



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 04:04 PM UTC

PDB ID : 4AUB / pdb_00004aub
Title : the complex Structure of the bacterial aldo-keto reductase AKR14A1 with NADP and citrate
Authors : Zhu, X.; Ellis, E.M.; Laphorn, A.
Deposited on : 2012-05-16
Resolution : 2.05 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

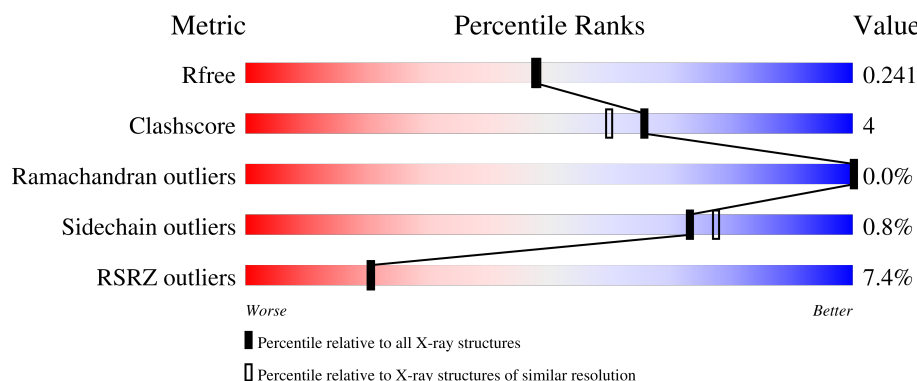
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	366	3% 76% 9% 15%
1	B	366	10% 83% 8% 8%
1	C	366	9% 82% 8% 10%
1	D	366	% 79% • 16%
1	E	366	9% 75% 6% 19%

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Mol	Chain	Length	Quality of chain
1	F	366	5% 75% 6% 19%
1	G	366	6% 84% 7% 8%
1	H	366	8% 78% 19%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21483 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 ALDO-KETO REDUCTASE AKR14A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	2	0
			2472	1561	436	465	10			
1	B	335	Total	C	N	O	S	0	1	0
			2655	1673	470	500	12			
1	C	330	Total	C	N	O	S	0	1	0
			2608	1646	457	493	12			
1	D	308	Total	C	N	O	S	0	0	0
			2430	1535	427	458	10			
1	E	297	Total	C	N	O	S	0	0	0
			2345	1484	411	440	10			
1	F	298	Total	C	N	O	S	0	0	0
			2359	1493	416	440	10			
1	G	335	Total	C	N	O	S	0	3	0
			2665	1681	471	501	12			
1	H	297	Total	C	N	O	S	0	0	0
			2348	1485	411	442	10			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q46851
A	-18	GLY	-	expression tag	UNP Q46851
A	-17	SER	-	expression tag	UNP Q46851
A	-16	SER	-	expression tag	UNP Q46851
A	-15	HIS	-	expression tag	UNP Q46851
A	-14	HIS	-	expression tag	UNP Q46851
A	-13	HIS	-	expression tag	UNP Q46851
A	-12	HIS	-	expression tag	UNP Q46851
A	-11	HIS	-	expression tag	UNP Q46851
A	-10	HIS	-	expression tag	UNP Q46851
A	-9	SER	-	expression tag	UNP Q46851
A	-8	SER	-	expression tag	UNP Q46851
A	-7	GLY	-	expression tag	UNP Q46851

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	expression tag	UNP Q46851
A	-5	VAL	-	expression tag	UNP Q46851
A	-4	PRO	-	expression tag	UNP Q46851
A	-3	ARG	-	expression tag	UNP Q46851
A	-2	GLY	-	expression tag	UNP Q46851
A	-1	SER	-	expression tag	UNP Q46851
A	0	HIS	-	expression tag	UNP Q46851
B	-19	MET	-	expression tag	UNP Q46851
B	-18	GLY	-	expression tag	UNP Q46851
B	-17	SER	-	expression tag	UNP Q46851
B	-16	SER	-	expression tag	UNP Q46851
B	-15	HIS	-	expression tag	UNP Q46851
B	-14	HIS	-	expression tag	UNP Q46851
B	-13	HIS	-	expression tag	UNP Q46851
B	-12	HIS	-	expression tag	UNP Q46851
B	-11	HIS	-	expression tag	UNP Q46851
B	-10	HIS	-	expression tag	UNP Q46851
B	-9	SER	-	expression tag	UNP Q46851
B	-8	SER	-	expression tag	UNP Q46851
B	-7	GLY	-	expression tag	UNP Q46851
B	-6	LEU	-	expression tag	UNP Q46851
B	-5	VAL	-	expression tag	UNP Q46851
B	-4	PRO	-	expression tag	UNP Q46851
B	-3	ARG	-	expression tag	UNP Q46851
B	-2	GLY	-	expression tag	UNP Q46851
B	-1	SER	-	expression tag	UNP Q46851
B	0	HIS	-	expression tag	UNP Q46851
C	-19	MET	-	expression tag	UNP Q46851
C	-18	GLY	-	expression tag	UNP Q46851
C	-17	SER	-	expression tag	UNP Q46851
C	-16	SER	-	expression tag	UNP Q46851
C	-15	HIS	-	expression tag	UNP Q46851
C	-14	HIS	-	expression tag	UNP Q46851
C	-13	HIS	-	expression tag	UNP Q46851
C	-12	HIS	-	expression tag	UNP Q46851
C	-11	HIS	-	expression tag	UNP Q46851
C	-10	HIS	-	expression tag	UNP Q46851
C	-9	SER	-	expression tag	UNP Q46851
C	-8	SER	-	expression tag	UNP Q46851
C	-7	GLY	-	expression tag	UNP Q46851
C	-6	LEU	-	expression tag	UNP Q46851
C	-5	VAL	-	expression tag	UNP Q46851

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	expression tag	UNP Q46851
C	-3	ARG	-	expression tag	UNP Q46851
C	-2	GLY	-	expression tag	UNP Q46851
C	-1	SER	-	expression tag	UNP Q46851
C	0	HIS	-	expression tag	UNP Q46851
D	-19	MET	-	expression tag	UNP Q46851
D	-18	GLY	-	expression tag	UNP Q46851
D	-17	SER	-	expression tag	UNP Q46851
D	-16	SER	-	expression tag	UNP Q46851
D	-15	HIS	-	expression tag	UNP Q46851
D	-14	HIS	-	expression tag	UNP Q46851
D	-13	HIS	-	expression tag	UNP Q46851
D	-12	HIS	-	expression tag	UNP Q46851
D	-11	HIS	-	expression tag	UNP Q46851
D	-10	HIS	-	expression tag	UNP Q46851
D	-9	SER	-	expression tag	UNP Q46851
D	-8	SER	-	expression tag	UNP Q46851
D	-7	GLY	-	expression tag	UNP Q46851
D	-6	LEU	-	expression tag	UNP Q46851
D	-5	VAL	-	expression tag	UNP Q46851
D	-4	PRO	-	expression tag	UNP Q46851
D	-3	ARG	-	expression tag	UNP Q46851
D	-2	GLY	-	expression tag	UNP Q46851
D	-1	SER	-	expression tag	UNP Q46851
D	0	HIS	-	expression tag	UNP Q46851
E	-19	MET	-	expression tag	UNP Q46851
E	-18	GLY	-	expression tag	UNP Q46851
E	-17	SER	-	expression tag	UNP Q46851
E	-16	SER	-	expression tag	UNP Q46851
E	-15	HIS	-	expression tag	UNP Q46851
E	-14	HIS	-	expression tag	UNP Q46851
E	-13	HIS	-	expression tag	UNP Q46851
E	-12	HIS	-	expression tag	UNP Q46851
E	-11	HIS	-	expression tag	UNP Q46851
E	-10	HIS	-	expression tag	UNP Q46851
E	-9	SER	-	expression tag	UNP Q46851
E	-8	SER	-	expression tag	UNP Q46851
E	-7	GLY	-	expression tag	UNP Q46851
E	-6	LEU	-	expression tag	UNP Q46851
E	-5	VAL	-	expression tag	UNP Q46851
E	-4	PRO	-	expression tag	UNP Q46851
E	-3	ARG	-	expression tag	UNP Q46851

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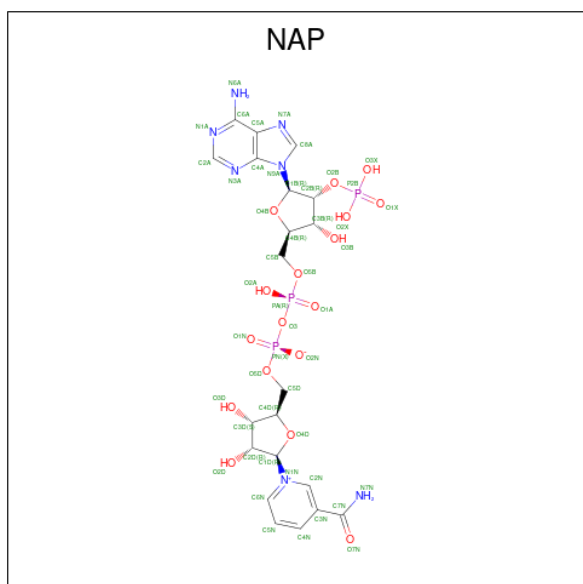
Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP Q46851
E	-1	SER	-	expression tag	UNP Q46851
E	0	HIS	-	expression tag	UNP Q46851
F	-19	MET	-	expression tag	UNP Q46851
F	-18	GLY	-	expression tag	UNP Q46851
F	-17	SER	-	expression tag	UNP Q46851
F	-16	SER	-	expression tag	UNP Q46851
F	-15	HIS	-	expression tag	UNP Q46851
F	-14	HIS	-	expression tag	UNP Q46851
F	-13	HIS	-	expression tag	UNP Q46851
F	-12	HIS	-	expression tag	UNP Q46851
F	-11	HIS	-	expression tag	UNP Q46851
F	-10	HIS	-	expression tag	UNP Q46851
F	-9	SER	-	expression tag	UNP Q46851
F	-8	SER	-	expression tag	UNP Q46851
F	-7	GLY	-	expression tag	UNP Q46851
F	-6	LEU	-	expression tag	UNP Q46851
F	-5	VAL	-	expression tag	UNP Q46851
F	-4	PRO	-	expression tag	UNP Q46851
F	-3	ARG	-	expression tag	UNP Q46851
F	-2	GLY	-	expression tag	UNP Q46851
F	-1	SER	-	expression tag	UNP Q46851
F	0	HIS	-	expression tag	UNP Q46851
G	-19	MET	-	expression tag	UNP Q46851
G	-18	GLY	-	expression tag	UNP Q46851
G	-17	SER	-	expression tag	UNP Q46851
G	-16	SER	-	expression tag	UNP Q46851
G	-15	HIS	-	expression tag	UNP Q46851
G	-14	HIS	-	expression tag	UNP Q46851
G	-13	HIS	-	expression tag	UNP Q46851
G	-12	HIS	-	expression tag	UNP Q46851
G	-11	HIS	-	expression tag	UNP Q46851
G	-10	HIS	-	expression tag	UNP Q46851
G	-9	SER	-	expression tag	UNP Q46851
G	-8	SER	-	expression tag	UNP Q46851
G	-7	GLY	-	expression tag	UNP Q46851
G	-6	LEU	-	expression tag	UNP Q46851
G	-5	VAL	-	expression tag	UNP Q46851
G	-4	PRO	-	expression tag	UNP Q46851
G	-3	ARG	-	expression tag	UNP Q46851
G	-2	GLY	-	expression tag	UNP Q46851
G	-1	SER	-	expression tag	UNP Q46851

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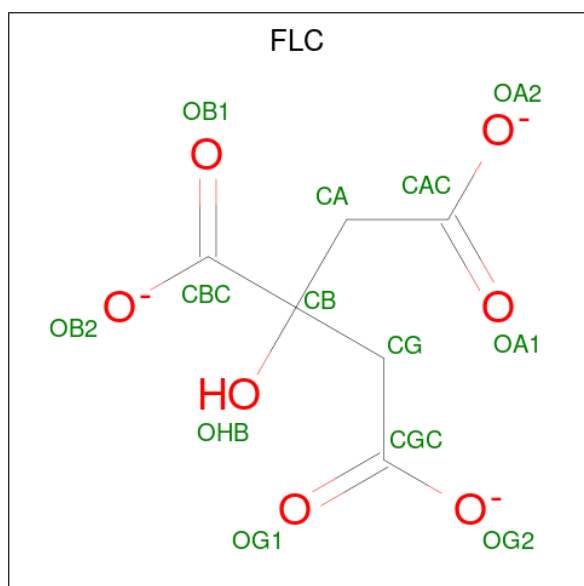
Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP Q46851
H	-19	MET	-	expression tag	UNP Q46851
H	-18	GLY	-	expression tag	UNP Q46851
H	-17	SER	-	expression tag	UNP Q46851
H	-16	SER	-	expression tag	UNP Q46851
H	-15	HIS	-	expression tag	UNP Q46851
H	-14	HIS	-	expression tag	UNP Q46851
H	-13	HIS	-	expression tag	UNP Q46851
H	-12	HIS	-	expression tag	UNP Q46851
H	-11	HIS	-	expression tag	UNP Q46851
H	-10	HIS	-	expression tag	UNP Q46851
H	-9	SER	-	expression tag	UNP Q46851
H	-8	SER	-	expression tag	UNP Q46851
H	-7	GLY	-	expression tag	UNP Q46851
H	-6	LEU	-	expression tag	UNP Q46851
H	-5	VAL	-	expression tag	UNP Q46851
H	-4	PRO	-	expression tag	UNP Q46851
H	-3	ARG	-	expression tag	UNP Q46851
H	-2	GLY	-	expression tag	UNP Q46851
H	-1	SER	-	expression tag	UNP Q46851
H	0	HIS	-	expression tag	UNP Q46851

- 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	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		

- Molecule 3 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	0
			13	6	7		
3	G	1	Total	C	O	0	0
			13	6	7		
3	H	1	Total	C	O	0	0
			13	6	7		

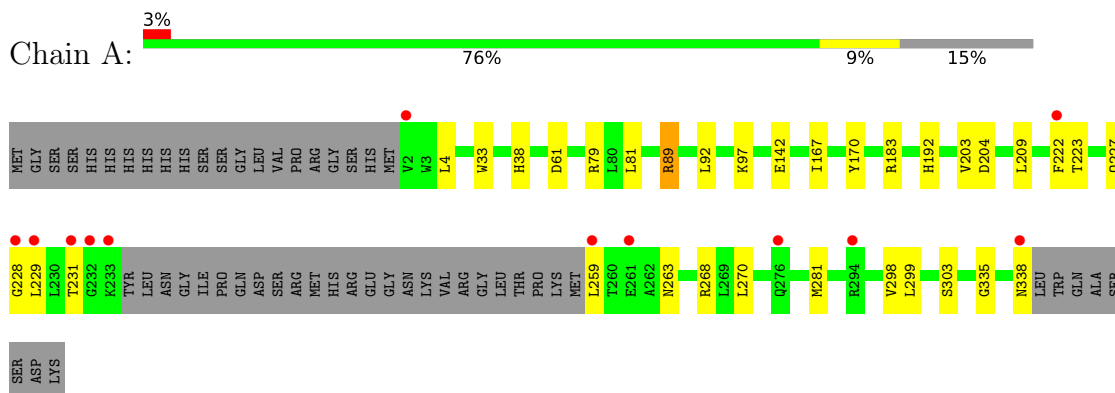
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	181	Total	O	0	0
			181	181		
4	B	155	Total	O	0	0
			155	155		
4	C	142	Total	O	0	0
			142	142		
4	D	161	Total	O	0	0
			161	161		
4	E	121	Total	O	0	0
			121	121		
4	F	156	Total	O	0	0
			156	156		
4	G	132	Total	O	0	0
			132	132		
4	H	113	Total	O	0	0
			113	113		

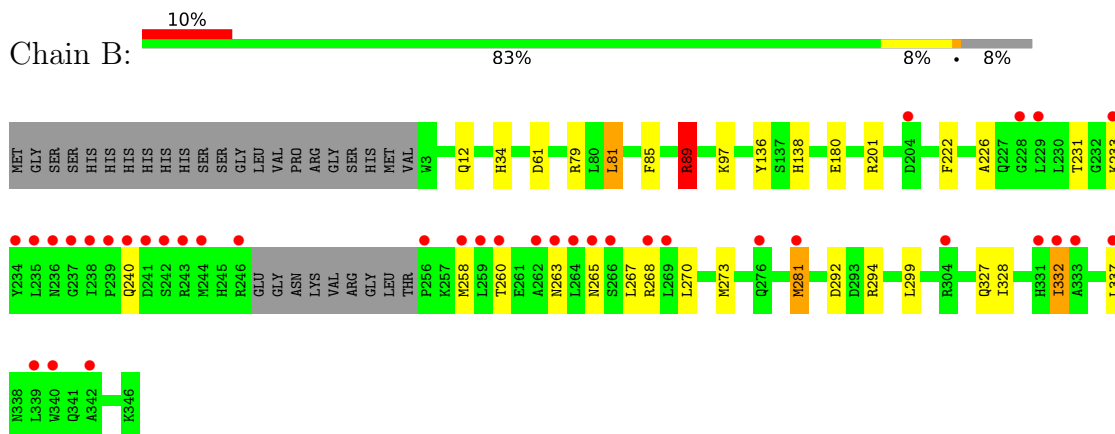
3 Residue-property plots

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.

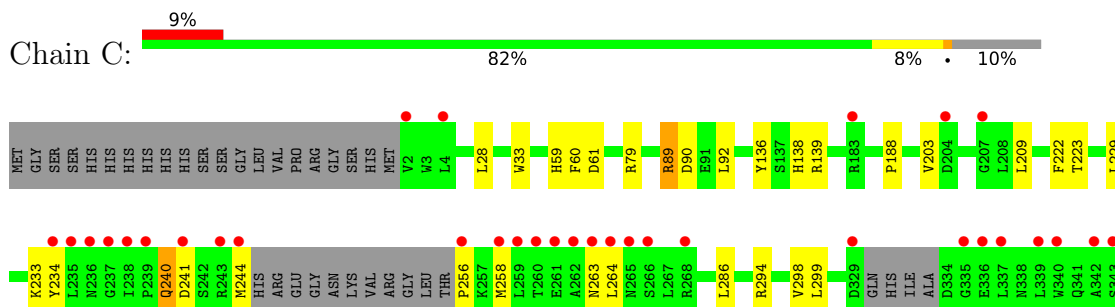
- Molecule 1: ALDO-KETO REDUCTASE AKR14A1



- Molecule 1: ALDO-KETO REDUCTASE AKR14A1

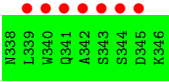
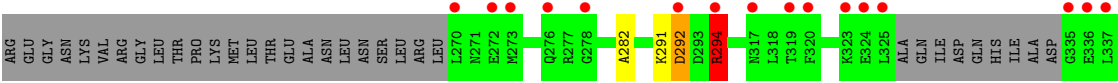
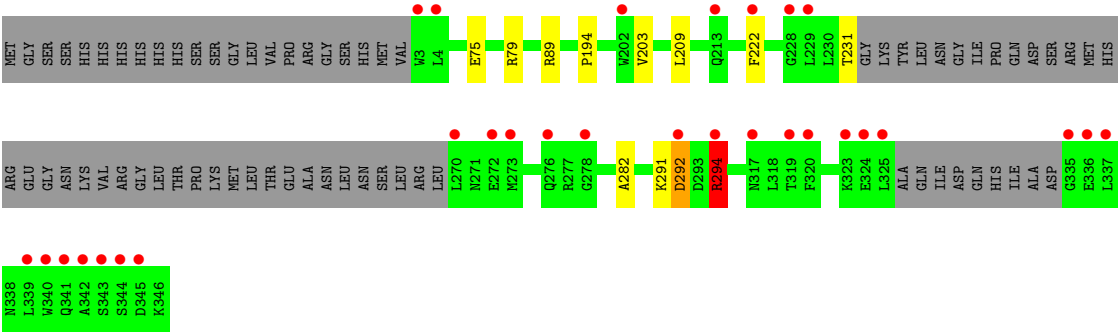
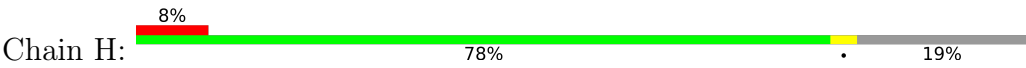


- Molecule 1: ALDO-KETO REDUCTASE AKR14A1





● Molecule 1: ALDO-KETO REDUCTASE AKR14A1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.81Å 191.09Å 97.30Å 90.00° 105.97° 90.00°	Depositor
Resolution (Å)	95.35 – 2.05 95.35 – 2.05	Depositor EDS
% Data completeness (in resolution range)	92.2 (95.35-2.05) 92.2 (95.35-2.05)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.34 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.202 , 0.238 0.203 , 0.241	Depositor DCC
R_{free} test set	10115 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21483	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% 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: FLC, NAP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.24	4/2528 (0.2%)	1.00	2/3421 (0.1%)
1	B	1.21	2/2716 (0.1%)	0.97	2/3672 (0.1%)
1	C	1.22	4/2664 (0.2%)	0.97	3/3601 (0.1%)
1	D	1.30	6/2480 (0.2%)	1.00	2/3358 (0.1%)
1	E	1.13	3/2395 (0.1%)	0.95	2/3239 (0.1%)
1	F	1.21	6/2409 (0.2%)	0.99	2/3261 (0.1%)
1	G	1.19	5/2733 (0.2%)	1.01	3/3694 (0.1%)
1	H	1.14	0/2398	0.96	3/3243 (0.1%)
All	All	1.21	30/20323 (0.1%)	0.98	19/27489 (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	A	0	1
1	B	0	2
1	C	0	2
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
All	All	0	9

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	222	PHE	CA-CB	7.39	1.64	1.53
1	F	76	ASN	N-CA	6.58	1.54	1.46
1	D	331	HIS	CG-CD2	6.48	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	138	HIS	ND1-CE1	6.35	1.38	1.32
1	D	138	HIS	CG-CD2	6.16	1.42	1.35
1	D	202	TRP	CD2-CE2	6.15	1.51	1.41
1	F	126	ARG	C-O	-5.91	1.17	1.24
1	C	138	HIS	CG-CD2	5.89	1.42	1.35
1	D	193	GLN	CA-C	5.74	1.59	1.52
1	B	138	HIS	CG-CD2	5.64	1.42	1.35
1	F	43	GLU	C-O	-5.61	1.17	1.24
1	A	38	HIS	ND1-CE1	5.51	1.38	1.32
1	E	138	HIS	ND1-CE1	5.46	1.38	1.32
1	G	125	LYS	C-O	-5.46	1.17	1.24
1	G	138	HIS	CG-CD2	5.46	1.41	1.35
1	E	59	HIS	CE1-NE2	5.38	1.38	1.32
1	D	192	HIS	CG-ND1	-5.35	1.32	1.38
1	A	223	THR	N-CA	5.25	1.50	1.46
1	E	138	HIS	CG-CD2	5.25	1.41	1.35
1	G	331	HIS	CG-CD2	5.22	1.41	1.35
1	F	59	HIS	CG-CD2	5.21	1.41	1.35
1	F	38	HIS	CE1-NE2	5.20	1.37	1.32
1	G	38	HIS	CG-CD2	5.10	1.41	1.35
1	F	38	HIS	CG-CD2	5.09	1.41	1.35
1	C	90	ASP	N-CA	-5.06	1.39	1.46
1	C	59	HIS	ND1-CE1	5.03	1.37	1.32
1	B	34	HIS	CG-ND1	-5.03	1.32	1.38
1	A	192	HIS	CG-ND1	-5.01	1.32	1.38
1	A	92	LEU	N-CA	5.01	1.51	1.45
1	G	291	LYS	CA-C	5.01	1.59	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	240	GLN	N-CA-C	-9.69	97.74	110.53
1	C	264	LEU	N-CA-C	7.31	119.88	111.11
1	E	89	ARG	CG-CD-NE	7.18	127.80	112.00
1	H	294	ARG	CG-CD-NE	6.96	127.31	112.00
1	B	89	ARG	CG-CD-NE	6.89	127.16	112.00
1	C	89	ARG	CG-CD-NE	6.81	126.97	112.00
1	H	89	ARG	CG-CD-NE	6.80	126.95	112.00
1	F	292	ASP	CB-CA-C	-6.78	96.51	109.66
1	H	292	ASP	CB-CA-C	-6.76	96.55	109.66
1	G	272	GLU	CB-CA-C	-6.73	100.26	110.90
1	D	89	ARG	CG-CD-NE	6.70	126.75	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	ARG	CG-CD-NE	6.70	126.74	112.00
1	G	89	ARG	CG-CD-NE	6.49	126.29	112.00
1	F	89	ARG	CG-CD-NE	6.42	126.13	112.00
1	G	276	GLN	CA-CB-CG	5.79	125.67	114.10
1	E	118	ALA	N-CA-C	-5.50	105.36	111.36
1	D	227	GLN	CB-CA-C	-5.42	104.19	111.89
1	B	332	ILE	N-CA-C	5.32	115.18	106.72
1	A	227	GLN	CB-CA-C	-5.25	104.44	111.89

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	89	ARG	Sidechain
1	B	136	TYR	Peptide
1	B	89	ARG	Sidechain
1	C	136	TYR	Peptide
1	C	89	ARG	Sidechain
1	D	89	ARG	Sidechain
1	E	89	ARG	Sidechain
1	F	89	ARG	Sidechain
1	G	89	ARG	Sidechain

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	2472	0	2446	25	0
1	B	2655	0	2617	30	0
1	C	2608	0	2577	22	0
1	D	2430	0	2396	8	0
1	E	2345	0	2305	20	0
1	F	2359	0	2332	17	0
1	G	2665	0	2634	31	0
1	H	2348	0	2307	7	0
2	A	48	0	25	6	0
2	B	48	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	48	0	25	5	0
2	E	48	0	25	2	0
2	F	48	0	25	2	0
2	G	48	0	25	1	0
2	H	48	0	25	1	0
3	A	13	0	5	0	0
3	B	13	0	5	0	0
3	C	13	0	5	0	0
3	D	13	0	5	0	0
3	E	13	0	5	1	0
3	F	13	0	5	3	0
3	G	13	0	5	1	0
3	H	13	0	5	1	0
4	A	181	0	0	3	0
4	B	155	0	0	2	0
4	C	142	0	0	3	0
4	D	161	0	0	2	0
4	E	121	0	0	0	0
4	F	156	0	0	1	0
4	G	132	0	0	1	0
4	H	113	0	0	0	0
All	All	21483	0	19829	153	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 (153) 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:180:GLU:HG2	4:B:2124:HOH:O	1.59	1.02
1:B:328:ILE:HG23	1:B:332:ILE:HD12	1.40	1.02
1:D:142:GLU:HB3	4:D:2095:HOH:O	1.63	0.97
1:A:79:ARG:NH1	1:G:79:ARG:CZ	2.27	0.97
1:F:292:ASP:HB3	1:F:294:ARG:HG2	1.50	0.93
1:F:332:ILE:HD12	1:F:332:ILE:O	1.67	0.93
1:F:270:LEU:HD11	1:F:332:ILE:HG21	1.51	0.90
1:B:328:ILE:HG23	1:B:332:ILE:CD1	2.04	0.86
1:G:76:ASN:OD1	1:G:79:ARG:NH1	2.08	0.85
1:G:201:ARG:HH22	1:G:328:ILE:HG22	1.45	0.81
1:G:271:ASN:OD1	1:G:281:MET:HE2	1.83	0.77
1:A:222:PHE:CE1	2:A:500:NAP:C4N	2.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:ILE:CG2	1:B:332:ILE:HD12	2.17	0.74
1:B:267:LEU:HD22	1:B:281:MET:CE	2.17	0.73
1:B:267:LEU:CD2	1:B:281:MET:HE1	2.17	0.73
1:F:270:LEU:HD11	1:F:332:ILE:CG2	2.17	0.73
1:H:231:THR:HG22	1:H:282:ALA:HB2	1.71	0.71
3:F:501:FLC:CBC	3:F:501:FLC:OA2	2.39	0.70
1:C:244:MET:C	4:C:2117:HOH:O	2.34	0.70
1:B:201:ARG:HH22	1:B:328:ILE:HG22	1.56	0.70
1:E:292:ASP:HB3	1:E:294:ARG:HG3	1.73	0.70
1:A:79:ARG:NH1	1:G:79:ARG:NH2	2.40	0.69
1:C:233:LYS:HE3	1:C:234:TYR:CZ	2.28	0.69
1:C:222:PHE:CE1	2:C:500:NAP:C4N	2.75	0.69
1:B:267:LEU:HD22	1:B:281:MET:HE1	1.73	0.68
1:B:265:ASN:O	1:B:268:ARG:HG2	1.94	0.68
1:A:79:ARG:CZ	1:G:79:ARG:NE	2.57	0.67
1:E:270:LEU:HB3	1:E:281:MET:HE1	1.76	0.67
1:B:270:LEU:HD21	1:B:332:ILE:HD11	1.77	0.67
1:F:292:ASP:CB	1:F:294:ARG:HG2	2.23	0.67
1:C:258:MET:O	1:C:263:ASN:ND2	2.28	0.66
1:B:267:LEU:CD2	1:B:281:MET:CE	2.75	0.64
1:B:222:PHE:CE1	2:B:500:NAP:C4N	2.80	0.64
1:G:271:ASN:HB2	1:G:281:MET:HE1	1.81	0.63
1:A:79:ARG:CZ	1:G:79:ARG:CZ	2.79	0.61
3:E:501:FLC:CBC	3:E:501:FLC:OA2	2.49	0.60
1:C:233:LYS:NZ	2:C:500:NAP:O1X	2.31	0.60
1:G:201:ARG:HH21	1:G:332:ILE:HD11	1.67	0.60
1:A:79:ARG:HH11	1:G:79:ARG:NH2	1.99	0.59
1:E:222:PHE:CE1	2:E:500:NAP:C4N	2.84	0.59
1:F:222:PHE:CE1	2:F:500:NAP:C4N	2.86	0.59
1:H:292:ASP:HB3	1:H:294:ARG:HG3	1.85	0.58
1:B:270:LEU:HD21	1:B:332:ILE:CD1	2.33	0.58
1:F:231:THR:HG22	1:F:282:ALA:HB2	1.85	0.57
1:F:332:ILE:O	1:F:332:ILE:CD1	2.48	0.57
1:B:292:ASP:OD1	1:B:294:ARG:HB2	2.05	0.57
1:A:142:GLU:HG2	4:A:2117:HOH:O	2.06	0.56
1:D:142:GLU:HG2	4:D:2093:HOH:O	2.05	0.56
1:B:273:MET:HE1	1:B:327:GLN:HB3	1.88	0.56
1:G:330:GLN:HG3	1:G:331:HIS:CE1	2.41	0.56
1:C:79:ARG:CD	1:E:79:ARG:CZ	2.84	0.56
1:G:222:PHE:CE1	2:G:500:NAP:C4N	2.89	0.56
1:E:146:MET:HE1	1:E:177:LYS:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:TYR:CG	1:D:203:VAL:HG21	2.44	0.53
1:G:42:LEU:HD13	1:G:79:ARG:NH1	2.24	0.53
1:G:292:ASP:OD1	1:G:294:ARG:HB2	2.07	0.53
1:F:294:ARG:HG3	1:F:294:ARG:HH11	1.72	0.53
1:A:222:PHE:CD1	2:A:500:NAP:C4N	2.91	0.53
1:B:267:LEU:HD23	1:B:281:MET:HE1	1.89	0.53
1:D:286:LEU:HD22	1:D:298:VAL:HG21	1.90	0.52
1:G:201:ARG:HH22	1:G:328:ILE:CG2	2.17	0.52
1:E:61:ASP:HB3	1:E:299:LEU:HD11	1.90	0.52
1:F:264:LEU:HA	1:F:267:LEU:HD12	1.91	0.52
1:D:42:LEU:HD22	1:F:79:ARG:HH22	1.74	0.52
1:A:259:LEU:N	4:A:2157:HOH:O	2.42	0.52
1:C:233:LYS:HE3	1:C:234:TYR:CE2	2.46	0.51
1:F:327:GLN:HG3	4:F:2154:HOH:O	2.11	0.51
1:B:79:ARG:CD	1:H:79:ARG:CZ	2.88	0.51
1:G:330:GLN:HB3	1:G:331:HIS:CD2	2.45	0.51
1:G:241:ASP:OD1	1:G:304[A]:ARG:NH2	2.45	0.50
1:B:201:ARG:NH2	1:B:328:ILE:HG22	2.24	0.50
1:A:268:ARG:HD3	4:A:2159:HOH:O	2.12	0.50
1:B:81:LEU:HD12	1:B:85:PHE:HB2	1.94	0.50
1:C:28:LEU:HD12	1:C:28:LEU:N	2.26	0.49
1:A:33:TRP:HB2	2:A:500:NAP:H2D	1.93	0.49
1:H:222:PHE:CE1	2:H:500:NAP:C4N	2.95	0.49
1:E:31:GLY:C	1:E:32:LEU:HD12	2.38	0.49
1:C:139:ARG:NE	4:C:2060:HOH:O	2.46	0.49
1:E:146:MET:CE	1:E:177:LYS:HG2	2.43	0.49
1:E:146:MET:HE3	1:E:177:LYS:CG	2.44	0.48
1:A:61:ASP:HB3	1:A:299:LEU:HD11	1.94	0.48
1:A:263:ASN:ND2	1:A:335:GLY:O	2.45	0.48
1:D:196:TYR:CD1	1:D:203:VAL:CG2	2.96	0.48
1:A:203:VAL:HG12	1:A:209:LEU:HG	1.96	0.48
1:G:232:GLY:HA3	1:G:281:MET:HE3	1.95	0.48
1:G:76:ASN:OD1	1:G:79:ARG:CZ	2.61	0.48
1:G:281:MET:HE2	1:G:281:MET:HB2	1.54	0.48
1:C:209:LEU:HD13	1:C:294:ARG:HB3	1.96	0.48
1:A:299:LEU:O	2:A:500:NAP:H51N	2.13	0.48
1:B:258:MET:O	1:B:263:ASN:ND2	2.47	0.48
1:C:60:PHE:HE2	1:C:92:LEU:HD22	1.79	0.48
1:G:330:GLN:CG	1:G:331:HIS:NE2	2.77	0.47
1:B:61:ASP:OD2	1:B:97:LYS:NZ	2.47	0.47
1:E:203:VAL:HG12	1:E:209:LEU:HG	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:330:GLN:HG2	1:G:331:HIS:NE2	2.29	0.47
1:A:303:SER:OG	2:A:500:NAP:O3X	2.25	0.47
1:E:32:LEU:HD12	1:E:32:LEU:N	2.30	0.47
1:B:273:MET:CE	1:B:327:GLN:HB3	2.45	0.46
1:G:232:GLY:CA	1:G:281:MET:HE3	2.46	0.46
1:A:204:ASP:OD1	1:A:209:LEU:HD11	2.16	0.46
1:E:146:MET:CE	1:E:177:LYS:CG	2.94	0.45
1:G:328:ILE:HG23	1:G:332:ILE:HG12	1.97	0.45
1:G:198:LEU:HD22	1:G:332:ILE:CD1	2.48	0.44
3:G:501:FLC:OA2	3:G:501:FLC:CBC	2.65	0.44
1:B:267:LEU:HD22	1:B:281:MET:HE2	1.99	0.44
2:F:500:NAP:C4N	3:F:501:FLC:CGC	2.95	0.44
1:C:79:ARG:HD2	1:E:79:ARG:CZ	2.47	0.44
1:C:188:PRO:HG2	4:C:2105:HOH:O	2.17	0.44
1:C:286:LEU:HD22	1:C:298:VAL:HG21	2.00	0.43
1:A:270:LEU:HB3	1:A:281:MET:HE1	2.01	0.43
1:A:298:VAL:O	1:A:298:VAL:HG23	2.18	0.43
1:G:270:LEU:HD21	1:G:332:ILE:HG21	1.99	0.43
1:H:291:LYS:HG2	1:H:292:ASP:OD1	2.18	0.43
1:B:226:ALA:HB1	1:B:337:LEU:HD22	2.01	0.43
1:C:61:ASP:HB3	1:C:299:LEU:HD11	2.00	0.43
1:C:240:GLN:O	1:C:241:ASP:HB2	2.19	0.43
1:E:117:LEU:HD23	1:E:117:LEU:HA	1.86	0.43
1:G:201:ARG:NH2	1:G:328:ILE:CG2	2.81	0.43
1:G:323:LYS:HG3	4:G:2128:HOH:O	2.17	0.43
1:C:79:ARG:HD2	1:E:79:ARG:NE	2.34	0.43
1:E:232:GLY:O	1:E:233:LYS:C	2.61	0.43
1:A:167:ILE:HD12	1:A:170:TYR:CG	2.54	0.42
1:C:244:MET:HE2	1:C:256:PRO:N	2.34	0.42
1:E:193:GLN:OE1	2:E:500:NAP:H2N	2.19	0.42
1:G:76:ASN:OD1	1:G:79:ARG:NH2	2.52	0.42
1:B:231:THR:OG1	1:B:233:LYS:HB2	2.19	0.42
1:A:61:ASP:CB	1:A:299:LEU:HD11	2.49	0.42
1:C:203:VAL:CG1	1:C:209:LEU:HG	2.49	0.42
1:H:203:VAL:CG1	1:H:209:LEU:HG	2.50	0.42
1:G:286:LEU:HD22	1:G:298:VAL:HG21	2.01	0.42
1:A:222:PHE:CD1	2:A:500:NAP:C5N	3.02	0.41
1:B:79:ARG:NH2	1:H:75:GLU:OE1	2.52	0.41
1:B:12:GLN:HG2	4:B:2004:HOH:O	2.20	0.41
1:B:61:ASP:HB3	1:B:299:LEU:HD11	2.02	0.41
1:F:291:LYS:HG2	1:F:292:ASP:OD1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:77:PHE:CE2	1:F:81:LEU:HD12	2.56	0.41
1:B:260:THR:H	1:B:263:ASN:HD22	1.68	0.41
1:B:267:LEU:HD23	1:B:281:MET:CE	2.50	0.41
1:G:330:GLN:CG	1:G:331:HIS:CD2	3.04	0.41
1:C:222:PHE:CD1	2:C:500:NAP:C5N	3.04	0.41
3:H:501:FLC:OA2	3:H:501:FLC:CB	2.69	0.41
1:C:33:TRP:HB2	2:C:500:NAP:H2D	2.02	0.40
1:E:146:MET:HE1	1:E:177:LYS:CB	2.48	0.40
1:F:100:TYR:CG	3:F:501:FLC:HA1	2.56	0.40
1:C:223:THR:HG22	2:C:500:NAP:O2N	2.20	0.40
1:D:51:LYS:NZ	1:D:309:GLU:OE2	2.38	0.40
1:D:192:HIS:CE1	1:D:208:LEU:HD21	2.57	0.40
1:F:60:PHE:HE2	1:F:92:LEU:HD22	1.86	0.40
1:A:61:ASP:OD2	1:A:97:LYS:NZ	2.46	0.40
1:F:209:LEU:HD13	1:F:294:ARG:HB3	2.04	0.40
1:A:228:GLY:HA2	1:A:231:THR:HG23	2.03	0.40
1:A:4:LEU:HD12	1:E:4:LEU:HD12	2.03	0.40
1:E:167:ILE:HG21	1:E:167:ILE:HD13	1.88	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	310/366 (85%)	300 (97%)	10 (3%)	0	100	100
1	B	332/366 (91%)	322 (97%)	10 (3%)	0	100	100
1	C	325/366 (89%)	314 (97%)	11 (3%)	0	100	100
1	D	304/366 (83%)	297 (98%)	7 (2%)	0	100	100
1	E	291/366 (80%)	282 (97%)	9 (3%)	0	100	100
1	F	294/366 (80%)	287 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	332/366 (91%)	322 (97%)	10 (3%)	0	100	100
1	H	291/366 (80%)	283 (97%)	7 (2%)	1 (0%)	36	30
All	All	2479/2928 (85%)	2407 (97%)	71 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	194	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	262/307 (85%)	257 (98%)	5 (2%)	50	50
1	B	282/307 (92%)	278 (99%)	4 (1%)	59	60
1	C	278/307 (91%)	277 (100%)	1 (0%)	84	88
1	D	257/307 (84%)	256 (100%)	1 (0%)	84	88
1	E	247/307 (80%)	246 (100%)	1 (0%)	84	88
1	F	250/307 (81%)	247 (99%)	3 (1%)	63	65
1	G	284/307 (92%)	282 (99%)	2 (1%)	76	80
1	H	248/307 (81%)	247 (100%)	1 (0%)	84	88
All	All	2108/2456 (86%)	2090 (99%)	18 (1%)	73	75

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	LEU
1	A	183[A]	ARG
1	A	183[B]	ARG
1	A	229	LEU
1	A	338	ASN
1	B	81	LEU

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Mol	Chain	Res	Type
1	B	89	ARG
1	B	240	GLN
1	B	281	MET
1	C	229	LEU
1	D	229	LEU
1	E	281	MET
1	F	81	LEU
1	F	265	ASN
1	F	332	ILE
1	G	269	LEU
1	G	281	MET
1	H	294	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	213	GLN
1	B	12	GLN
1	B	240	GLN
1	B	245	HIS
1	B	263	ASN
1	B	275	GLN
1	C	12	GLN
1	D	12	GLN
1	D	215	ASN
1	D	275	GLN
1	E	12	GLN
1	E	215	ASN
1	F	12	GLN
1	F	313	GLN
1	G	12	GLN
1	G	176	GLN
1	G	215	ASN
1	G	275	GLN
1	G	331	HIS
1	H	12	GLN
1	H	215	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

15 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FLC	G	501	-	12,12,12	0.95	0	17,17,17	1.55	5 (29%)
3	FLC	A	501	-	12,12,12	1.07	0	17,17,17	1.75	4 (23%)
2	NAP	E	500	-	50,52,52	1.23	4 (8%)	71,80,80	1.96	17 (23%)
2	NAP	F	500	-	50,52,52	1.61	10 (20%)	71,80,80	1.85	15 (21%)
2	NAP	A	500	-	50,52,52	1.52	9 (18%)	71,80,80	2.03	19 (26%)
3	FLC	C	501	-	12,12,12	1.02	1 (8%)	17,17,17	1.83	4 (23%)
3	FLC	B	501	-	12,12,12	1.12	1 (8%)	17,17,17	2.16	5 (29%)
2	NAP	B	500	-	50,52,52	1.71	12 (24%)	71,80,80	1.81	15 (21%)
2	NAP	G	500	-	50,52,52	1.82	8 (16%)	71,80,80	2.00	16 (22%)
3	FLC	D	501	-	12,12,12	1.37	1 (8%)	17,17,17	2.30	7 (41%)
3	FLC	H	501	-	12,12,12	1.06	0	17,17,17	2.01	5 (29%)
3	FLC	E	501	-	12,12,12	1.11	0	17,17,17	1.40	4 (23%)
2	NAP	H	500	-	50,52,52	1.40	8 (16%)	71,80,80	1.78	15 (21%)
2	NAP	C	500	-	50,52,52	1.63	9 (18%)	71,80,80	1.80	18 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FLC	F	501	-	12,12,12	1.07	1 (8%)	17,17,17	2.29	6 (35%)

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
3	FLC	G	501	-	-	1/16/16/16	-
3	FLC	A	501	-	-	6/16/16/16	-
2	NAP	E	500	-	-	3/35/67/67	0/5/5/5
2	NAP	F	500	-	-	3/35/67/67	0/5/5/5
2	NAP	A	500	-	-	4/35/67/67	0/5/5/5
3	FLC	C	501	-	-	8/16/16/16	-
3	FLC	B	501	-	-	6/16/16/16	-
2	NAP	B	500	-	-	3/35/67/67	0/5/5/5
2	NAP	G	500	-	-	2/35/67/67	0/5/5/5
3	FLC	D	501	-	-	7/16/16/16	-
3	FLC	H	501	-	-	3/16/16/16	-
3	FLC	E	501	-	-	0/16/16/16	-
2	NAP	H	500	-	-	3/35/67/67	0/5/5/5
2	NAP	C	500	-	-	2/35/67/67	0/5/5/5
3	FLC	F	501	-	-	1/16/16/16	-

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	500	NAP	PA-O3	8.27	1.68	1.59
2	B	500	NAP	C5A-C4A	5.72	1.49	1.39
2	C	500	NAP	C5A-C4A	5.22	1.48	1.39
2	F	500	NAP	C5A-C4A	5.16	1.48	1.39
2	E	500	NAP	C5A-C4A	4.93	1.47	1.39
2	A	500	NAP	C5A-C4A	4.72	1.47	1.39
2	H	500	NAP	C5A-C4A	4.60	1.47	1.39
2	F	500	NAP	PA-O3	4.43	1.64	1.59
2	C	500	NAP	PN-O3	4.15	1.64	1.59
2	C	500	NAP	O4D-C1D	4.13	1.46	1.40
2	G	500	NAP	C5A-C4A	3.90	1.46	1.39
2	G	500	NAP	O4D-C1D	3.89	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	NAP	PN-O3	3.78	1.63	1.59
2	B	500	NAP	PA-O3	3.76	1.63	1.59
2	C	500	NAP	PA-O3	3.69	1.63	1.59
2	F	500	NAP	PN-O3	3.51	1.63	1.59
2	G	500	NAP	PN-O3	3.39	1.63	1.59
2	H	500	NAP	C5A-C6A	3.22	1.49	1.41
2	A	500	NAP	PA-O3	3.20	1.62	1.59
2	F	500	NAP	C5A-C6A	3.15	1.49	1.41
2	G	500	NAP	C5A-C6A	3.05	1.49	1.41
2	H	500	NAP	PN-O3	3.04	1.62	1.59
2	A	500	NAP	C5A-C6A	3.03	1.49	1.41
2	B	500	NAP	C5A-C6A	3.03	1.49	1.41
2	B	500	NAP	C8A-N7A	3.02	1.37	1.31
2	C	500	NAP	C5A-C6A	2.97	1.49	1.41
2	A	500	NAP	PA-O1A	2.97	1.61	1.50
2	B	500	NAP	O4D-C1D	2.96	1.44	1.40
3	D	501	FLC	CB-CBC	2.95	1.56	1.53
2	A	500	NAP	PN-O3	2.93	1.62	1.59
2	E	500	NAP	PA-O3	2.86	1.62	1.59
2	B	500	NAP	C3N-C7N	2.84	1.54	1.50
2	F	500	NAP	O4D-C1D	2.81	1.44	1.40
2	E	500	NAP	C5A-C6A	2.71	1.48	1.41
2	H	500	NAP	O4D-C1D	2.64	1.44	1.40
2	H	500	NAP	PA-O3	2.64	1.62	1.59
2	B	500	NAP	C4N-C3N	2.59	1.43	1.39
2	A	500	NAP	O4D-C1D	2.52	1.44	1.40
2	A	500	NAP	C8A-N7A	2.51	1.36	1.31
2	G	500	NAP	C5A-N7A	-2.51	1.34	1.39
2	H	500	NAP	C8A-N7A	2.46	1.36	1.31
2	G	500	NAP	C8A-N7A	2.40	1.36	1.31
2	F	500	NAP	P2B-O2B	2.40	1.63	1.59
2	E	500	NAP	C4A-N3A	2.40	1.38	1.34
2	B	500	NAP	P2B-O2B	2.38	1.63	1.59
2	A	500	NAP	C4N-C3N	2.34	1.43	1.39
2	C	500	NAP	P2B-O2B	2.29	1.63	1.59
2	F	500	NAP	C4A-N3A	2.29	1.38	1.34
2	A	500	NAP	O2D-C2D	2.26	1.48	1.43
2	G	500	NAP	P2B-O2B	2.22	1.63	1.59
2	F	500	NAP	C8A-N7A	2.18	1.35	1.31
2	B	500	NAP	C7N-N7N	2.16	1.36	1.33
2	F	500	NAP	C2N-N1N	-2.15	1.32	1.35
3	C	501	FLC	OA2-CAC	-2.11	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	500	NAP	C4N-C3N	2.10	1.42	1.39
3	F	501	FLC	CB-CBC	2.09	1.55	1.53
2	C	500	NAP	C4A-N9A	-2.08	1.33	1.37
2	B	500	NAP	C5A-N7A	-2.08	1.35	1.39
2	H	500	NAP	C4A-N9A	-2.08	1.33	1.37
2	B	500	NAP	C1B-N9A	2.07	1.52	1.46
2	C	500	NAP	C8A-N7A	2.07	1.35	1.31
2	H	500	NAP	C5A-N7A	-2.02	1.35	1.39
3	B	501	FLC	OA1-CAC	2.02	1.28	1.22
2	C	500	NAP	C5A-N7A	-2.01	1.35	1.39

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	500	NAP	C5A-C4A-N3A	-6.86	117.28	126.72
2	G	500	NAP	C5A-C4A-N3A	-6.70	117.50	126.72
2	E	500	NAP	N3A-C4A-N9A	6.35	137.96	127.17
2	A	500	NAP	C5A-C4A-N3A	-6.16	118.24	126.72
2	G	500	NAP	N3A-C4A-N9A	5.58	136.65	127.17
2	F	500	NAP	O3-PA-O1A	-5.53	94.07	110.70
2	H	500	NAP	C5A-C4A-N3A	-5.46	119.20	126.72
2	B	500	NAP	C5A-C4A-N3A	-5.39	119.30	126.72
3	F	501	FLC	OB2-CBC-CB	5.22	123.15	113.14
3	B	501	FLC	OB2-CBC-CB	5.19	123.10	113.14
2	A	500	NAP	O3-PA-O1A	-4.98	95.73	110.70
2	A	500	NAP	N3A-C4A-N9A	4.97	135.62	127.17
2	C	500	NAP	C5A-C4A-N3A	-4.90	119.97	126.72
2	F	500	NAP	N3A-C4A-N9A	4.87	135.45	127.17
2	F	500	NAP	C5A-C4A-N3A	-4.78	120.13	126.72
2	H	500	NAP	N3A-C4A-N9A	4.78	135.30	127.17
3	D	501	FLC	OHB-CB-CBC	4.72	115.65	108.96
2	H	500	NAP	N3A-C2A-N1A	-4.66	121.52	128.58
2	C	500	NAP	N3A-C4A-N9A	4.66	135.09	127.17
2	G	500	NAP	C3N-C7N-N7N	4.60	123.41	117.74
3	D	501	FLC	OB2-CBC-CB	4.52	121.80	113.14
2	B	500	NAP	O3-PA-O1A	-4.51	97.15	110.70
2	E	500	NAP	N3A-C2A-N1A	-4.46	121.83	128.58
2	G	500	NAP	C2A-N3A-C4A	4.40	122.57	111.83
2	H	500	NAP	C2A-N3A-C4A	4.33	122.41	111.83
2	E	500	NAP	C2A-N3A-C4A	4.32	122.39	111.83
2	A	500	NAP	O2A-PA-O1A	4.29	132.40	112.44
2	F	500	NAP	C4A-N9A-C8A	4.23	110.18	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	FLC	OB2-CBC-CB	4.21	121.22	113.14
2	F	500	NAP	N3A-C2A-N1A	-4.19	122.24	128.58
2	B	500	NAP	C3N-C7N-N7N	4.19	122.90	117.74
2	B	500	NAP	N3A-C4A-N9A	4.19	134.29	127.17
2	A	500	NAP	C2A-N3A-C4A	4.18	122.03	111.83
2	C	500	NAP	N3A-C2A-N1A	-4.16	122.28	128.58
2	B	500	NAP	N3A-C2A-N1A	-4.15	122.30	128.58
2	G	500	NAP	C5A-N7A-C8A	4.14	109.96	103.45
2	C	500	NAP	C4D-O4D-C1D	4.11	113.69	109.92
3	H	501	FLC	OB2-CBC-CB	4.09	120.99	113.14
3	F	501	FLC	OHB-CB-CBC	4.08	114.75	108.96
2	A	500	NAP	N3A-C2A-N1A	-4.04	122.47	128.58
3	H	501	FLC	OHB-CB-CBC	3.95	114.57	108.96
2	G	500	NAP	N3A-C2A-N1A	-3.88	122.71	128.58
2	C	500	NAP	O3-PA-O1A	-3.85	99.12	110.70
2	A	500	NAP	C4A-C5A-N7A	-3.83	106.20	110.58
2	G	500	NAP	C4A-C5A-N7A	-3.82	106.21	110.58
2	B	500	NAP	O2A-PA-O1A	3.75	129.89	112.44
2	B	500	NAP	C2A-N3A-C4A	3.75	120.98	111.83
2	C	500	NAP	C2A-N3A-C4A	3.62	120.67	111.83
2	G	500	NAP	N9A-C8A-N7A	-3.62	108.81	113.94
2	C	500	NAP	C4A-N9A-C8A	3.60	109.51	105.74
2	F	500	NAP	C2A-N3A-C4A	3.59	120.60	111.83
3	B	501	FLC	OG1-CGC-CG	-3.38	113.37	122.95
3	A	501	FLC	OG1-CGC-CG	-3.37	113.40	122.95
3	C	501	FLC	OB1-CBC-CB	-3.37	115.57	122.09
2	A	500	NAP	C5A-N7A-C8A	3.36	108.72	103.45
2	E	500	NAP	O3-PA-O1A	-3.35	100.64	110.70
3	A	501	FLC	OB2-CBC-CB	3.31	119.48	113.14
2	C	500	NAP	O7N-C7N-C3N	3.27	123.60	119.60
2	G	500	NAP	C4A-N9A-C8A	3.25	109.15	105.74
2	A	500	NAP	C4A-N9A-C8A	3.23	109.13	105.74
3	C	501	FLC	OG1-CGC-CG	-3.22	113.83	122.95
3	B	501	FLC	OG2-CGC-CG	3.21	124.50	114.35
2	C	500	NAP	O2A-PA-O1A	3.18	127.23	112.44
2	H	500	NAP	C3N-C7N-N7N	3.16	121.63	117.74
3	A	501	FLC	OG2-CGC-CG	3.15	124.31	114.35
2	F	500	NAP	O2A-PA-O1A	3.12	126.97	112.44
2	H	500	NAP	O2A-PA-O1A	3.10	126.88	112.44
3	D	501	FLC	OG1-CGC-CG	-3.07	114.25	122.95
2	G	500	NAP	O7N-C7N-N7N	-3.06	118.19	122.62
3	D	501	FLC	OG2-CGC-CG	3.06	124.03	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	NAP	C2B-C1B-N9A	3.04	118.76	113.75
2	E	500	NAP	C4A-N9A-C8A	3.01	108.90	105.74
3	F	501	FLC	CB-CA-CAC	-3.01	105.70	113.92
2	B	500	NAP	C4A-C5A-N7A	-3.00	107.15	110.58
2	H	500	NAP	O7N-C7N-C3N	-3.00	115.93	119.60
2	E	500	NAP	O2B-P2B-O1X	-2.98	98.70	109.33
2	H	500	NAP	C4A-N9A-C8A	2.97	108.85	105.74
2	A	500	NAP	C4D-O4D-C1D	2.93	112.61	109.92
2	E	500	NAP	O3X-P2B-O2B	2.93	117.25	105.85
2	H	500	NAP	O3-PA-O1A	-2.91	101.95	110.70
2	A	500	NAP	N9A-C8A-N7A	-2.91	109.81	113.94
2	C	500	NAP	C2A-N1A-C6A	2.90	123.50	118.73
2	B	500	NAP	C2A-N1A-C6A	2.89	123.47	118.73
2	E	500	NAP	C6N-N1N-C2N	-2.89	119.42	121.88
2	F	500	NAP	N9A-C8A-N7A	-2.88	109.85	113.94
3	F	501	FLC	OG1-CGC-CG	-2.86	114.85	122.95
2	E	500	NAP	C4A-C5A-N7A	-2.85	107.32	110.58
2	F	500	NAP	C5A-N7A-C8A	2.85	107.93	103.45
2	A	500	NAP	C6A-C5A-N7A	2.80	137.49	132.09
3	D	501	FLC	OHB-CB-CA	-2.77	103.05	109.38
3	B	501	FLC	CA-CB-CBC	2.75	116.11	110.03
2	A	500	NAP	O2N-PN-O1N	2.73	125.17	112.44
2	H	500	NAP	O2N-PN-O3	2.73	114.64	107.27
2	F	500	NAP	C2A-N1A-C6A	2.69	123.15	118.73
2	F	500	NAP	C6N-N1N-C2N	-2.65	119.62	121.88
2	E	500	NAP	O2X-P2B-O2B	-2.63	95.59	105.85
2	F	500	NAP	C4A-C5A-N7A	-2.59	107.62	110.58
2	E	500	NAP	O2A-PA-O1A	2.57	124.38	112.44
2	A	500	NAP	O2D-C2D-C3D	2.55	119.98	111.82
2	G	500	NAP	O3-PA-O1A	-2.55	103.04	110.70
2	E	500	NAP	C2A-N1A-C6A	2.52	122.87	118.73
3	G	501	FLC	OA2-CAC-CA	2.51	122.31	114.35
2	C	500	NAP	C4A-C5A-N7A	-2.50	107.72	110.58
2	A	500	NAP	C6N-N1N-C2N	-2.50	119.75	121.88
3	C	501	FLC	OG2-CGC-CG	2.50	122.25	114.35
2	A	500	NAP	O2B-P2B-O1X	-2.48	100.50	109.33
2	A	500	NAP	O4D-C4D-C5D	-2.46	101.44	109.33
2	B	500	NAP	C5A-N7A-C8A	2.44	107.29	103.45
2	G	500	NAP	O2N-PN-O3	2.44	113.86	107.27
2	B	500	NAP	O7N-C7N-N7N	-2.43	119.11	122.62
2	E	500	NAP	C5A-N7A-C8A	2.39	107.21	103.45
2	C	500	NAP	O2B-P2B-O1X	-2.37	100.87	109.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	NAP	O7N-C7N-N7N	-2.34	119.23	122.62
3	H	501	FLC	OA2-CAC-CA	2.34	121.75	114.35
2	B	500	NAP	O2N-PN-O3	2.32	113.54	107.27
3	E	501	FLC	OHB-CB-CBC	2.30	112.23	108.96
3	H	501	FLC	OHB-CB-CA	-2.28	104.17	109.38
3	A	501	FLC	OHB-CB-CBC	2.26	112.16	108.96
2	E	500	NAP	O2X-P2B-O1X	2.25	119.62	110.83
3	D	501	FLC	OA2-CAC-CA	2.25	121.48	114.35
2	C	500	NAP	N6A-C6A-N1A	2.25	123.38	118.38
3	G	501	FLC	OHB-CB-CBC	2.24	112.14	108.96
2	G	500	NAP	O4B-C4B-C5B	-2.24	102.17	109.33
2	G	500	NAP	O2A-PA-O1A	2.23	122.80	112.44
3	G	501	FLC	OG2-CGC-CG	2.22	121.39	114.35
2	A	500	NAP	P2B-O2B-C2B	2.22	129.35	123.43
2	H	500	NAP	C5A-C6A-N6A	-2.21	117.80	123.29
2	B	500	NAP	C6A-C5A-N7A	2.20	136.34	132.09
2	E	500	NAP	C1B-N9A-C8A	-2.20	122.21	127.09
3	F	501	FLC	OHB-CB-CG	-2.15	104.47	109.38
3	H	501	FLC	OA2-CAC-OA1	-2.15	117.81	123.33
2	H	500	NAP	C6A-C5A-N7A	2.14	136.22	132.09
2	F	500	NAP	N6A-C6A-N1A	2.14	123.14	118.38
3	G	501	FLC	OG1-CGC-CG	-2.13	116.91	122.95
2	F	500	NAP	O2N-PN-O1N	2.13	122.35	112.44
2	A	500	NAP	C3N-C7N-N7N	2.12	120.35	117.74
2	C	500	NAP	C5A-N7A-C8A	2.11	106.77	103.45
2	F	500	NAP	C6A-C5A-N7A	2.11	136.16	132.09
2	C	500	NAP	C2N-C3N-C4N	-2.09	115.82	118.26
2	E	500	NAP	C4D-O4D-C1D	2.06	111.81	109.92
3	E	501	FLC	OA1-CAC-CA	-2.06	117.11	122.95
3	F	501	FLC	OA1-CAC-CA	-2.04	117.17	122.95
2	G	500	NAP	O3X-P2B-O2X	2.04	115.46	107.80
2	B	500	NAP	C2N-C3N-C4N	-2.04	115.89	118.26
3	D	501	FLC	OB2-CBC-OB1	-2.04	117.34	123.86
2	C	500	NAP	C6N-N1N-C2N	-2.04	120.14	121.88
3	G	501	FLC	CA-CB-CBC	-2.03	105.54	110.03
2	H	500	NAP	C4A-C5A-N7A	-2.03	108.26	110.58
2	C	500	NAP	N9A-C8A-N7A	-2.03	111.06	113.94
2	H	500	NAP	C2A-N1A-C6A	2.02	122.04	118.73
3	E	501	FLC	CB-CA-CAC	-2.01	108.41	113.92
2	H	500	NAP	N6A-C6A-N1A	2.01	122.86	118.38
2	G	500	NAP	O2B-P2B-O1X	-2.01	102.18	109.33
3	E	501	FLC	CG-CB-CBC	-2.00	105.60	110.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	FLC	OHB-CB-CBC	2.00	111.80	108.96

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	500	NAP	PN-O3-PA-O5B
3	B	501	FLC	OHB-CB-CBC-OB1
3	B	501	FLC	OHB-CB-CBC-OB2
3	C	501	FLC	OHB-CB-CBC-OB1
3	D	501	FLC	OHB-CB-CBC-OB1
3	B	501	FLC	CG-CB-CBC-OB1
3	C	501	FLC	CG-CB-CBC-OB1
3	C	501	FLC	CG-CB-CBC-OB2
2	B	500	NAP	PN-O3-PA-O1A
2	F	500	NAP	PN-O3-PA-O1A
2	H	500	NAP	PN-O3-PA-O1A
3	A	501	FLC	OHB-CB-CBC-OB1
3	C	501	FLC	OHB-CB-CBC-OB2
3	C	501	FLC	CA-CB-CBC-OB2
3	D	501	FLC	OHB-CB-CG-CGC
2	B	500	NAP	PN-O3-PA-O5B
2	E	500	NAP	PN-O3-PA-O5B
2	F	500	NAP	PN-O3-PA-O5B
2	G	500	NAP	PN-O3-PA-O5B
2	H	500	NAP	PN-O3-PA-O5B
2	G	500	NAP	PN-O3-PA-O1A
3	B	501	FLC	CA-CB-CBC-OB2
3	B	501	FLC	CG-CB-CBC-OB2
3	D	501	FLC	CA-CB-CBC-OB1
2	A	500	NAP	C5D-O5D-PN-O3
2	A	500	NAP	C5D-O5D-PN-O1N
2	B	500	NAP	C5D-O5D-PN-O1N
2	C	500	NAP	C5D-O5D-PN-O1N
2	E	500	NAP	C5D-O5D-PN-O1N
2	F	500	NAP	C5D-O5D-PN-O1N
3	D	501	FLC	OHB-CB-CBC-OB2
3	A	501	FLC	CA-CB-CBC-OB1
3	A	501	FLC	CA-CB-CBC-OB2
3	A	501	FLC	CG-CB-CBC-OB1
3	A	501	FLC	CG-CB-CBC-OB2
3	C	501	FLC	CA-CB-CBC-OB1

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Mol	Chain	Res	Type	Atoms
3	D	501	FLC	CA-CB-CBC-OB2
3	D	501	FLC	CG-CB-CBC-OB1
3	D	501	FLC	CG-CB-CBC-OB2
3	C	501	FLC	CAC-CA-CB-OHB
3	F	501	FLC	OHB-CB-CG-CGC
3	C	501	FLC	CAC-CA-CB-CBC
3	B	501	FLC	CA-CB-CBC-OB1
2	A	500	NAP	PA-O3-PN-O1N
3	A	501	FLC	OHB-CB-CBC-OB2
3	H	501	FLC	CB-CA-CAC-OA1
3	H	501	FLC	CB-CA-CAC-OA2
3	G	501	FLC	CA-CB-CBC-OB2
2	A	500	NAP	C2B-O2B-P2B-O3X
2	E	500	NAP	O4D-C4D-C5D-O5D
3	H	501	FLC	CAC-CA-CB-OHB
2	H	500	NAP	C2B-O2B-P2B-O1X

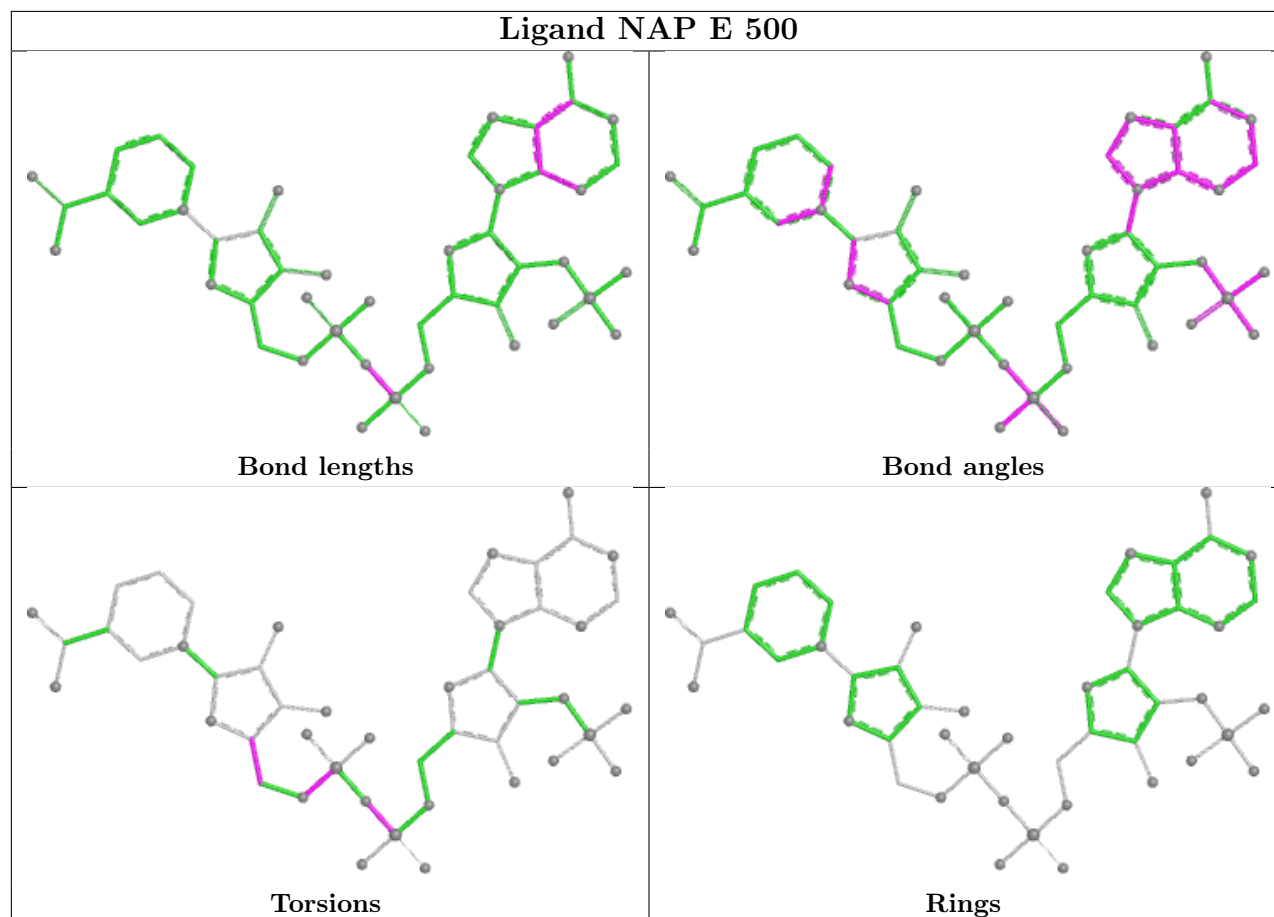
There are no ring outliers.

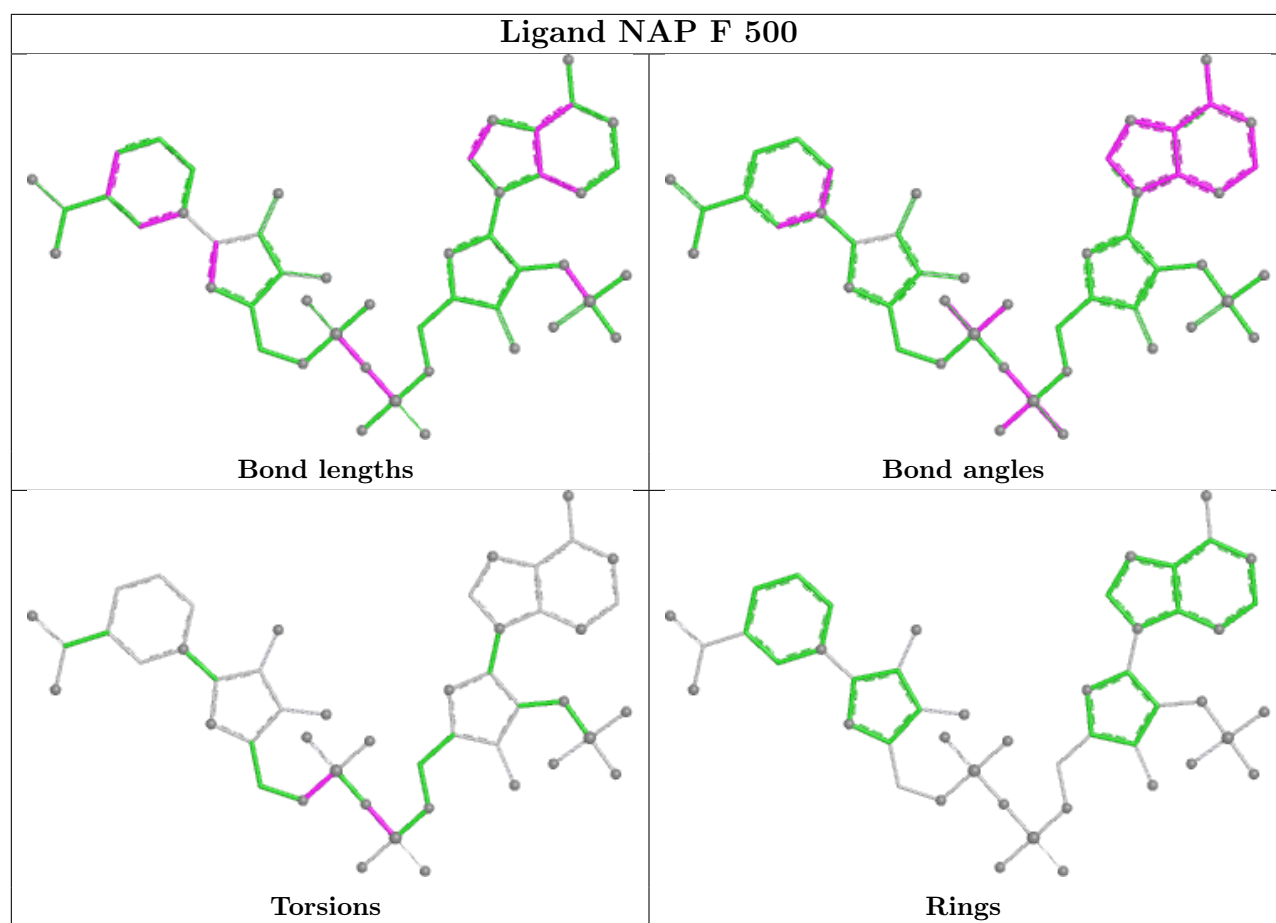
11 monomers are involved in 23 short contacts:

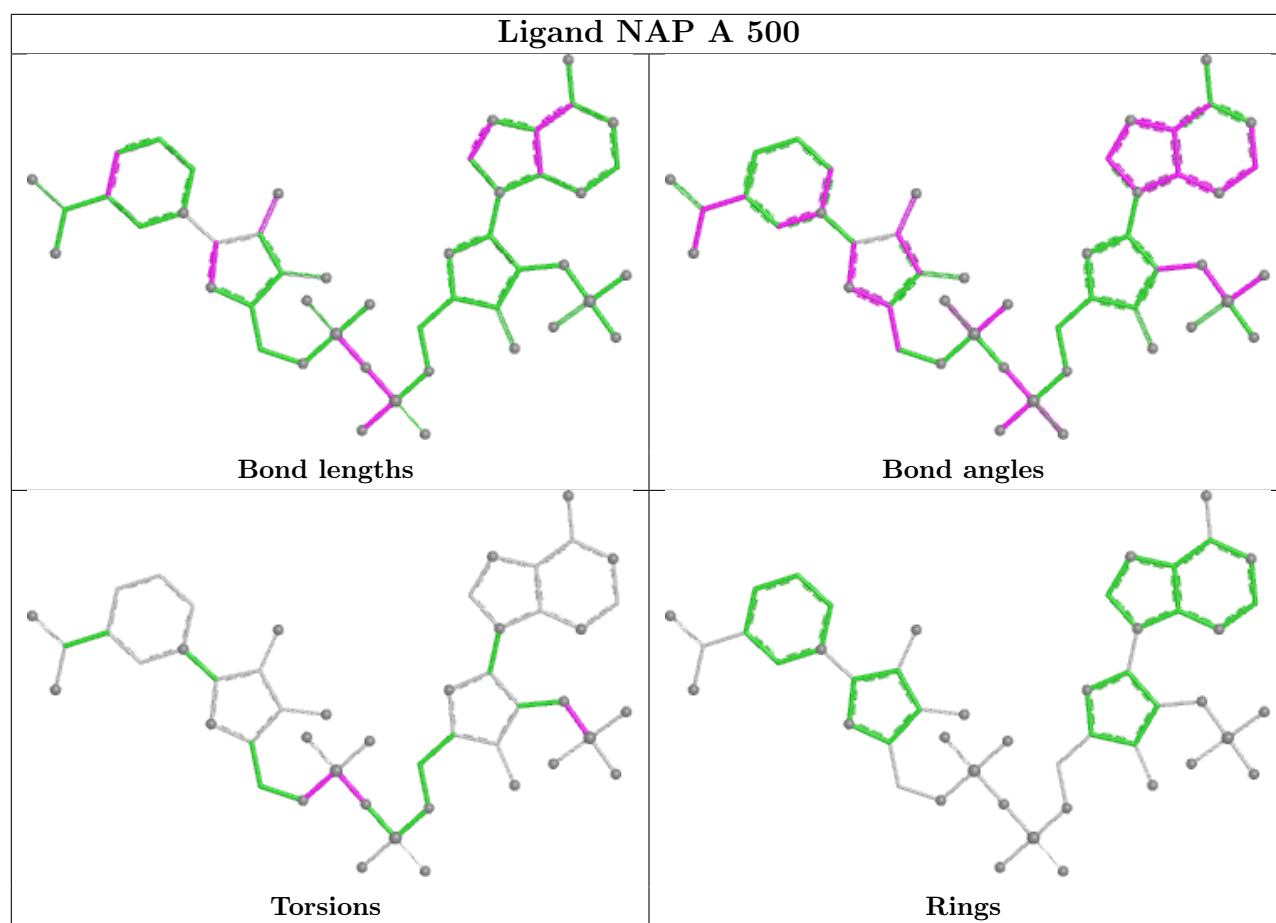
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	501	FLC	1	0
2	E	500	NAP	2	0
2	F	500	NAP	2	0
2	A	500	NAP	6	0
2	B	500	NAP	1	0
2	G	500	NAP	1	0
3	H	501	FLC	1	0
3	E	501	FLC	1	0
2	H	500	NAP	1	0
2	C	500	NAP	5	0
3	F	501	FLC	3	0

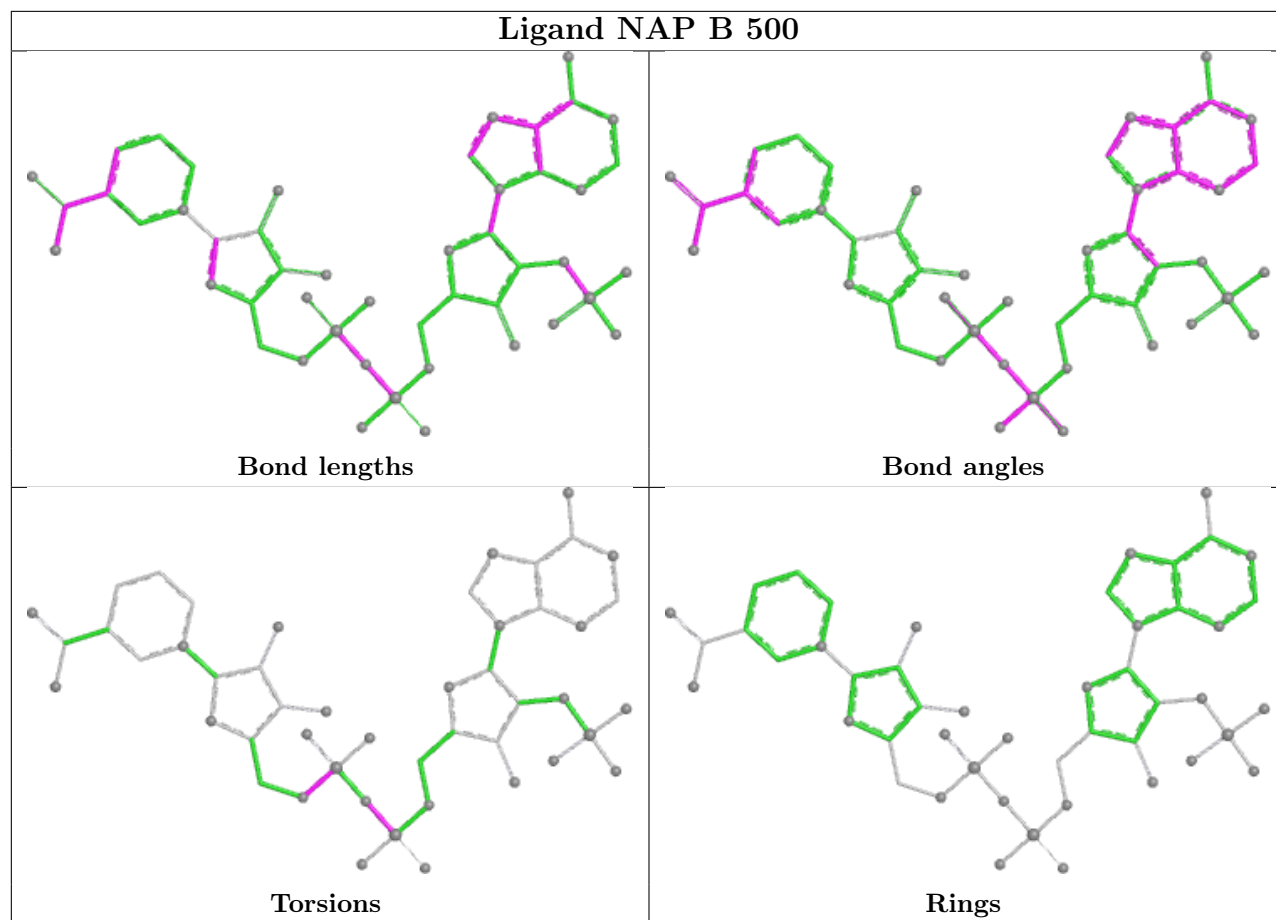
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

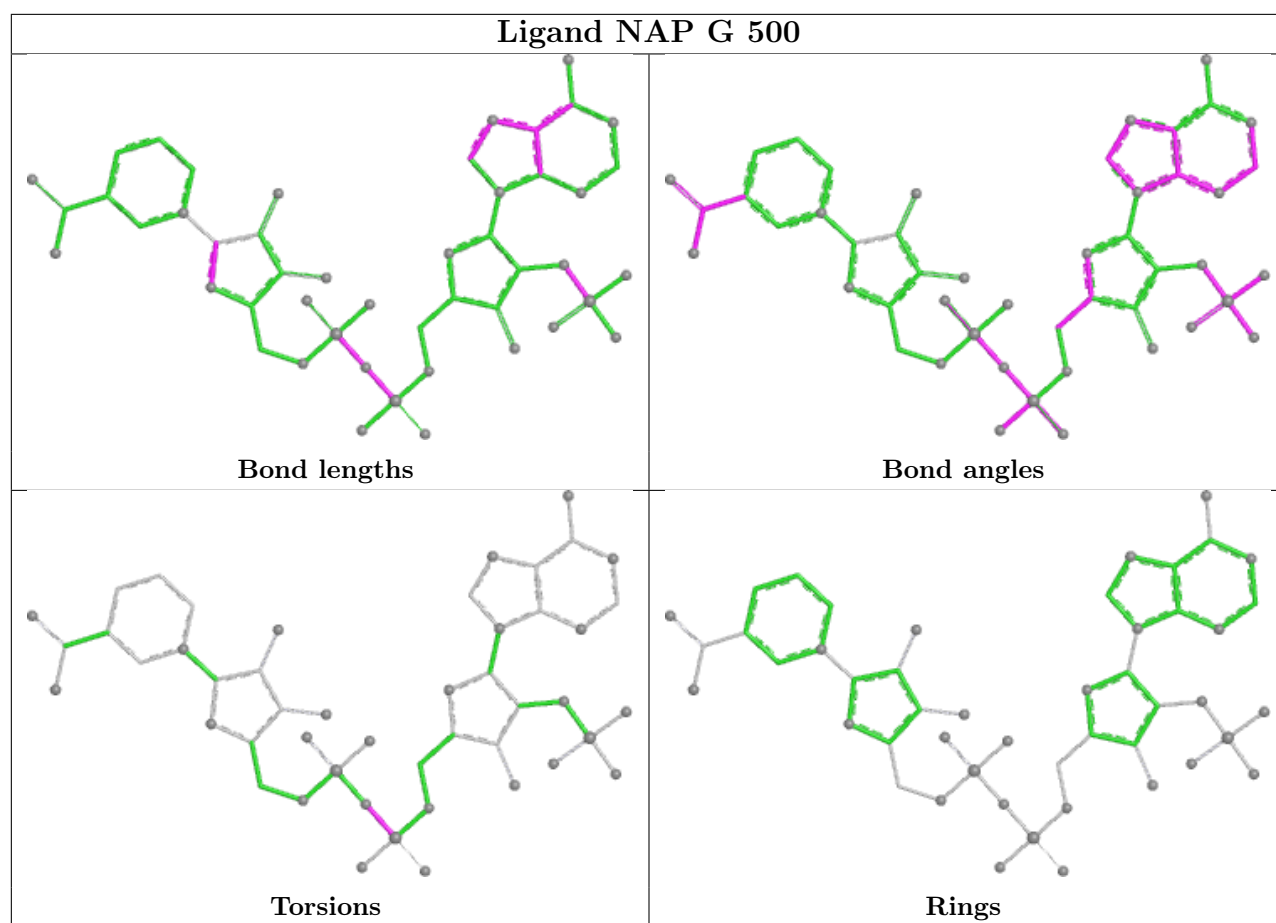
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

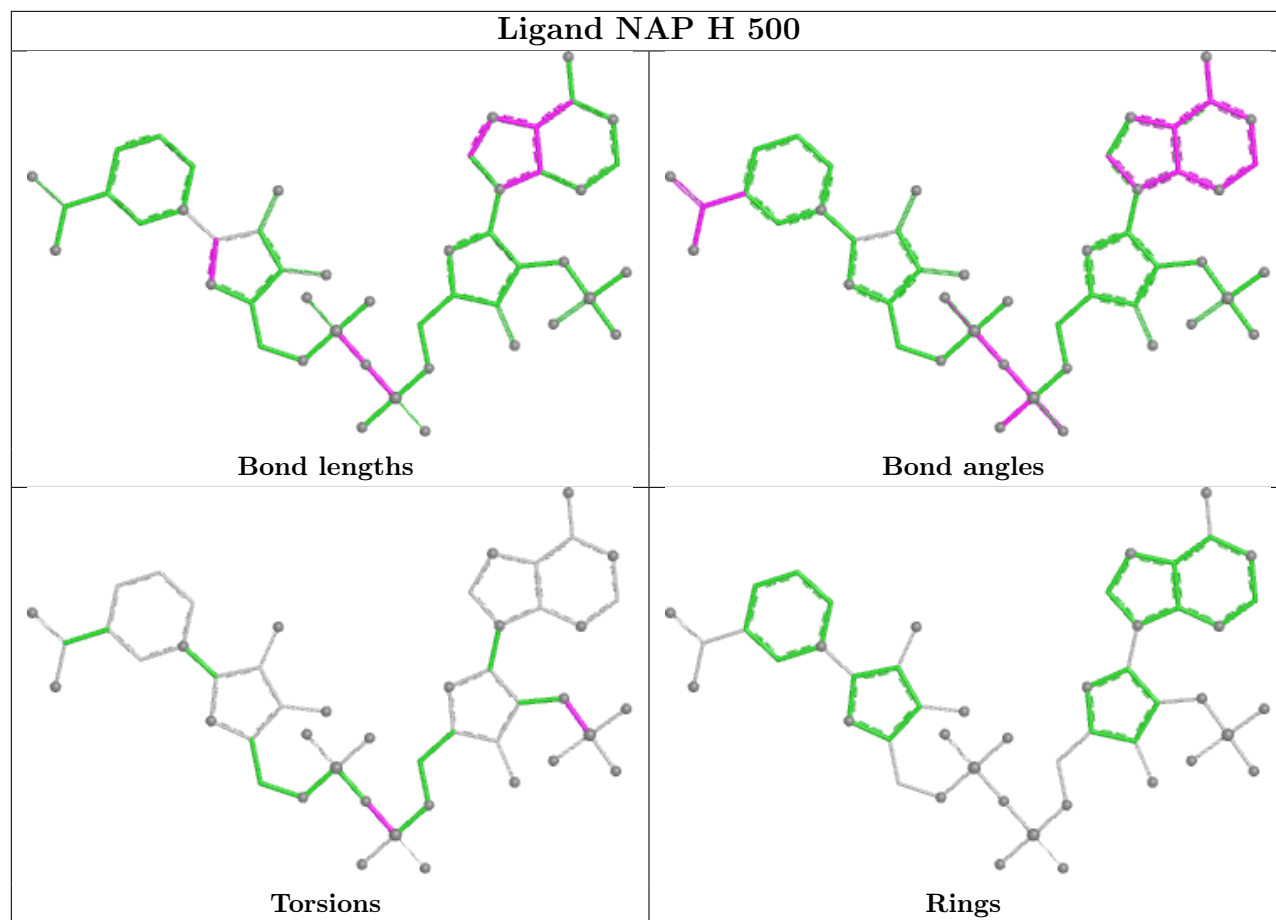


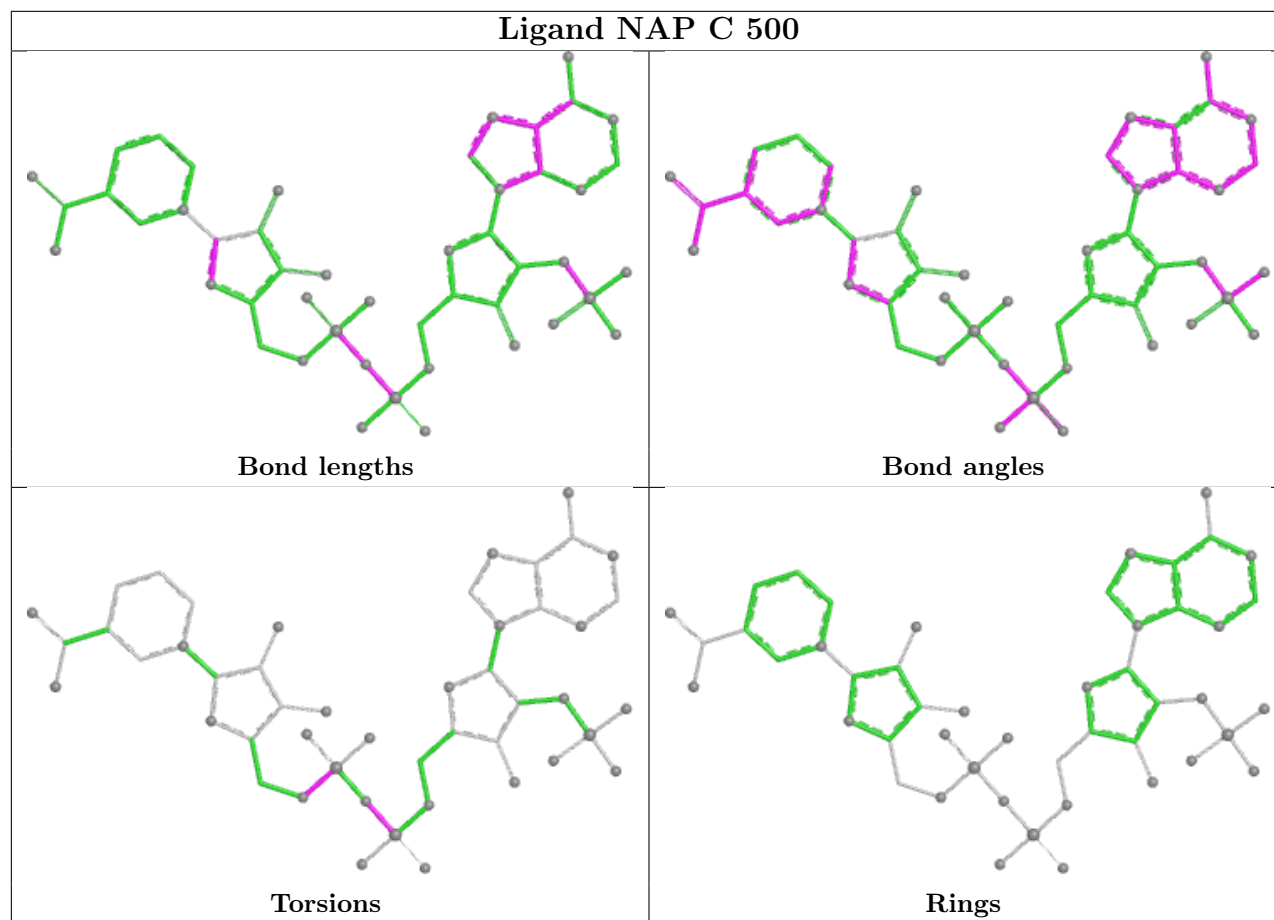












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	312/366 (85%)	-0.07	12 (3%)	44	44	12, 21, 46, 77	3 (0%)
1	B	335/366 (91%)	0.36	37 (11%)	10	10	14, 26, 73, 97	2 (0%)
1	C	330/366 (90%)	0.25	33 (10%)	12	12	11, 24, 67, 98	2 (0%)
1	D	308/366 (84%)	-0.19	4 (1%)	75	76	12, 20, 41, 55	1 (0%)
1	E	297/366 (81%)	0.41	32 (10%)	11	10	16, 28, 65, 81	0
1	F	298/366 (81%)	0.03	18 (6%)	27	28	13, 22, 47, 78	1 (0%)
1	G	335/366 (91%)	0.18	21 (6%)	26	26	14, 24, 59, 84	3 (0%)
1	H	297/366 (81%)	0.32	30 (10%)	12	12	15, 26, 59, 79	2 (0%)
All	All	2512/2928 (85%)	0.16	187 (7%)	20	21	11, 24, 59, 98	14 (0%)

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	272	GLU	8.0
1	C	268	ARG	7.4
1	H	276	GLN	7.3
1	F	268	ARG	7.1
1	C	262	ALA	6.9
1	A	261	GLU	6.9
1	F	264	LEU	6.3
1	E	269	LEU	5.6
1	B	276	GLN	5.5
1	B	235	LEU	5.1
1	C	237	GLY	4.9
1	C	260	THR	4.7
1	C	263	ASN	4.7
1	D	202	TRP	4.7
1	C	265	ASN	4.7
1	E	228	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	263	ASN	4.5
1	B	262	ALA	4.4
1	G	262	ALA	4.4
1	B	269	LEU	4.3
1	B	264	LEU	4.3
1	C	339	LEU	4.3
1	A	228	GLY	4.3
1	B	228	GLY	4.3
1	D	276	GLN	4.3
1	B	266	SER	4.2
1	B	333	ALA	4.1
1	F	332	ILE	4.1
1	E	270	LEU	4.0
1	H	292	ASP	4.0
1	H	344	SER	3.9
1	C	337	LEU	3.9
1	E	271	ASN	3.8
1	H	335	GLY	3.8
1	B	258	MET	3.7
1	C	234	TYR	3.7
1	C	343	SER	3.7
1	C	244	MET	3.6
1	H	340	TRP	3.6
1	F	207	GLY	3.6
1	F	292	ASP	3.6
1	C	342	ALA	3.6
1	G	259	LEU	3.6
1	B	256	PRO	3.5
1	B	259	LEU	3.5
1	E	339	LEU	3.5
1	C	239	PRO	3.5
1	G	269	LEU	3.5
1	E	345	ASP	3.5
1	B	260	THR	3.5
1	E	340	TRP	3.4
1	H	337	LEU	3.4
1	B	238	ILE	3.4
1	F	228	GLY	3.4
1	C	238	ILE	3.4
1	H	323	LYS	3.3
1	C	259	LEU	3.3
1	H	325	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	292	ASP	3.3
1	C	256	PRO	3.3
1	E	344	SER	3.3
1	H	270	LEU	3.3
1	C	340	TRP	3.2
1	C	261	GLU	3.2
1	B	265	ASN	3.2
1	A	229	LEU	3.2
1	E	337	LEU	3.2
1	C	258	MET	3.2
1	H	342	ALA	3.2
1	E	232	GLY	3.2
1	B	332	ILE	3.1
1	F	269	LEU	3.1
1	A	233	LYS	3.1
1	E	231	THR	3.1
1	F	267	LEU	3.1
1	C	266	SER	3.1
1	B	242	SER	3.1
1	E	334	ASP	3.1
1	C	2	VAL	3.1
1	G	332	ILE	3.1
1	B	234	TYR	3.0
1	B	246	ARG	3.0
1	C	241	ASP	3.0
1	H	339	LEU	3.0
1	C	329	ASP	3.0
1	E	273	MET	3.0
1	H	319	THR	2.9
1	E	233	LYS	2.9
1	H	4	LEU	2.9
1	A	2	VAL	2.9
1	B	337	LEU	2.9
1	B	239	PRO	2.9
1	B	340	TRP	2.9
1	C	243	ARG	2.8
1	C	336	GLU	2.8
1	C	183	ARG	2.8
1	B	237	GLY	2.8
1	E	209	LEU	2.8
1	F	4	LEU	2.8
1	H	229	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	294	ARG	2.7
1	A	338	ASN	2.7
1	G	238	ILE	2.7
1	E	229	LEU	2.7
1	F	229	LEU	2.7
1	H	341	GLN	2.7
1	B	339	LEU	2.7
1	E	320	PHE	2.6
1	B	331	HIS	2.6
1	H	228	GLY	2.6
1	E	202	TRP	2.6
1	G	270	LEU	2.6
1	F	265	ASN	2.6
1	E	343	SER	2.6
1	E	204	ASP	2.6
1	G	234	TYR	2.5
1	B	233	LYS	2.5
1	H	345	ASP	2.5
1	G	258	MET	2.5
1	G	331	HIS	2.5
1	H	317	ASN	2.5
1	G	239	PRO	2.5
1	C	335	GLY	2.5
1	E	341	GLN	2.5
1	B	229	LEU	2.5
1	C	264	LEU	2.5
1	H	278	GLY	2.5
1	E	276	GLN	2.4
1	H	343	SER	2.4
1	B	240	GLN	2.4
1	E	288	TRP	2.4
1	E	281	MET	2.4
1	A	232	GLY	2.4
1	B	241	ASP	2.4
1	G	2	VAL	2.4
1	B	243	ARG	2.4
1	F	331	HIS	2.4
1	E	275	GLN	2.4
1	G	327	GLN	2.4
1	F	328	ILE	2.4
1	A	222	PHE	2.3
1	E	294	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	328	ILE	2.3
1	G	256	PRO	2.3
1	E	335	GLY	2.3
1	B	268	ARG	2.3
1	G	79	ARG	2.3
1	G	245	HIS	2.3
1	E	304	ARG	2.3
1	B	342	ALA	2.3
1	B	281	MET	2.3
1	D	337	LEU	2.3
1	G	242	SER	2.2
1	H	213	GLN	2.2
1	F	222	PHE	2.2
1	C	204	ASP	2.2
1	C	235	LEU	2.2
1	G	340	TRP	2.2
1	A	231	THR	2.2
1	B	244	MET	2.2
1	C	4	LEU	2.2
1	G	330	GLN	2.2
1	B	304	ARG	2.2
1	G	183	ARG	2.2
1	E	2	VAL	2.2
1	B	204	ASP	2.2
1	H	324	GLU	2.1
1	A	294	ARG	2.1
1	F	183	ARG	2.1
1	D	231	THR	2.1
1	H	320	PHE	2.1
1	C	207	GLY	2.1
1	A	259	LEU	2.1
1	H	273	MET	2.1
1	F	327	GLN	2.1
1	H	222	PHE	2.1
1	F	266	SER	2.1
1	B	236	ASN	2.0
1	E	319	THR	2.0
1	H	336	GLU	2.0
1	G	244	MET	2.0
1	H	3	TRP	2.0
1	H	202	TRP	2.0
1	C	236	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	276	GLN	2.0
1	F	276	GLN	2.0
1	E	277	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

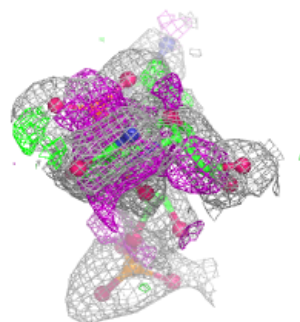
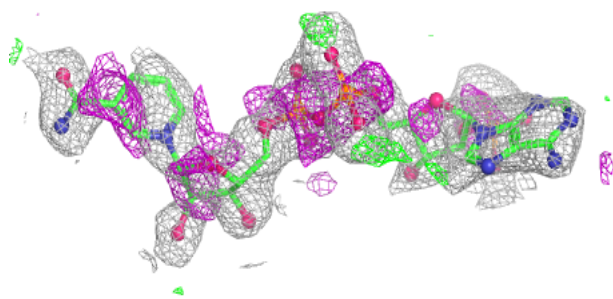
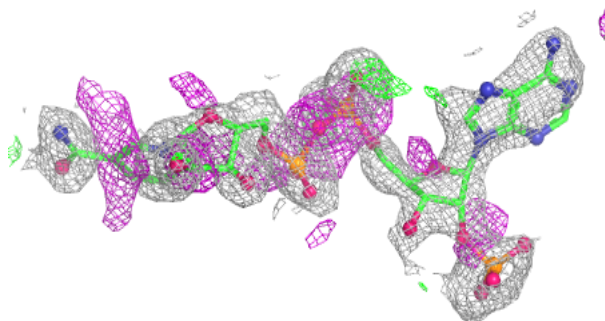
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAP	A	500	48/48	0.80	0.17	28,55,79,82	0
3	FLC	A	501	13/13	0.80	0.16	46,57,63,65	0
3	FLC	D	501	13/13	0.86	0.12	42,51,56,59	0
3	FLC	F	501	13/13	0.87	0.11	32,43,49,50	0
3	FLC	C	501	13/13	0.88	0.11	33,42,48,58	0
2	NAP	F	500	48/48	0.89	0.12	22,43,56,60	0
2	NAP	H	500	48/48	0.89	0.11	33,44,50,52	0
3	FLC	H	501	13/13	0.89	0.10	38,46,49,49	0
3	FLC	B	501	13/13	0.90	0.10	34,37,45,51	0
2	NAP	E	500	48/48	0.91	0.11	28,43,50,57	0
3	FLC	G	501	13/13	0.91	0.10	34,39,46,51	0
3	FLC	E	501	13/13	0.91	0.09	38,42,48,50	0
2	NAP	C	500	48/48	0.92	0.11	19,40,51,53	0
2	NAP	B	500	48/48	0.92	0.10	27,43,58,61	0
2	NAP	G	500	48/48	0.96	0.07	21,30,37,40	0

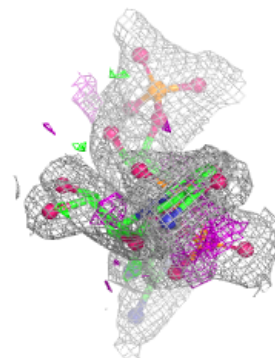
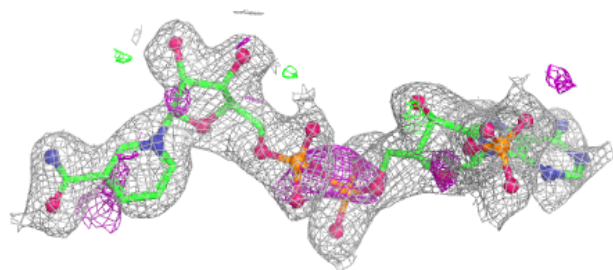
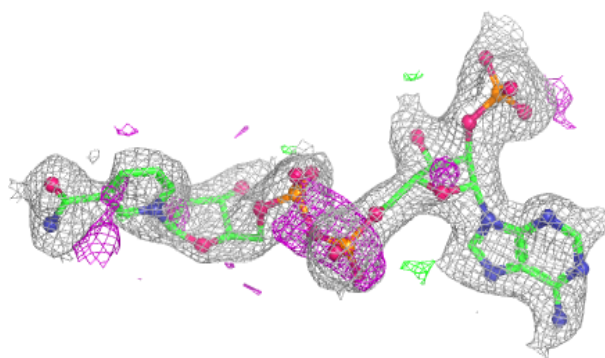
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP A 500:

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

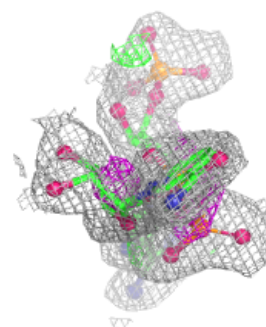
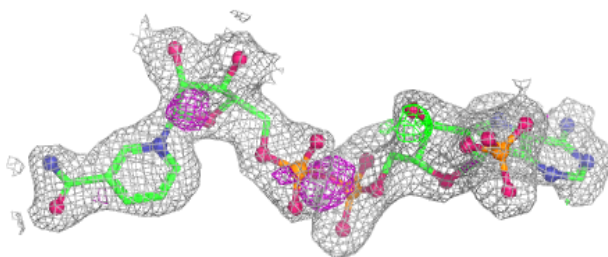
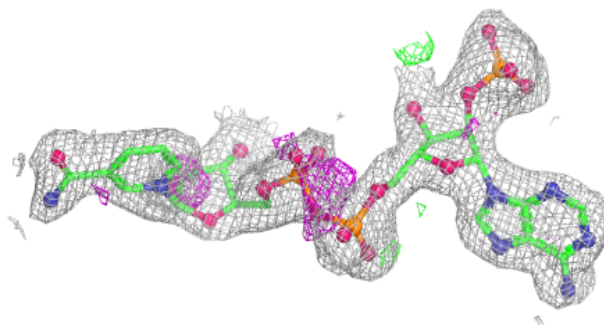
**Electron density around NAP F 500:**

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

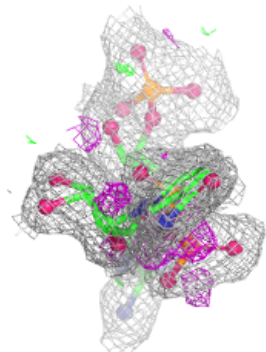
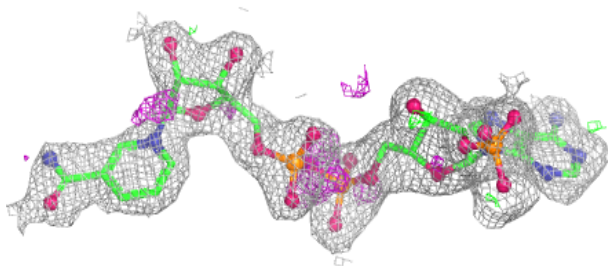
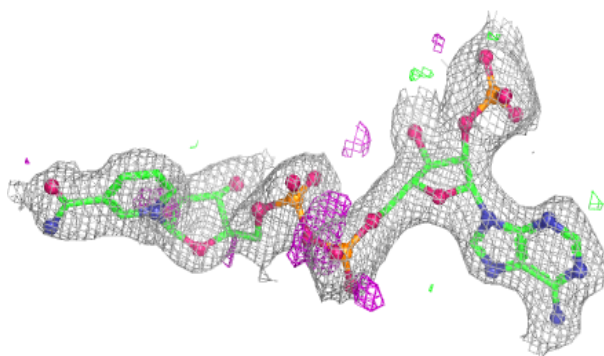


Electron density around NAP H 500:

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

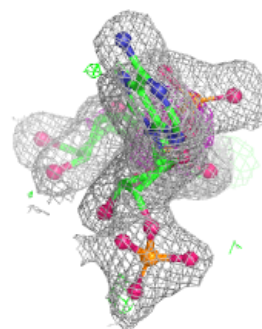
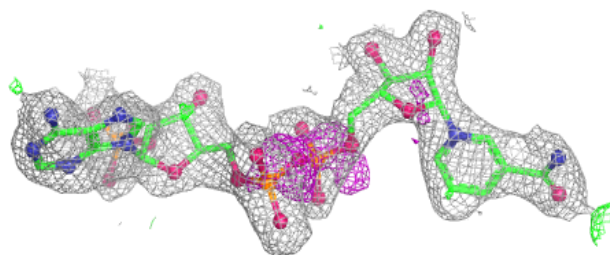
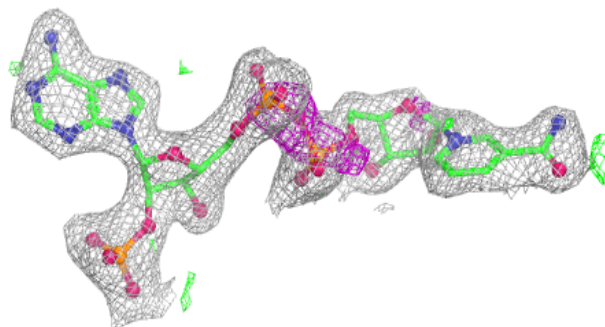
**Electron density around NAP E 500:**

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

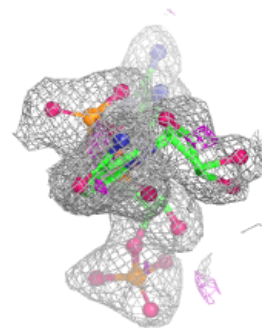
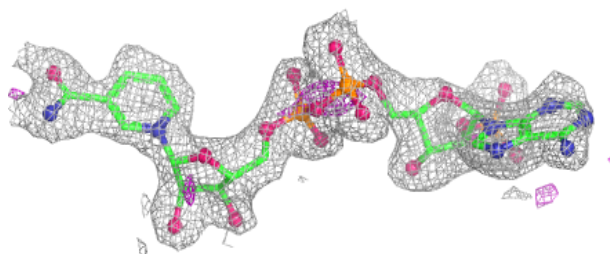
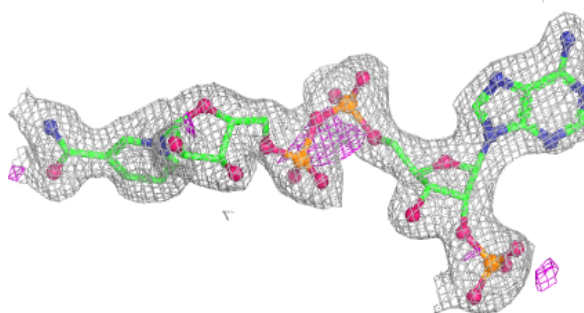


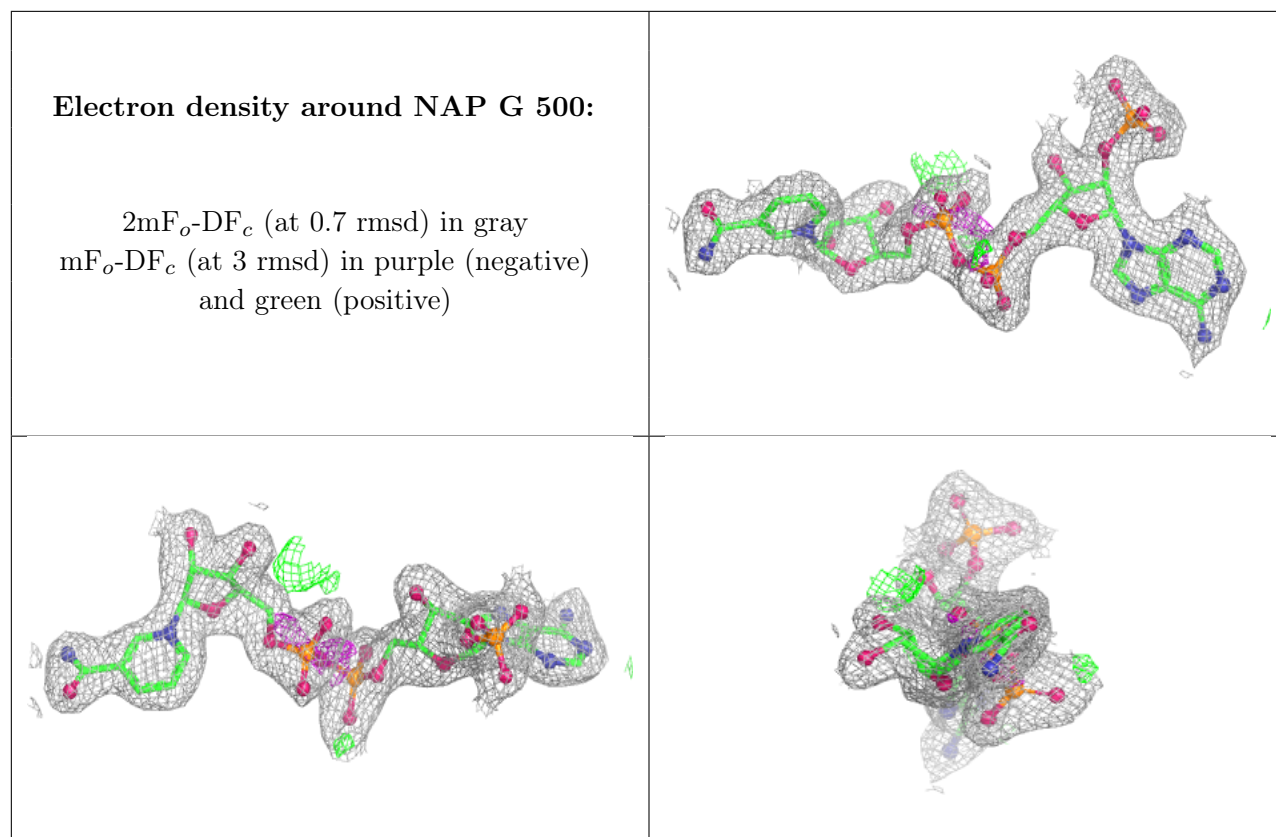
Electron density around NAP C 500:

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

**Electron density around NAP B 500:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.