	117.18
2	F	501	NAP	O2B-P2B-O1X	-2.24	101.34	109.33
2	H	501	NAP	C4D-O4D-C1D	-2.24	107.88	109.92
2	B	501	NAP	C2B-C1B-N9A	-2.23	110.08	113.75
2	E	501	NAP	O3X-P2B-O2X	2.22	116.13	107.80
2	F	501	NAP	C5A-C6A-N6A	-2.21	117.82	123.29
3	H	502	AKG	O4-C5-O3	2.20	128.99	123.33
3	G	502	AKG	C3-C2-C1	-2.18	112.16	115.86
2	G	501	NAP	C6N-N1N-C2N	-2.17	120.03	121.88
3	J	502	AKG	O5-C2-C3	-2.16	116.53	121.17
2	B	501	NAP	C2A-N1A-C6A	2.13	122.23	118.73
2	H	501	NAP	O3D-C3D-C4D	-2.12	105.00	111.08
2	C	501	NAP	O3-PA-O1A	-2.10	104.39	110.70
3	J	502	AKG	O2-C1-O1	-2.09	118.91	123.90
2	A	501	NAP	C1B-N9A-C8A	-2.06	122.52	127.09
2	H	501	NAP	O5D-PN-O1N	2.02	116.92	108.94
2	E	501	NAP	O3-PN-O1N	-2.01	104.64	110.70
2	C	501	NAP	C6N-C5N-C4N	2.01	122.35	119.45
3	H	502	AKG	C4-C3-C2	-2.01	109.14	112.91
2	H	501	NAP	O7N-C7N-N7N	-2.01	119.71	122.62
2	H	501	NAP	O2N-PN-O5D	-2.00	98.49	107.57

There are no chirality outliers.

All (99) 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	B	501	NAP	O4D-C1D-N1N-C2N
2	B	501	NAP	O4D-C1D-N1N-C6N
2	C	501	NAP	O4D-C1D-N1N-C2N
2	D	501	NAP	O4D-C1D-N1N-C2N
2	E	501	NAP	C5D-O5D-PN-O2N
2	E	501	NAP	O4D-C1D-N1N-C2N
2	E	501	NAP	O4D-C1D-N1N-C6N
2	F	501	NAP	O4D-C1D-N1N-C2N
2	F	501	NAP	O4D-C1D-N1N-C6N
2	G	501	NAP	C5D-O5D-PN-O3
2	G	501	NAP	O4D-C1D-N1N-C2N
2	H	501	NAP	O4D-C1D-N1N-C2N
2	J	501	NAP	C5D-O5D-PN-O3
2	J	501	NAP	C5D-O5D-PN-O1N
3	A	502	AKG	O1-C1-C2-O5
3	A	502	AKG	O1-C1-C2-C3
3	A	502	AKG	O2-C1-C2-C3
3	A	502	AKG	C2-C3-C4-C5
3	B	502	AKG	O2-C1-C2-C3
3	C	502	AKG	O1-C1-C2-C3
3	C	502	AKG	O2-C1-C2-O5
3	C	502	AKG	O2-C1-C2-C3
3	C	502	AKG	C2-C3-C4-C5
3	D	502	AKG	C1-C2-C3-C4
3	E	502	AKG	O1-C1-C2-O5
3	E	502	AKG	O1-C1-C2-C3
3	E	502	AKG	O2-C1-C2-C3
3	E	502	AKG	C2-C3-C4-C5
3	F	502	AKG	O1-C1-C2-O5
3	F	502	AKG	O1-C1-C2-C3
3	F	502	AKG	O2-C1-C2-C3
3	F	502	AKG	C2-C3-C4-C5
3	G	502	AKG	O1-C1-C2-C3
3	G	502	AKG	O2-C1-C2-C3
3	H	502	AKG	O2-C1-C2-C3
3	J	502	AKG	C1-C2-C3-C4
3	J	502	AKG	O5-C2-C3-C4
3	J	502	AKG	C2-C3-C4-C5
3	G	502	AKG	C2-C3-C4-C5
2	G	501	NAP	O4D-C4D-C5D-O5D
3	D	502	AKG	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	H	502	AKG	C2-C3-C4-C5
2	F	501	NAP	O4B-C4B-C5B-O5B
3	B	502	AKG	O1-C1-C2-O5
3	C	502	AKG	O1-C1-C2-O5
3	G	502	AKG	O1-C1-C2-O5
3	J	502	AKG	O1-C1-C2-O5
2	F	501	NAP	C3B-C4B-C5B-O5B
3	B	502	AKG	O1-C1-C2-C3
3	J	502	AKG	O1-C1-C2-C3
2	J	501	NAP	C2N-C3N-C7N-N7N
2	J	501	NAP	C2N-C3N-C7N-O7N
2	H	501	NAP	O4D-C4D-C5D-O5D
2	G	501	NAP	C5D-O5D-PN-O1N
2	J	501	NAP	C5D-O5D-PN-O2N
3	B	502	AKG	O2-C1-C2-O5
3	F	502	AKG	O2-C1-C2-O5
3	J	502	AKG	O2-C1-C2-O5
2	J	501	NAP	C2B-C1B-N9A-C8A
2	J	501	NAP	C4N-C3N-C7N-N7N
2	B	501	NAP	C2B-O2B-P2B-O3X
2	C	501	NAP	C2B-O2B-P2B-O2X
2	G	501	NAP	C2B-O2B-P2B-O2X
3	J	502	AKG	O2-C1-C2-C3
3	G	502	AKG	C3-C4-C5-O4
2	E	501	NAP	C2D-C1D-N1N-C6N
2	F	501	NAP	C2D-C1D-N1N-C6N
2	J	501	NAP	C4N-C3N-C7N-O7N
3	G	502	AKG	C3-C4-C5-O3
3	E	502	AKG	C3-C4-C5-O3
3	C	502	AKG	C3-C4-C5-O3
3	C	502	AKG	C3-C4-C5-O4
3	E	502	AKG	C3-C4-C5-O4
2	C	501	NAP	O4D-C1D-N1N-C6N
2	D	501	NAP	O4D-C1D-N1N-C6N
2	G	501	NAP	O4D-C1D-N1N-C6N
2	H	501	NAP	O4D-C1D-N1N-C6N
3	F	502	AKG	C3-C4-C5-O4
2	A	501	NAP	C2B-O2B-P2B-O1X
2	B	501	NAP	C2B-O2B-P2B-O1X
2	H	501	NAP	C2B-O2B-P2B-O1X
3	F	502	AKG	C3-C4-C5-O3
3	H	502	AKG	C3-C4-C5-O3

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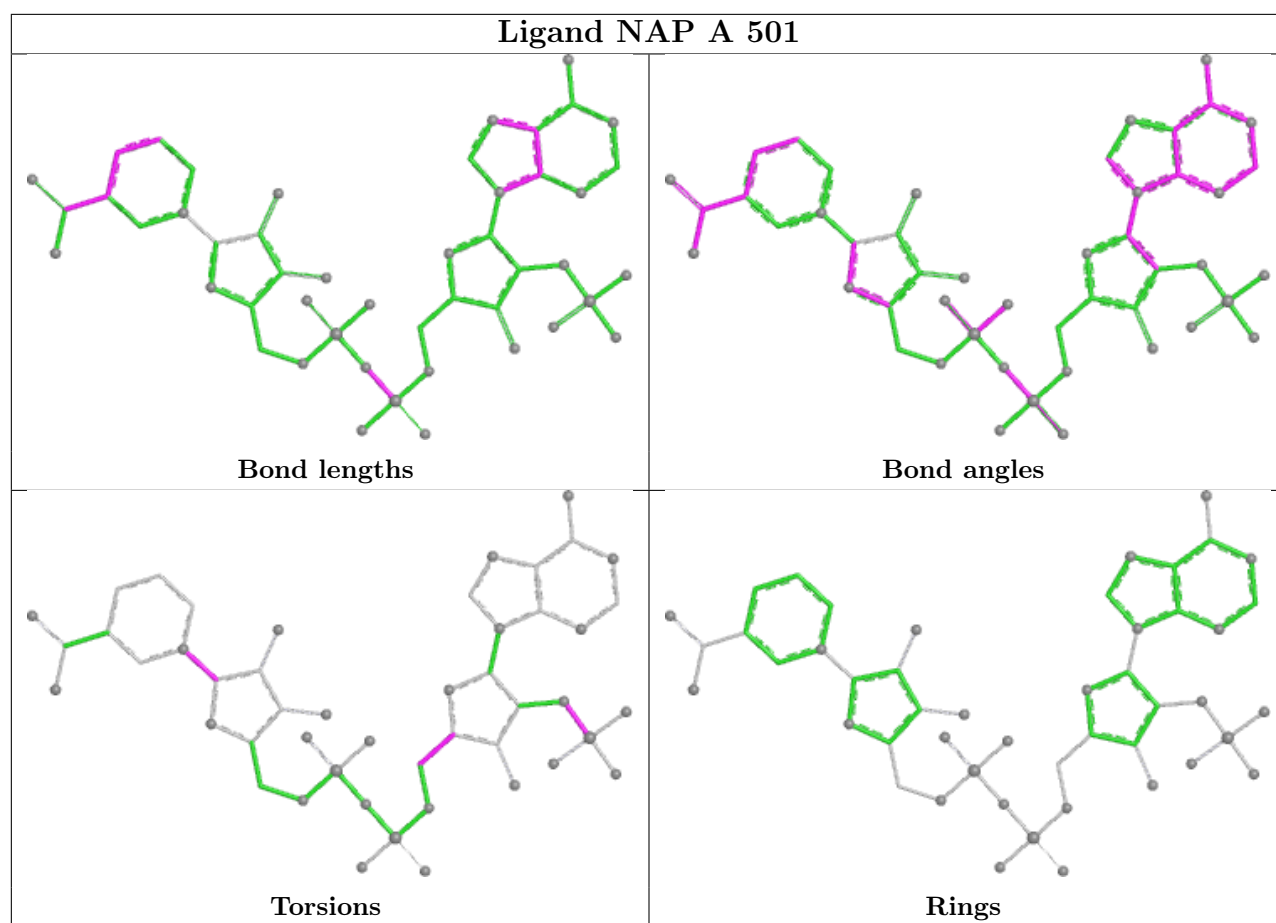
Mol	Chain	Res	Type	Atoms
3	H	502	AKG	C3-C4-C5-O4
3	F	502	AKG	C1-C2-C3-C4
2	D	501	NAP	O4B-C4B-C5B-O5B
3	A	502	AKG	C3-C4-C5-O3
3	A	502	AKG	C3-C4-C5-O4
2	E	501	NAP	O4B-C4B-C5B-O5B
2	B	501	NAP	O4B-C4B-C5B-O5B
2	J	501	NAP	O4B-C4B-C5B-O5B
2	B	501	NAP	C2B-O2B-P2B-O2X
2	A	501	NAP	O4B-C4B-C5B-O5B
2	J	501	NAP	O4B-C1B-N9A-C8A
2	F	501	NAP	C2B-O2B-P2B-O1X
2	G	501	NAP	PN-O3-PA-O1A
2	G	501	NAP	O4B-C4B-C5B-O5B

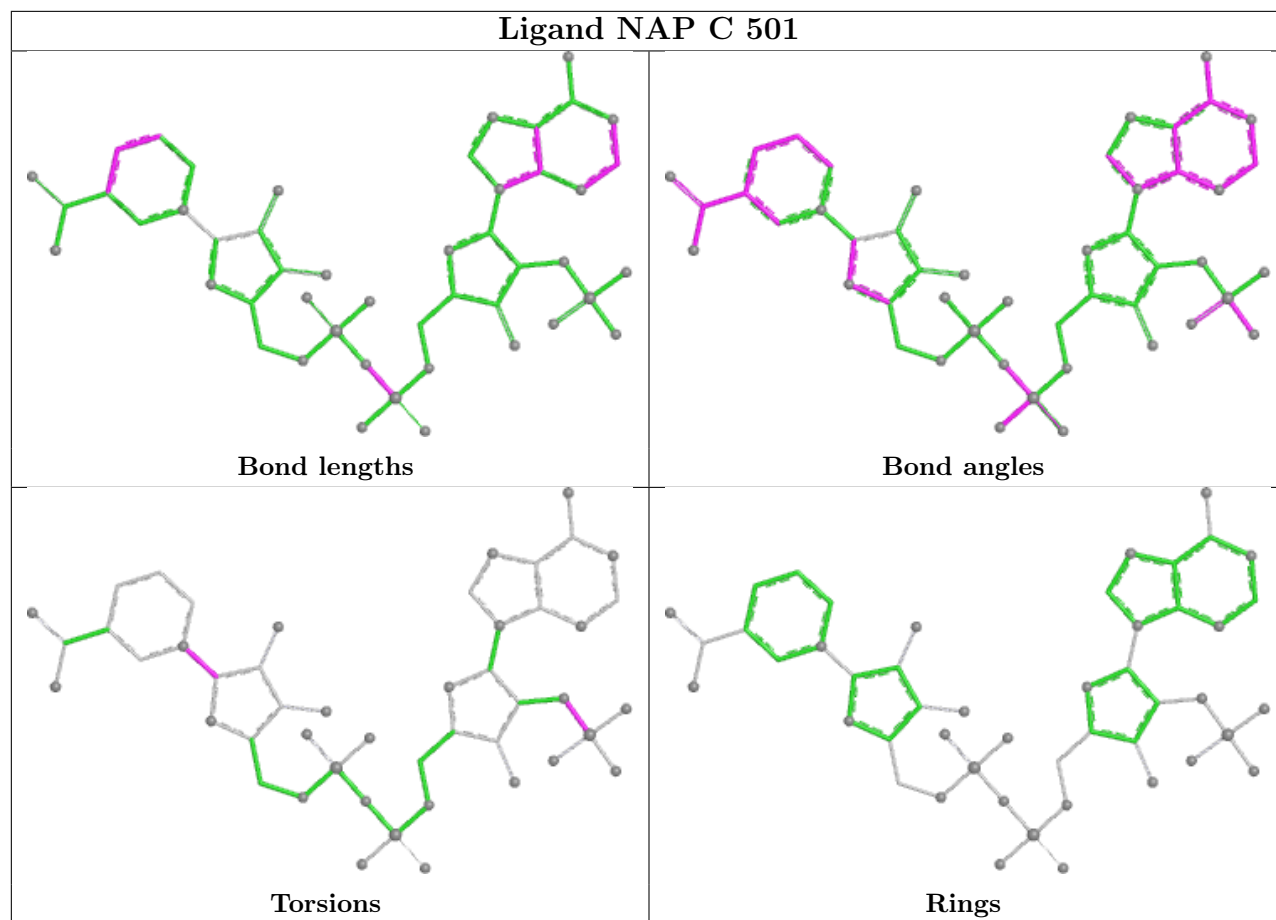
There are no ring outliers.

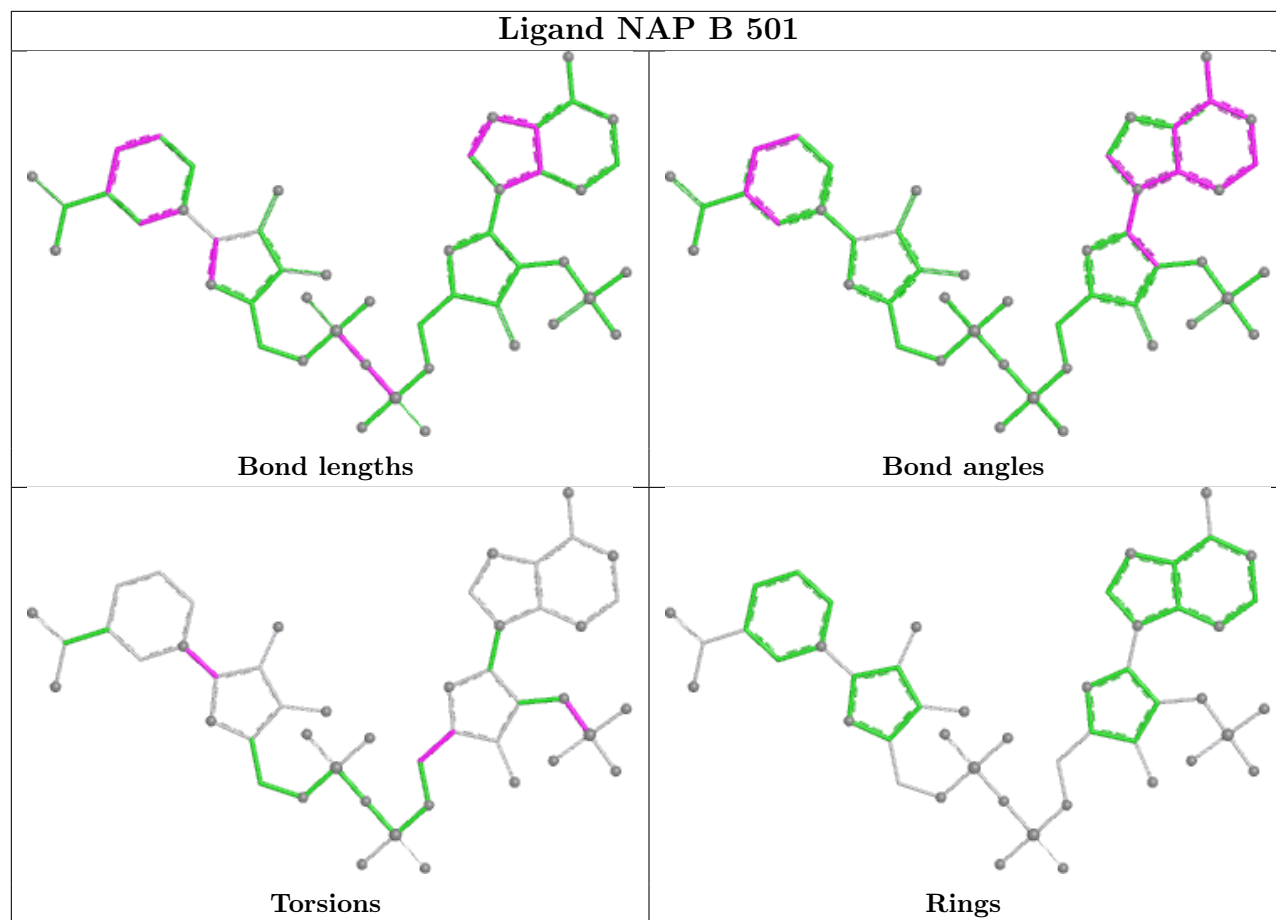
5 monomers are involved in 7 short contacts:

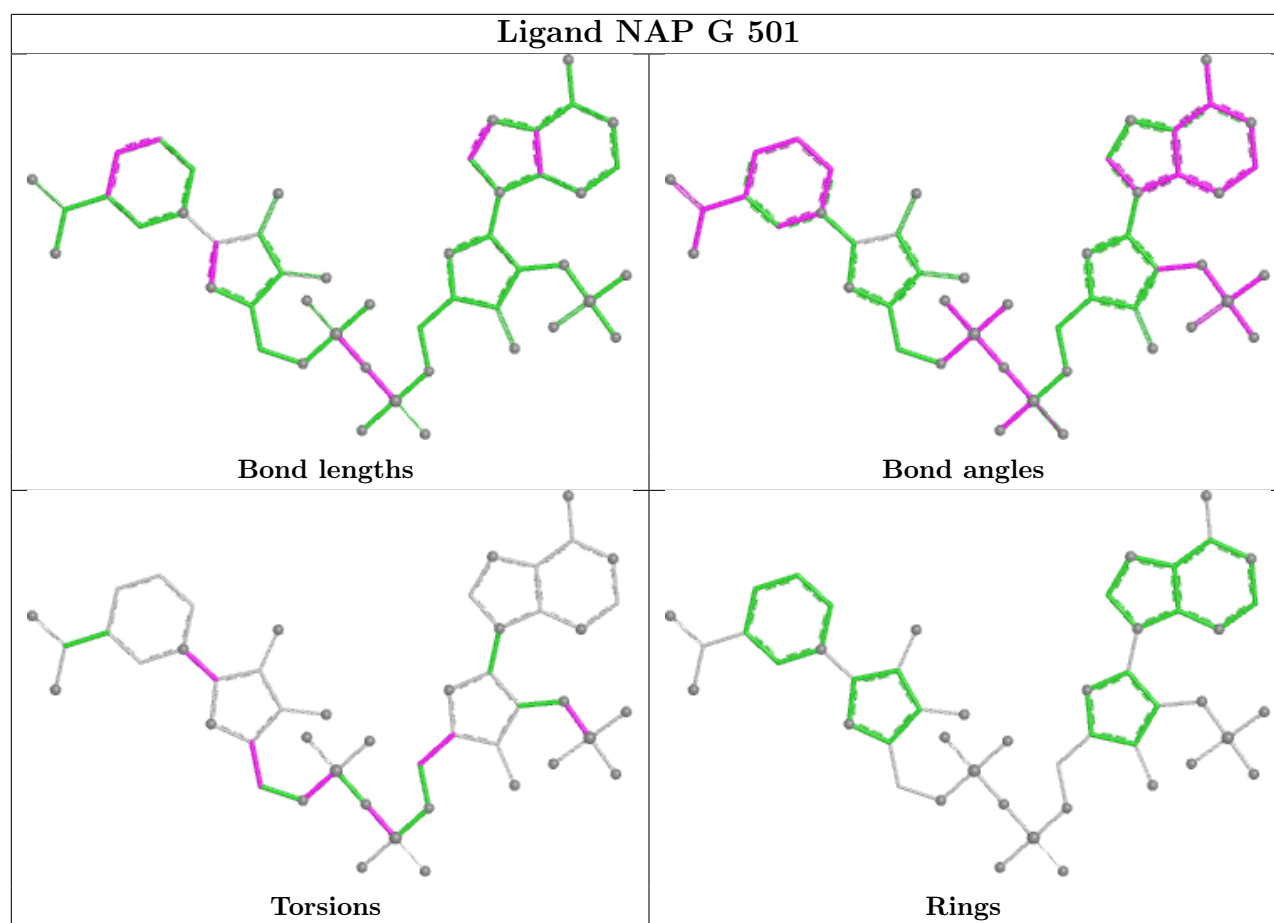
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	501	NAP	2	0
3	B	502	AKG	2	0
3	C	502	AKG	1	0
3	E	502	AKG	1	0
3	J	502	AKG	1	0

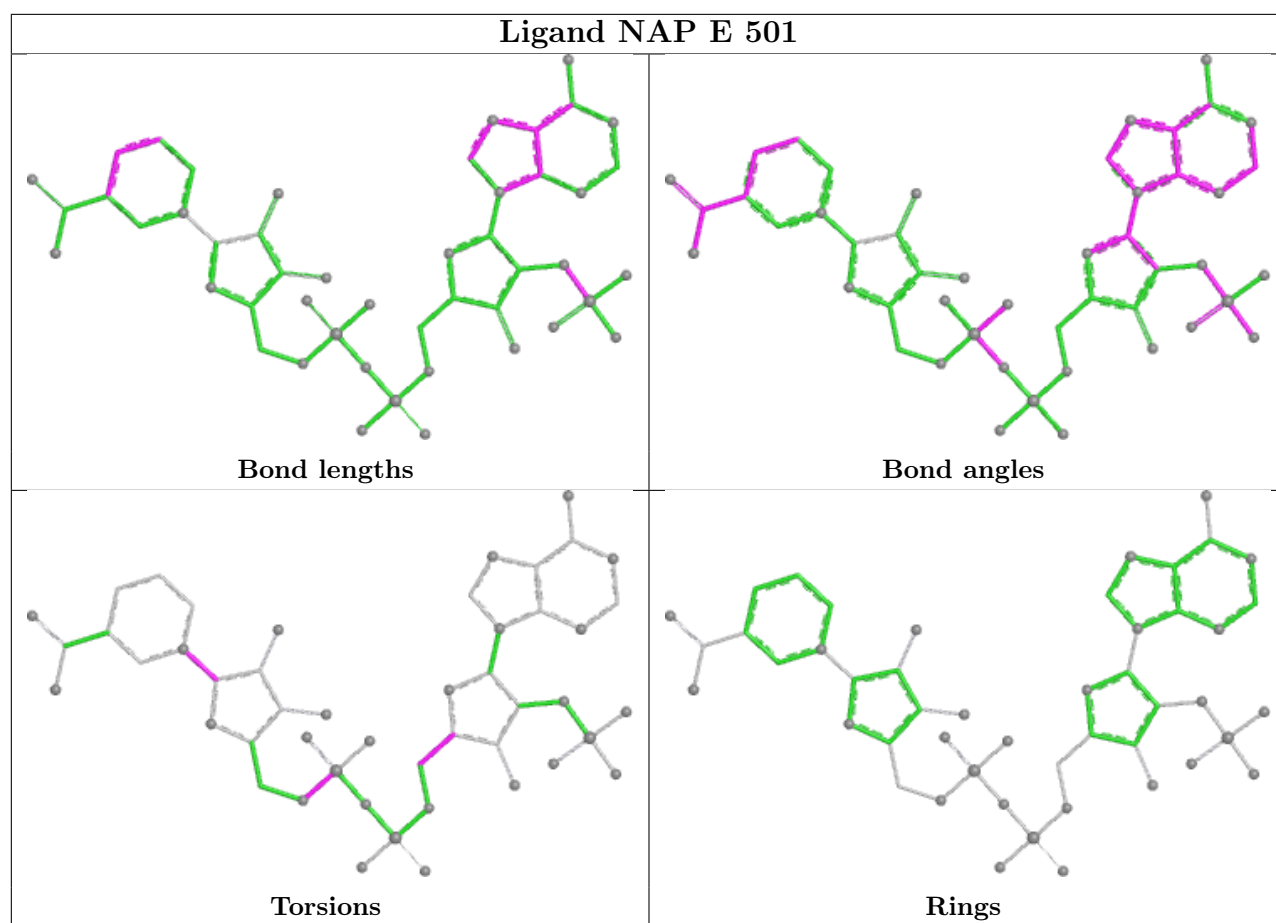
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

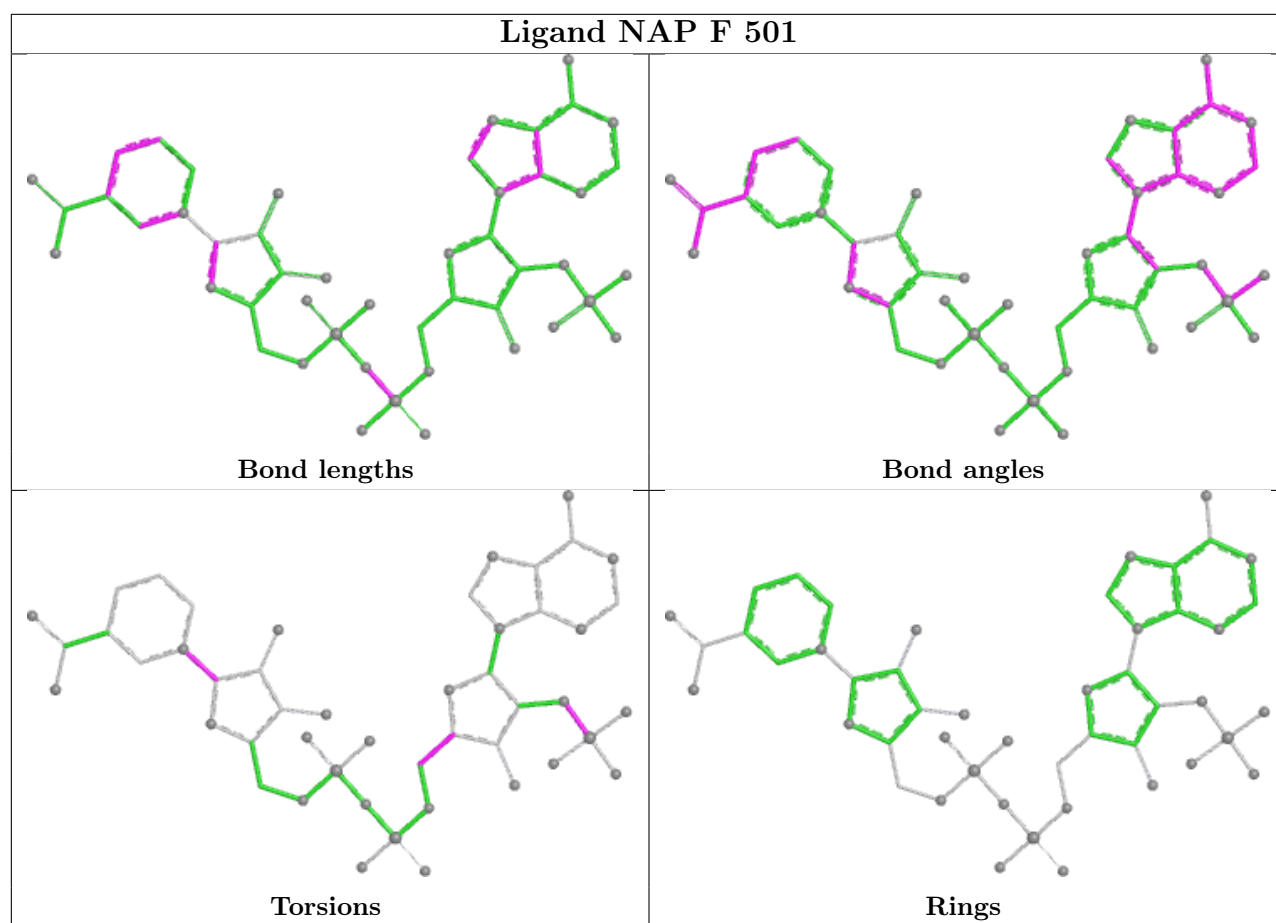


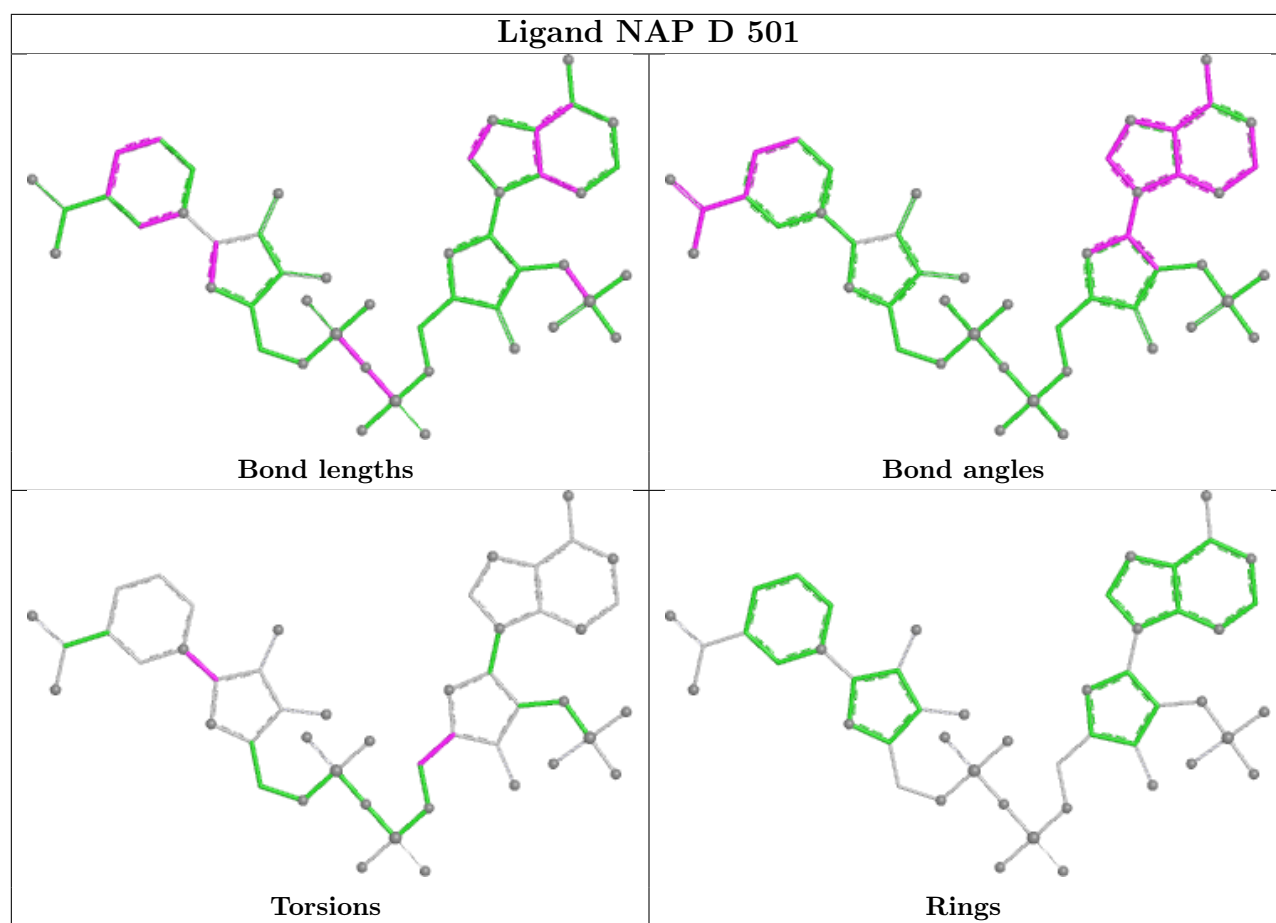


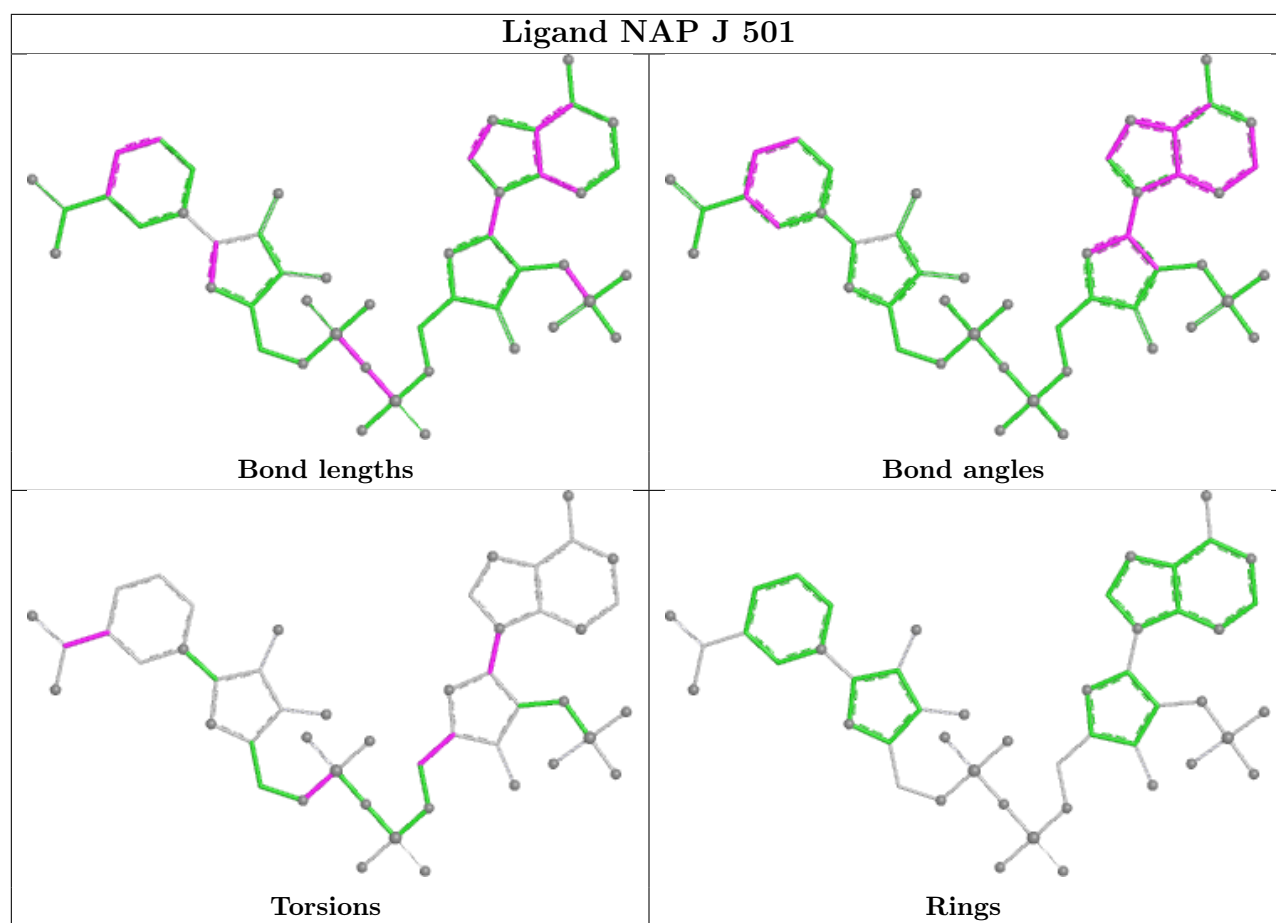


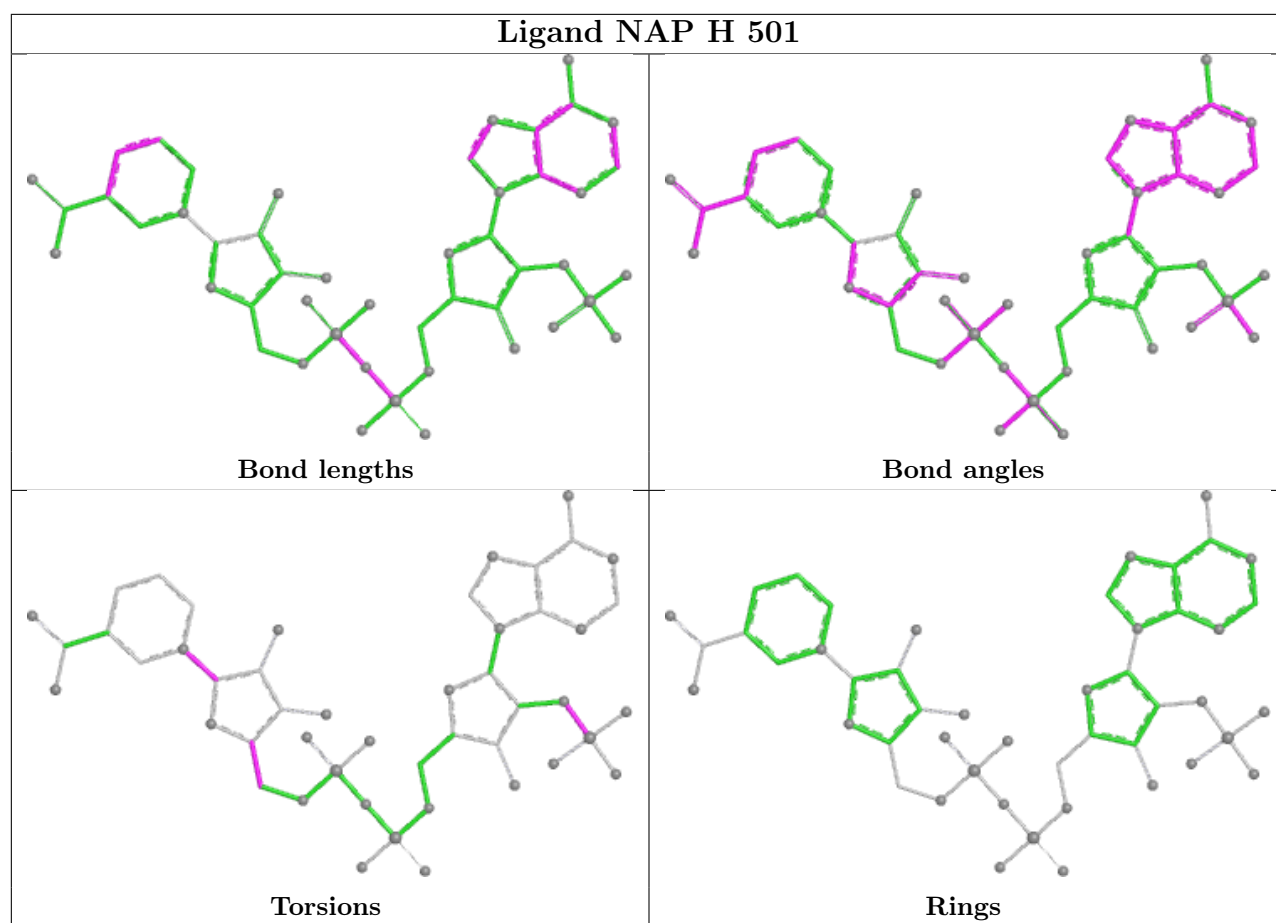












5.7 Other polymers [i](#)

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 ⓘ

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	447/447 (100%)	-0.58	1 (0%) 91 91	10, 16, 33, 63	0
1	B	447/447 (100%)	-0.63	1 (0%) 91 91	8, 15, 31, 61	0
1	C	447/447 (100%)	-0.60	2 (0%) 88 89	8, 15, 33, 67	0
1	D	447/447 (100%)	-0.53	5 (1%) 78 79	9, 16, 36, 70	0
1	E	447/447 (100%)	-0.54	2 (0%) 88 89	8, 17, 34, 76	0
1	F	447/447 (100%)	-0.50	3 (0%) 84 85	9, 18, 37, 53	0
1	G	447/447 (100%)	-0.50	1 (0%) 91 91	11, 19, 38, 77	0
1	H	447/447 (100%)	-0.31	3 (0%) 84 85	12, 22, 45, 66	0
1	I	447/447 (100%)	0.22	58 (12%) 7 8	8, 23, 69, 91	0
1	J	447/447 (100%)	1.44	165 (36%) 1 1	13, 45, 117, 146	0
1	K	304/447 (68%)	0.44	44 (14%) 6 7	17, 30, 75, 99	0
1	L	447/447 (100%)	-0.14	9 (2%) 65 66	12, 26, 54, 96	0
All	All	5221/5364 (97%)	-0.20	294 (5%) 30 32	8, 20, 65, 146	0

All (294) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	231	ILE	8.1
1	J	237	ILE	7.9
1	J	342	VAL	7.6
1	J	309	ILE	7.5
1	J	343	ALA	7.3
1	J	259	VAL	7.3
1	J	260	ILE	7.2
1	J	277	VAL	7.0
1	J	272	PRO	6.9
1	J	341	PHE	6.7
1	K	31	VAL	6.5

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Mol	Chain	Res	Type	RSRZ
1	J	275	VAL	6.3
1	J	283	ILE	6.3
1	J	274	GLY	6.2
1	J	320	CYS	6.1
1	J	286	VAL	5.9
1	J	328	GLY	5.8
1	J	345	GLY	5.7
1	J	317	ALA	5.5
1	J	365	PHE	5.4
1	J	319	PRO	5.3
1	J	294	TYR	5.3
1	K	3	VAL	5.2
1	J	269	VAL	5.1
1	J	244	VAL	5.1
1	J	247	TYR	5.1
1	J	324	ASN	5.0
1	J	316	ILE	5.0
1	J	302	THR	5.0
1	J	314	CYS	5.0
1	J	334	LEU	4.9
1	K	39	LEU	4.8
1	J	228	GLY	4.8
1	J	293	VAL	4.8
1	J	224	ILE	4.8
1	J	300	GLY	4.8
1	J	326	LEU	4.7
1	J	240	GLY	4.7
1	J	262	PHE	4.7
1	J	298	VAL	4.7
1	J	258	THR	4.7
1	J	303	TYR	4.7
1	J	223	MET	4.7
1	J	238	VAL	4.6
1	J	351	THR	4.6
1	J	3	VAL	4.5
1	J	301	ALA	4.5
1	J	321	ALA	4.5
1	J	340	ARG	4.5
1	K	32	LEU	4.5
1	J	216	CYS	4.5
1	A	1	MET	4.5
1	J	315	ASP	4.5

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Mol	Chain	Res	Type	RSRZ
1	J	218	TYR	4.4
1	J	291	VAL	4.4
1	L	3	VAL	4.4
1	J	270	HIS	4.4
1	J	339	CYS	4.4
1	J	268	TRP	4.4
1	E	1	MET	4.4
1	J	350	SER	4.4
1	K	7	VAL	4.4
1	K	218	TYR	4.4
1	J	344	GLU	4.3
1	J	318	LEU	4.3
1	J	276	ASP	4.3
1	J	349	PRO	4.3
1	J	366	GLY	4.3
1	J	236	ILE	4.3
1	J	355	VAL	4.3
1	I	266	SER	4.3
1	J	255	LEU	4.2
1	J	278	ALA	4.2
1	K	35	LEU	4.2
1	D	1	MET	4.1
1	J	246	THR	4.1
1	G	1	MET	4.1
1	J	280	LEU	4.0
1	J	261	GLY	4.0
1	J	226	ALA	4.0
1	J	249	ILE	4.0
1	I	238	VAL	3.9
1	J	217	VAL	3.9
1	J	252	ALA	3.9
1	J	304	HIS	3.9
1	J	352	PRO	3.9
1	I	240	GLY	3.9
1	J	235	LYS	3.8
1	I	305	THR	3.8
1	K	1	MET	3.8
1	J	305	THR	3.8
1	K	216	CYS	3.8
1	C	1	MET	3.7
1	K	13	MET	3.7
1	J	358	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	I	1	MET	3.6
1	J	263	SER	3.6
1	L	13	MET	3.5
1	J	296	ASP	3.5
1	B	1	MET	3.5
1	J	1	MET	3.5
1	J	332	LYS	3.5
1	J	256	GLY	3.5
1	J	338	GLY	3.5
1	J	337	ASN	3.5
1	L	274	GLY	3.5
1	J	248	ALA	3.4
1	J	335	ALA	3.4
1	J	306	ASP	3.4
1	J	232	SER	3.4
1	J	290	ARG	3.4
1	K	29	ALA	3.4
1	K	22	PRO	3.3
1	J	361	ARG	3.3
1	J	267	GLY	3.3
1	J	279	LYS	3.3
1	J	368	GLY	3.3
1	F	1	MET	3.3
1	I	336	ASP	3.3
1	J	266	SER	3.3
1	J	333	THR	3.3
1	J	264	ASP	3.2
1	I	239	SER	3.2
1	J	348	MET	3.2
1	J	251	LYS	3.2
1	J	347	ASN	3.2
1	K	217	VAL	3.2
1	J	35	LEU	3.2
1	J	271	THR	3.2
1	J	230	SER	3.1
1	J	285	GLU	3.1
1	I	355	VAL	3.1
1	K	426	VAL	3.1
1	J	353	GLU	3.1
1	J	287	ARG	3.1
1	K	10	TYR	3.0
1	K	224	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	I	267	GLY	3.0
1	J	311	ASP	3.0
1	J	295	ALA	3.0
1	I	241	SER	3.0
1	I	361	ARG	3.0
1	J	273	ASN	3.0
1	I	301	ALA	3.0
1	J	331	ALA	3.0
1	J	250	GLU	3.0
1	K	23	GLU	3.0
1	K	33	GLU	3.0
1	J	220	VAL	2.9
1	I	332	LYS	2.9
1	J	363	ILE	2.9
1	K	219	PHE	2.9
1	J	44	HIS	2.9
1	K	223	MET	2.9
1	J	233	GLY	2.9
1	L	44	HIS	2.9
1	K	220	VAL	2.9
1	J	364	ARG	2.9
1	J	426	VAL	2.9
1	J	322	THR	2.9
1	J	227	LYS	2.8
1	I	359	ARG	2.8
1	I	354	ALA	2.8
1	J	257	ALA	2.8
1	I	243	ASN	2.8
1	I	228	GLY	2.8
1	J	241	SER	2.8
1	J	367	PRO	2.8
1	I	360	GLU	2.8
1	J	243	ASN	2.8
1	J	327	ASN	2.8
1	I	242	GLY	2.8
1	K	43	PRO	2.8
1	H	13	MET	2.8
1	J	219	PHE	2.8
1	K	9	ASN	2.8
1	I	338	GLY	2.8
1	J	289	ALA	2.8
1	D	306	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	272	PRO	2.7
1	J	354	ALA	2.7
1	J	417	ALA	2.7
1	K	2	THR	2.7
1	J	239	SER	2.7
1	K	214	TYR	2.7
1	I	3	VAL	2.7
1	K	34	SER	2.7
1	J	310	TRP	2.7
1	K	409	PHE	2.7
1	J	357	VAL	2.7
1	J	2	THR	2.7
1	J	307	GLY	2.7
1	J	359	ARG	2.7
1	I	6	GLN	2.6
1	J	346	ALA	2.6
1	H	10	TYR	2.6
1	J	297	GLU	2.6
1	K	403	VAL	2.6
1	I	233	GLY	2.6
1	I	260	ILE	2.6
1	J	43	PRO	2.6
1	K	8	SER	2.6
1	J	254	GLU	2.6
1	I	307	GLY	2.6
1	L	43	PRO	2.6
1	J	312	LEU	2.6
1	J	234	GLN	2.5
1	J	245	ALA	2.5
1	J	292	SER	2.5
1	I	363	ILE	2.5
1	L	1	MET	2.5
1	K	44	HIS	2.5
1	J	282	GLU	2.5
1	J	425	TYR	2.5
1	I	286	VAL	2.4
1	J	413	ALA	2.4
1	I	300	GLY	2.4
1	F	2	THR	2.4
1	H	1	MET	2.4
1	I	255	LEU	2.4
1	D	2	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	337	ASN	2.4
1	J	329	GLU	2.4
1	J	416	ALA	2.4
1	K	27	ALA	2.4
1	K	417	ALA	2.4
1	J	313	LYS	2.4
1	C	164	VAL	2.4
1	I	304	HIS	2.4
1	J	371	ALA	2.3
1	J	13	MET	2.3
1	I	339	CYS	2.3
1	I	358	PHE	2.3
1	I	296	ASP	2.3
1	I	327	ASN	2.3
1	I	268	TRP	2.3
1	J	225	LYS	2.3
1	I	274	GLY	2.3
1	J	242	GLY	2.3
1	K	420	GLY	2.3
1	E	2	THR	2.3
1	J	221	SER	2.3
1	K	37	ILE	2.3
1	I	256	GLY	2.3
1	I	293	VAL	2.3
1	I	306	ASP	2.3
1	I	311	ASP	2.3
1	J	415	THR	2.3
1	I	8	SER	2.3
1	I	270	HIS	2.3
1	K	28	VAL	2.3
1	I	288	ARG	2.2
1	I	10	TYR	2.2
1	L	228	GLY	2.2
1	J	229	GLU	2.2
1	K	40	GLU	2.2
1	D	164	VAL	2.2
1	I	357	VAL	2.2
1	K	5	GLU	2.2
1	K	371	ALA	2.2
1	J	308	SER	2.2
1	I	313	LYS	2.2
1	J	40	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	26	GLN	2.2
1	I	331	ALA	2.2
1	J	288	ARG	2.1
1	J	330	ASN	2.1
1	L	300	GLY	2.1
1	I	289	ALA	2.1
1	J	265	SER	2.1
1	F	13	MET	2.1
1	J	409	PHE	2.1
1	K	6	GLN	2.1
1	J	411	THR	2.1
1	I	353	GLU	2.1
1	J	222	GLU	2.1
1	J	299	GLU	2.1
1	I	309	ILE	2.1
1	J	253	GLN	2.1
1	K	24	PHE	2.1
1	I	314	CYS	2.1
1	K	16	LYS	2.1
1	I	316	ILE	2.1
1	K	366	GLY	2.1
1	I	334	LEU	2.0
1	J	39	LEU	2.0
1	J	336	ASP	2.0
1	I	277	VAL	2.0
1	D	307	GLY	2.0
1	J	284	LYS	2.0
1	K	227	LYS	2.0
1	L	2	THR	2.0
1	I	335	ALA	2.0
1	I	44	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 ⓘ

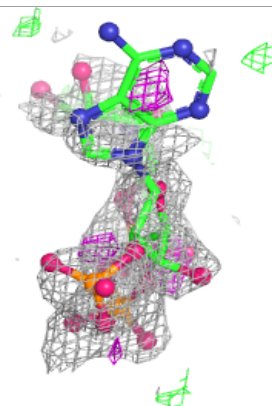
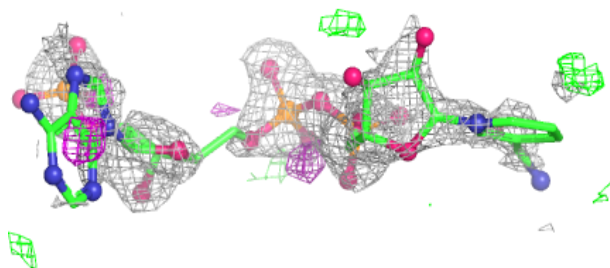
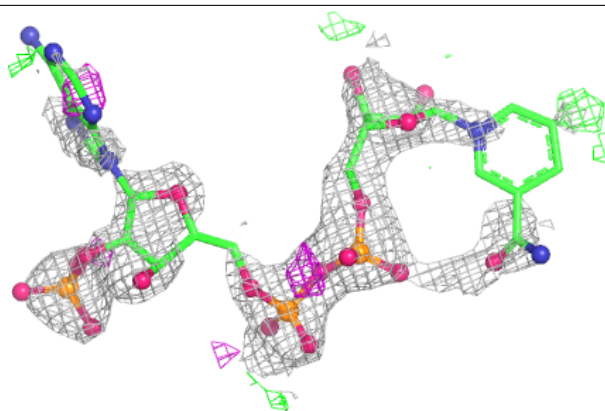
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAP	J	501	48/48	0.71	0.18	69,96,113,116	0
3	AKG	J	502	10/10	0.77	0.17	40,58,69,71	0
3	AKG	E	502	10/10	0.87	0.17	24,35,41,43	0
3	AKG	D	502	10/10	0.87	0.15	22,28,42,56	0
3	AKG	B	502	10/10	0.88	0.15	30,33,41,43	0
3	AKG	A	502	10/10	0.91	0.12	23,31,36,39	0
3	AKG	H	502	10/10	0.92	0.10	25,33,38,39	0
3	AKG	F	502	10/10	0.92	0.12	21,32,40,43	0
3	AKG	G	502	10/10	0.93	0.14	21,32,44,48	0
3	AKG	C	502	10/10	0.94	0.10	21,30,35,35	0
2	NAP	H	501	48/48	0.96	0.07	17,24,43,50	0
2	NAP	G	501	48/48	0.97	0.06	14,18,31,36	0
2	NAP	D	501	48/48	0.98	0.06	12,17,29,32	0
2	NAP	E	501	48/48	0.98	0.06	13,18,37,42	0
2	NAP	F	501	48/48	0.98	0.05	11,16,25,27	0
2	NAP	A	501	48/48	0.98	0.05	12,16,28,32	0
2	NAP	C	501	48/48	0.98	0.06	12,16,27,32	0
2	NAP	B	501	48/48	0.99	0.04	9,11,21,22	0

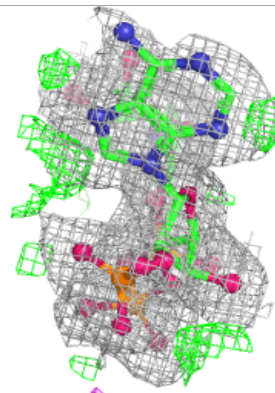
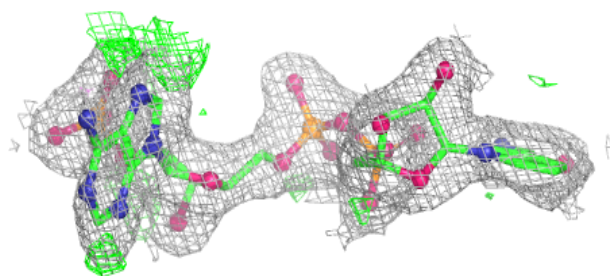
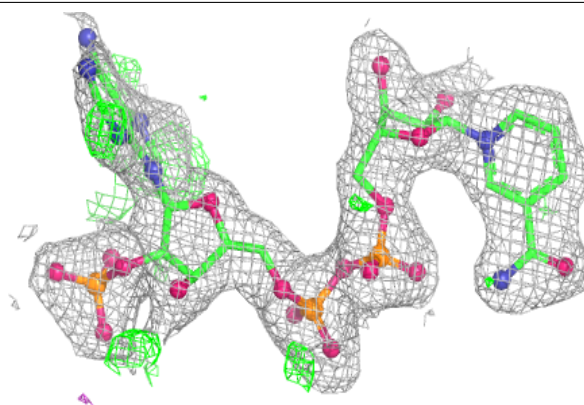
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP J 501:

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

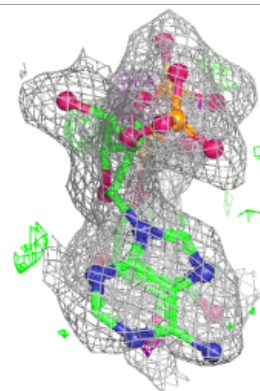
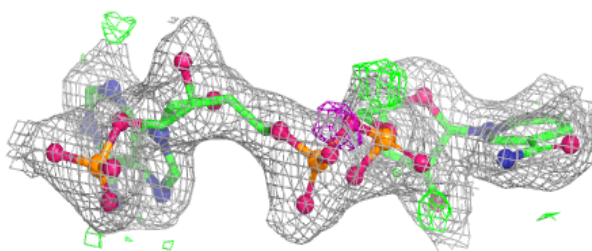
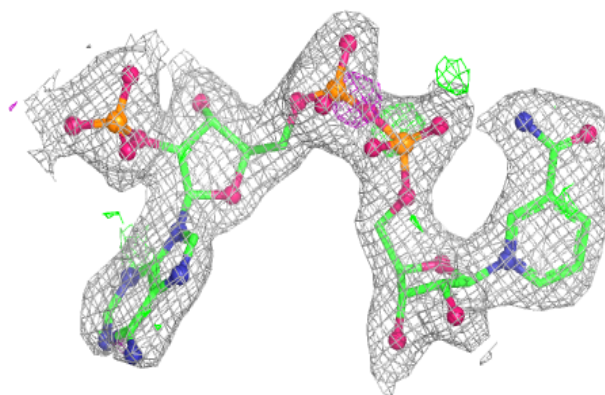
**Electron density around NAP H 501:**

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

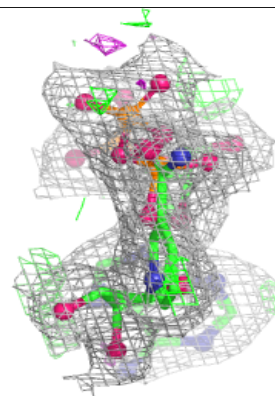
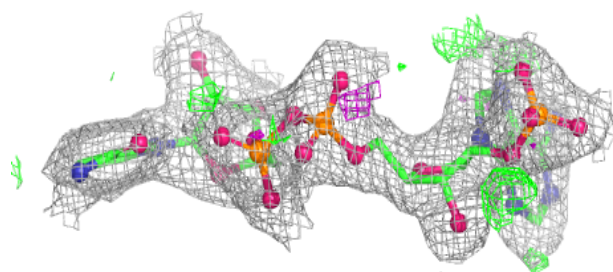
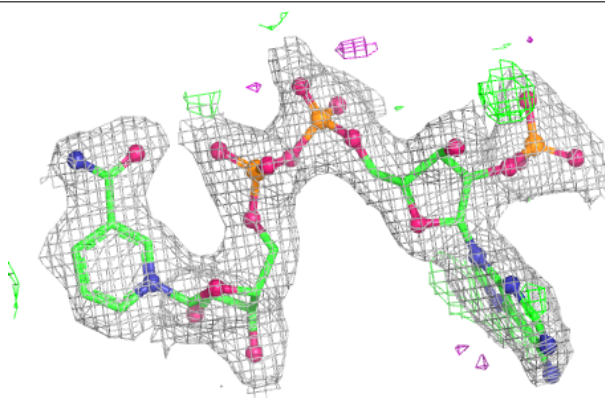


Electron density around NAP G 501:

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

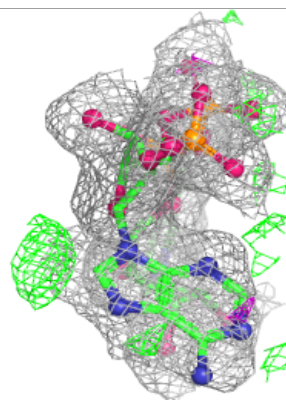
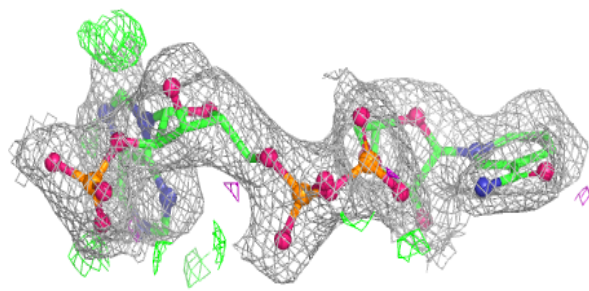
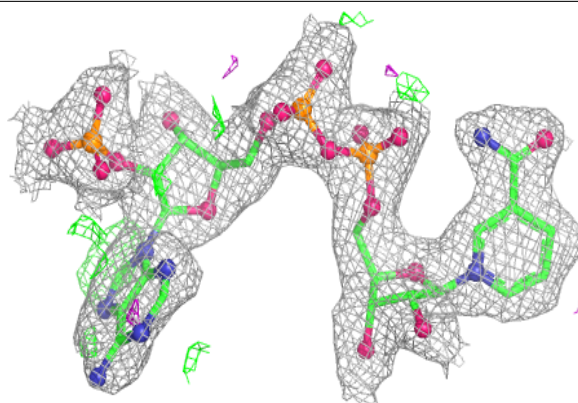
**Electron density around NAP D 501:**

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

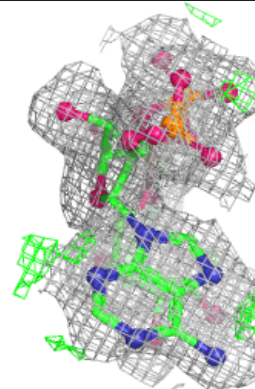
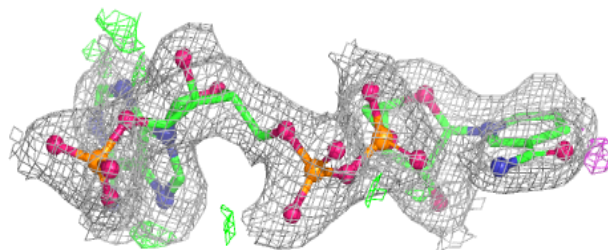
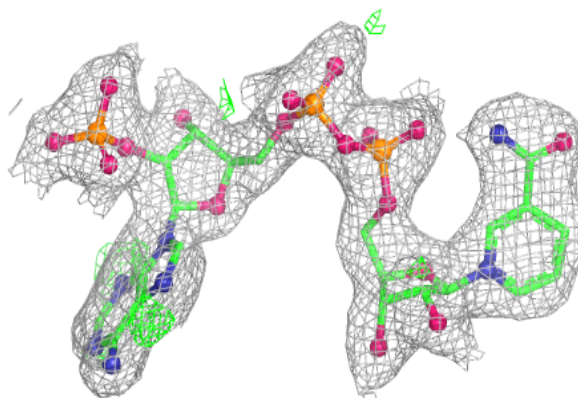


Electron density around NAP E 501:

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

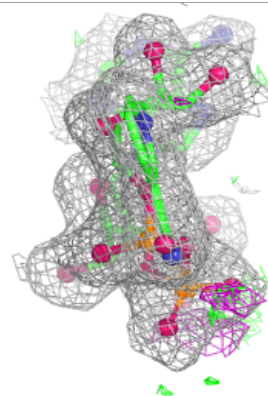
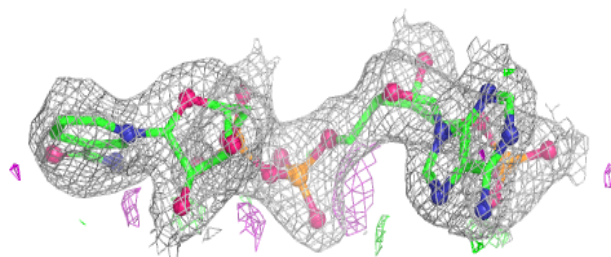
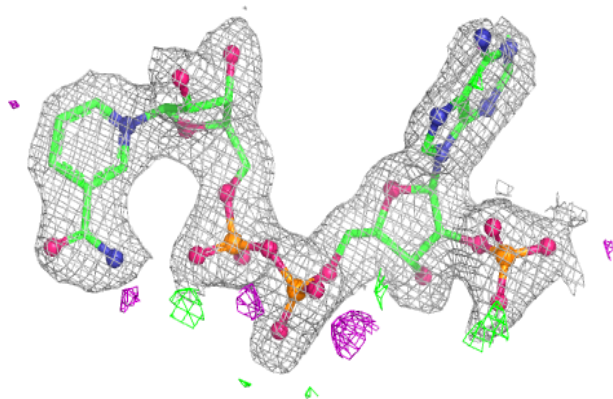
**Electron density around NAP F 501:**

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

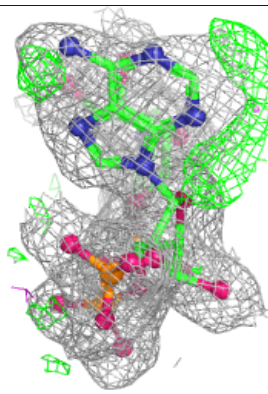
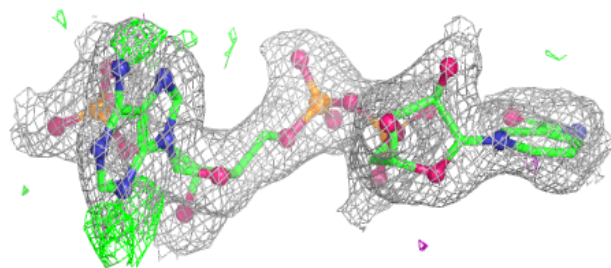
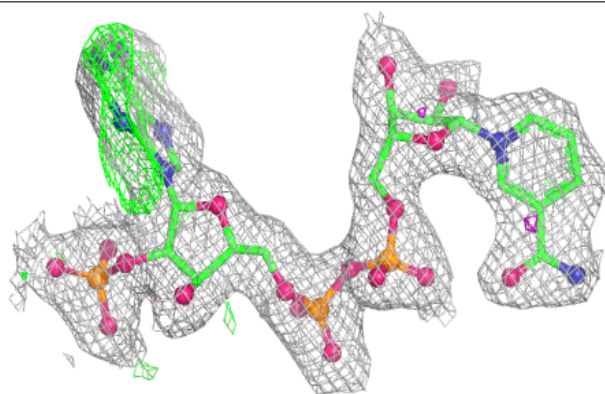


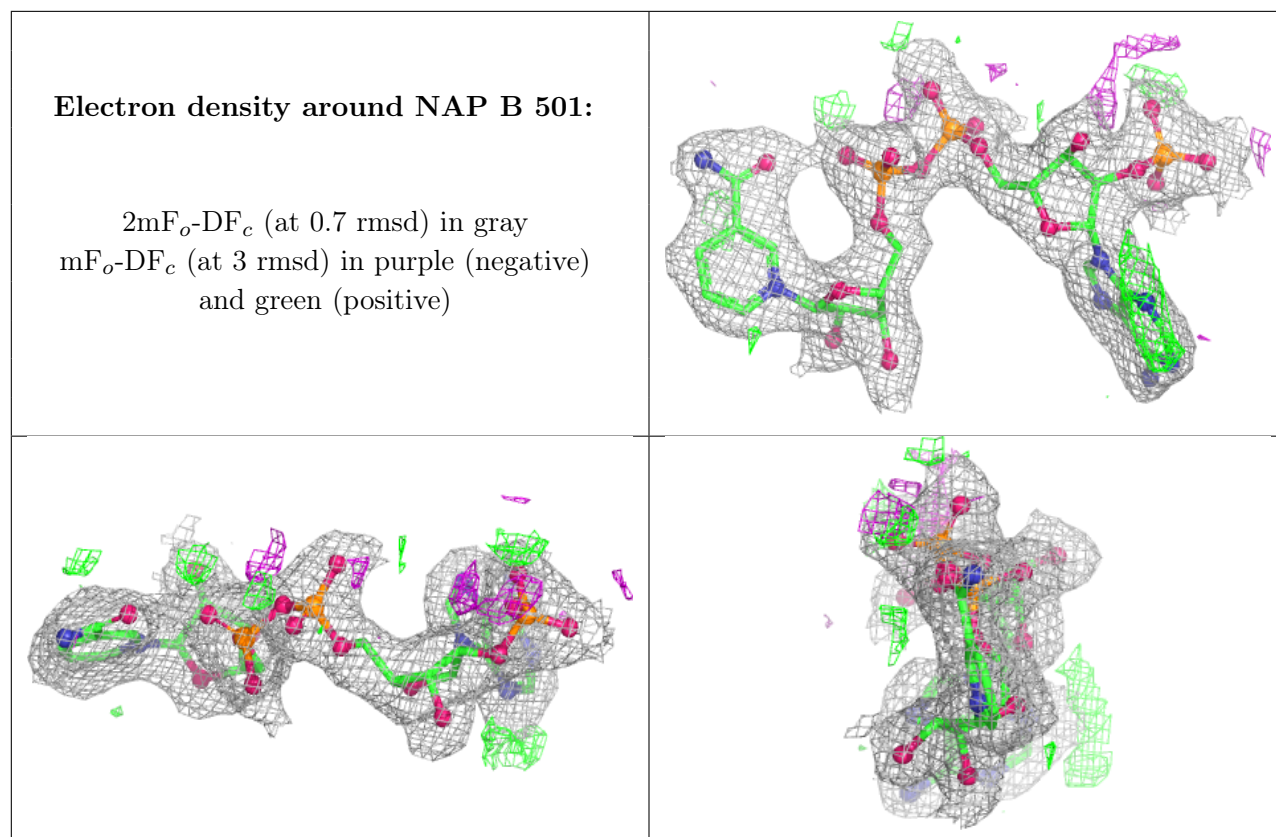
Electron density around NAP A 501:

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

**Electron density around NAP C 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.