



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:25 AM UTC

PDB ID : 2C91 / pdb_00002c91
Title : mouse succinic semialdehyde reductase, AKR7A5
Authors : Zhu, X.; Ellis, E.M.; Lapthorn, A.J.
Deposited on : 2005-12-08
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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

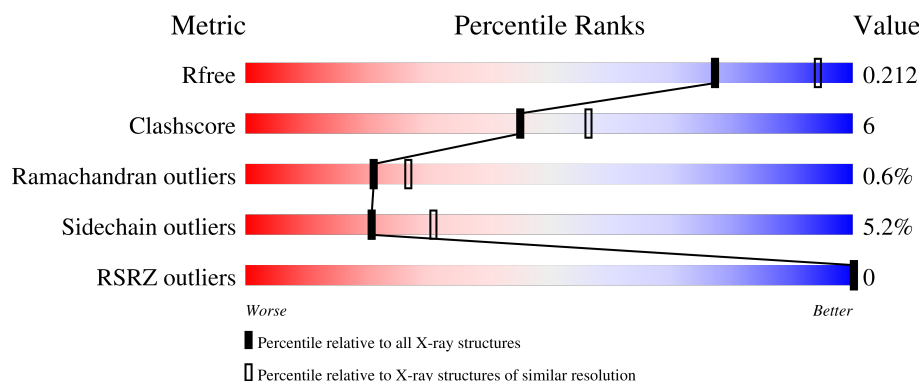
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	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	338	 80% 14% . .
1	B	338	 80% 13% . .
1	C	338	 83% 12% . .
1	D	338	 82% 11% . .
1	E	338	 82% 12% . .

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Mol	Chain	Length	Quality of chain
1	F	338	 82% 11% . . .
1	G	338	 75% 18% . . .
1	H	338	 82% 12% . .
1	I	338	 82% 12% . .
1	J	338	 82% 12% . .

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	TLA	C	360	-	-	X	-
4	GOL	G	364	-	X	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 28440 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 AFLATOXIN B1 ALDEHYDE REDUCTASE MEMBER 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	3	0
			2569	1617	454	480	18			
1	B	324	Total	C	N	O	S	0	0	0
			2545	1603	447	477	18			
1	C	324	Total	C	N	O	S	0	1	0
			2552	1608	447	479	18			
1	D	324	Total	C	N	O	S	0	2	0
			2564	1616	453	477	18			
1	E	324	Total	C	N	O	S	0	1	0
			2556	1611	450	477	18			
1	F	324	Total	C	N	O	S	0	0	0
			2548	1606	447	477	18			
1	G	324	Total	C	N	O	S	0	1	0
			2552	1608	447	479	18			
1	H	324	Total	C	N	O	S	0	1	0
			2538	1601	440	479	18			
1	I	324	Total	C	N	O	S	0	0	0
			2548	1606	447	477	18			
1	J	325	Total	C	N	O	S	0	1	0
			2559	1613	448	480	18			

There are 20 discrepancies between the modelled and reference sequences:

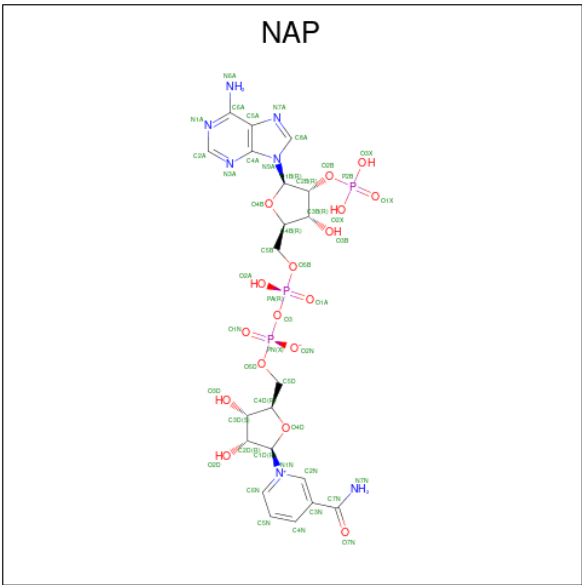
Chain	Residue	Modelled	Actual	Comment	Reference
A	87	ILE	VAL	conflict	UNP Q8CG76
A	122	CYS	ARG	conflict	UNP Q8CG76
B	87	ILE	VAL	conflict	UNP Q8CG76
B	122	CYS	ARG	conflict	UNP Q8CG76
C	87	ILE	VAL	conflict	UNP Q8CG76
C	122	CYS	ARG	conflict	UNP Q8CG76
D	87	ILE	VAL	conflict	UNP Q8CG76
D	122	CYS	ARG	conflict	UNP Q8CG76
E	87	ILE	VAL	conflict	UNP Q8CG76

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Chain	Residue	Modelled	Actual	Comment	Reference
E	122	CYS	ARG	conflict	UNP Q8CG76
F	87	ILE	VAL	conflict	UNP Q8CG76
F	122	CYS	ARG	conflict	UNP Q8CG76
G	87	ILE	VAL	conflict	UNP Q8CG76
G	122	CYS	ARG	conflict	UNP Q8CG76
H	87	ILE	VAL	conflict	UNP Q8CG76
H	122	CYS	ARG	conflict	UNP Q8CG76
I	87	ILE	VAL	conflict	UNP Q8CG76
I	122	CYS	ARG	conflict	UNP Q8CG76
J	87	ILE	VAL	conflict	UNP Q8CG76
J	122	CYS	ARG	conflict	UNP Q8CG76

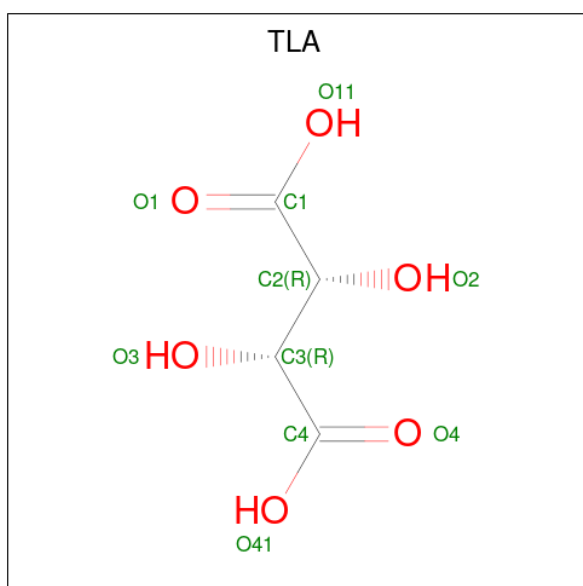
- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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	I	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 L(+)-TARTARIC ACID (CCD ID: TLA) (formula: C₄H₆O₆).



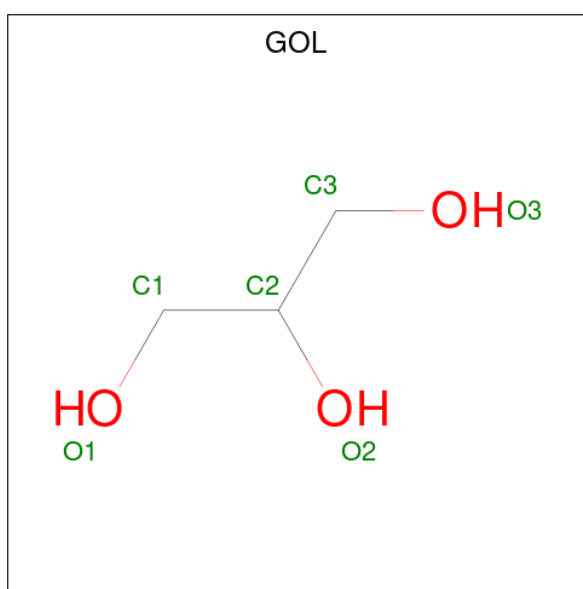
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	4	6		
3	B	1	Total	C	O	0	0
			10	4	6		
3	C	1	Total	C	O	0	0
			10	4	6		
3	D	1	Total	C	O	0	0
			10	4	6		
3	E	1	Total	C	O	0	0
			10	4	6		
3	F	1	Total	C	O	0	0
			10	4	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	C	O	0	0
			10	4	6		
3	H	1	Total	C	O	0	0
			10	4	6		
3	I	1	Total	C	O	0	0
			10	4	6		
3	J	1	Total	C	O	0	0
			10	4	6		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



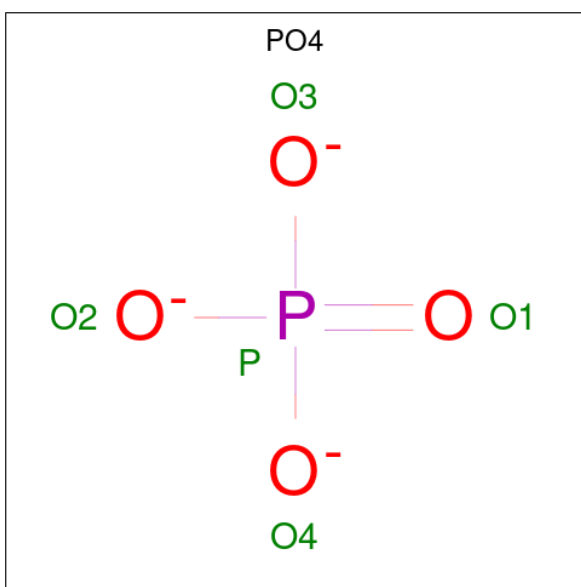
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

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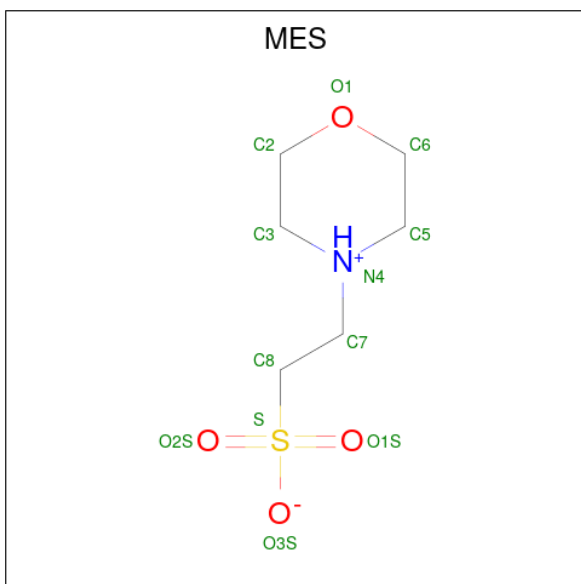
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	I	1	Total	C	O	0	0
			6	3	3		
4	I	1	Total	C	O	0	0
			6	3	3		
4	J	1	Total	C	O	0	0
			6	3	3		
4	J	1	Total	C	O	0	0
			6	3	3		
4	J	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	J	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	S	
			12	6	1	4	1	

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
6	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
6	I	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
6	J	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 7 is water.

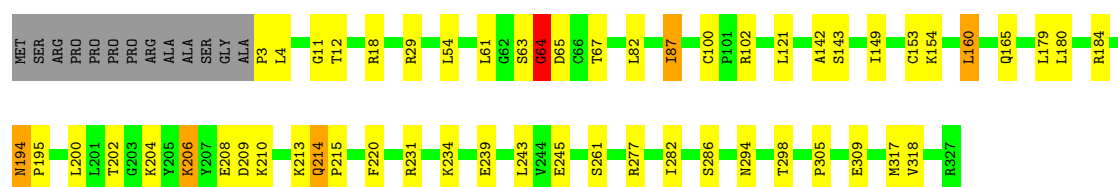
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	223	Total	O	0	0
			223	223		
7	B	131	Total	O	0	0
			131	131		
7	C	225	Total	O	0	0
			225	225		
7	D	272	Total	O	0	0
			272	272		
7	E	262	Total	O	0	0
			262	262		
7	F	214	Total	O	0	0
			214	214		
7	G	257	Total	O	0	0
			257	257		
7	H	159	Total	O	0	0
			159	159		
7	I	164	Total	O	0	0
			164	164		
7	J	202	Total	O	0	0
			202	202		

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.

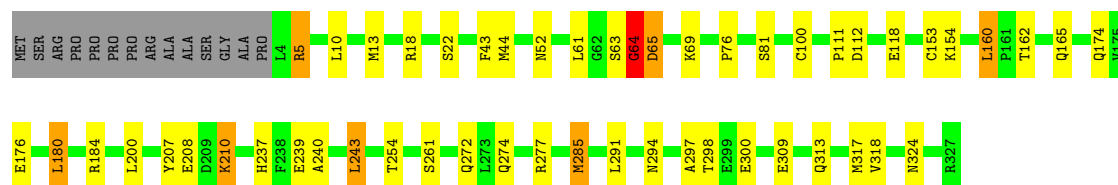
• Molecule 1: AFLATOXIN B1 ALDEHYDE REDUCTASE MEMBER 2

Chain A: 



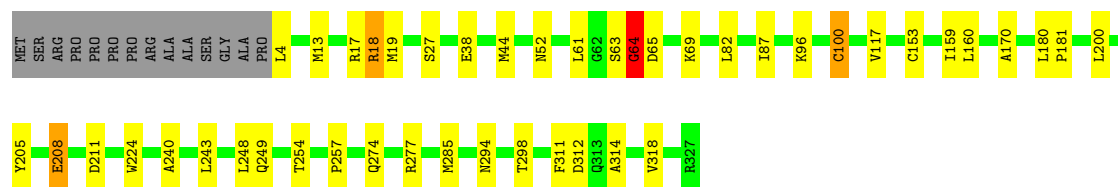
• Molecule 1: AFLATOXIN B1 ALDEHYDE REDUCTASE MEMBER 2

Chain B: 



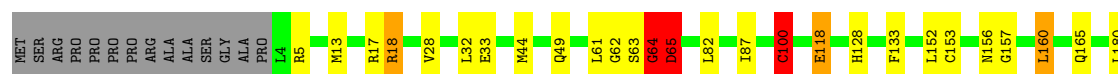
• Molecule 1: AFLATOXIN B1 ALDEHYDE REDUCTASE MEMBER 2

Chain C: 



• Molecule 1: AFLATOXIN B1 ALDEHYDE REDUCTASE MEMBER 2

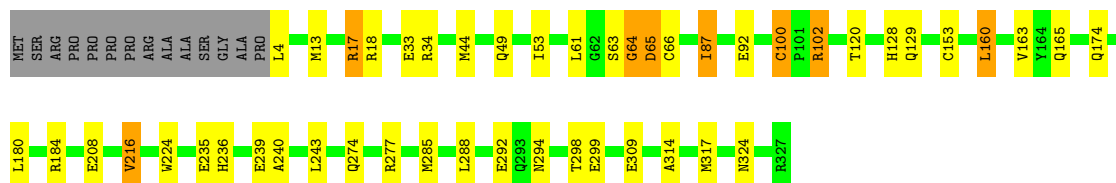
Chain D: 





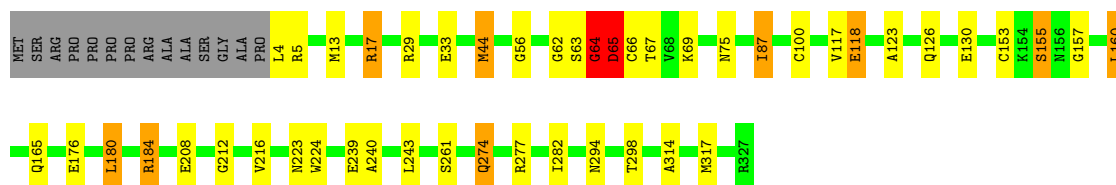
• Molecule 1: AFLATOXIN B1 ALDEHYDE REDUCTASE MEMBER 2

Chain E: 82% 12% . .



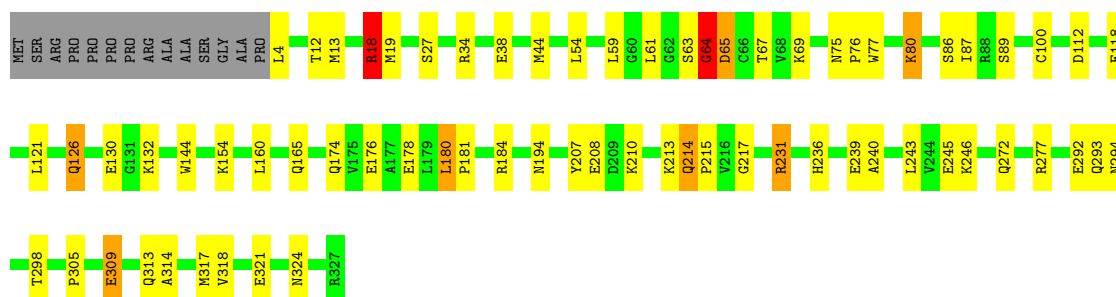
• Molecule 1: AFLATOXIN B1 ALDEHYDE REDUCTASE MEMBER 2

Chain F: 82% 11% . . .



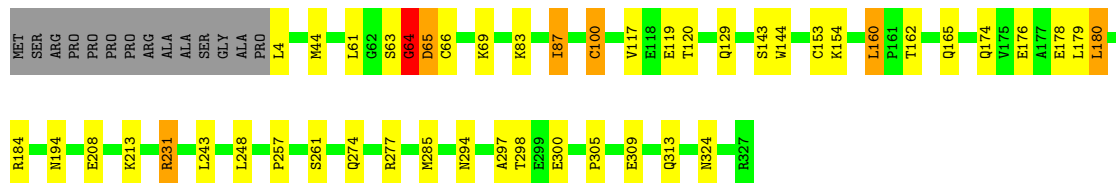
• Molecule 1: AFLATOXIN B1 ALDEHYDE REDUCTASE MEMBER 2

Chain G: 75% 18% . . .



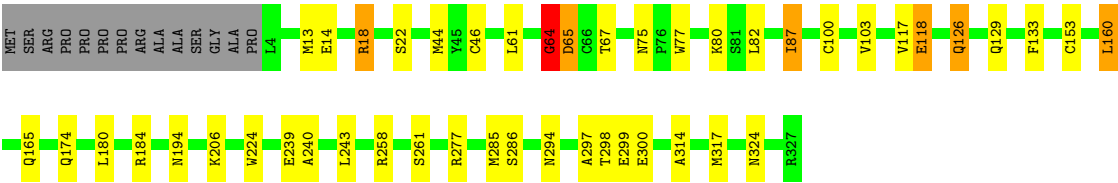
• Molecule 1: AFLATOXIN B1 ALDEHYDE REDUCTASE MEMBER 2

Chain H: 82% 12% . .

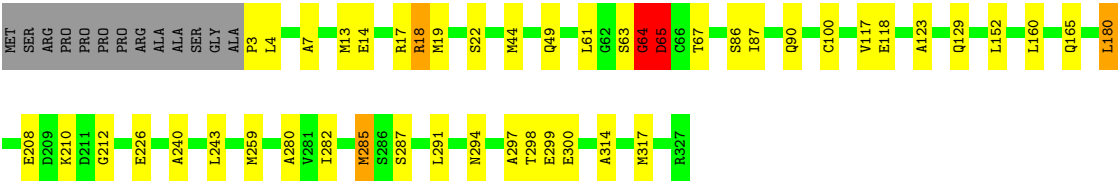
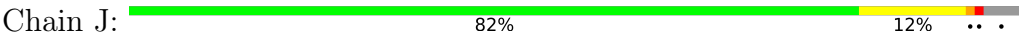


• Molecule 1: AFLATOXIN B1 ALDEHYDE REDUCTASE MEMBER 2

Chain I: 82% 12% . .



● Molecule 1: AFLATOXIN B1 ALDEHYDE REDUCTASE MEMBER 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	98.53Å 159.24Å 96.70Å 90.02° 119.40° 78.50°	Depositor
Resolution (Å)	45.00 – 2.30 45.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.8 (45.00-2.30) 89.7 (45.00-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.160 , 0.208 0.170 , 0.212	Depositor DCC
R_{free} test set	9982 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 22.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.458 for -h-l,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	28440	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: GOL, PO4, MES, TLA, 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	1.37	8/2647 (0.3%)	1.11	1/3584 (0.0%)
1	B	1.10	2/2608 (0.1%)	1.05	3/3533 (0.1%)
1	C	1.23	2/2620 (0.1%)	1.07	0/3549
1	D	1.35	11/2633 (0.4%)	1.13	3/3565 (0.1%)
1	E	1.32	6/2622 (0.2%)	1.14	3/3552 (0.1%)
1	F	1.24	3/2611 (0.1%)	1.09	4/3537 (0.1%)
1	G	1.33	5/2620 (0.2%)	1.10	5/3549 (0.1%)
1	H	1.14	1/2604 (0.0%)	1.02	2/3531 (0.1%)
1	I	1.20	2/2611 (0.1%)	1.07	1/3537 (0.0%)
1	J	1.17	2/2625 (0.1%)	1.06	4/3556 (0.1%)
All	All	1.25	42/26201 (0.2%)	1.08	26/35493 (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	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	1
All	All	0	10

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	194	ASN	C-O	18.55	1.32	1.23
1	D	17	ARG	CA-C	11.04	1.59	1.52
1	A	214	GLN	C-O	-10.56	1.19	1.23
1	D	214	GLN	C-O	-8.63	1.19	1.23
1	G	214	GLN	CA-CB	7.39	1.57	1.52
1	J	282	ILE	CA-CB	7.06	1.61	1.53
1	A	87	ILE	CA-CB	6.98	1.62	1.54
1	E	53	ILE	C-O	-6.94	1.16	1.24
1	G	318	VAL	CA-CB	6.57	1.61	1.54
1	D	18	ARG	CG-CD	6.56	1.72	1.52
1	I	87	ILE	CA-CB	6.31	1.61	1.54
1	E	163	VAL	C-O	-6.29	1.17	1.24
1	H	313	GLN	CG-CD	6.14	1.67	1.52
1	D	192	ALA	CA-CB	6.04	1.61	1.53
1	A	142	ALA	CA-CB	-5.97	1.44	1.53
1	D	254	THR	CA-CB	5.93	1.63	1.53
1	D	194	ASN	CA-C	5.88	1.57	1.53
1	F	75	ASN	N-CA	5.80	1.50	1.45
1	G	184	ARG	CZ-NH1	5.66	1.40	1.32
1	J	180	LEU	C-O	-5.59	1.19	1.24
1	F	56	GLY	C-O	-5.56	1.16	1.24
1	A	318	VAL	CA-CB	5.55	1.60	1.54
1	E	49	GLN	C-O	-5.50	1.17	1.24
1	A	206	LYS	CE-NZ	5.46	1.65	1.49
1	I	118	GLU	CG-CD	5.45	1.65	1.52
1	G	194	ASN	C-O	5.45	1.26	1.23
1	B	111	PRO	C-O	5.29	1.30	1.23
1	D	5	ARG	CZ-NH2	5.26	1.40	1.33
1	D	309	GLU	CG-CD	5.22	1.65	1.52
1	A	213	LYS	CE-NZ	5.21	1.65	1.49
1	D	100	CYS	C-O	-5.21	1.18	1.24
1	G	231	ARG	N-CA	-5.20	1.40	1.46
1	D	49	GLN	C-O	-5.17	1.17	1.24
1	E	235	GLU	C-O	-5.16	1.18	1.24
1	E	92	GLU	C-O	-5.14	1.18	1.24
1	C	159	ILE	CA-CB	5.14	1.60	1.54
1	A	220	PHE	CA-C	-5.13	1.46	1.52
1	D	18	ARG	CB-CG	5.13	1.67	1.52
1	F	184	ARG	CZ-NH2	5.08	1.40	1.33
1	E	17	ARG	CA-C	5.07	1.55	1.52
1	B	313	GLN	CG-CD	5.01	1.64	1.52
1	C	318	VAL	C-O	-5.01	1.19	1.24

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	309	GLU	CB-CA-C	10.30	127.89	110.79
1	E	216	VAL	CB-CA-C	-9.13	96.44	111.32
1	D	216	VAL	CB-CA-C	-8.44	97.56	111.32
1	A	3	PRO	N-CA-CB	7.65	111.41	103.00
1	J	3	PRO	N-CA-CB	7.47	111.21	103.00
1	G	80	LYS	CD-CE-NZ	-7.13	89.09	111.90
1	H	87	ILE	CB-CA-C	-6.63	103.48	111.97
1	I	87	ILE	N-CA-CB	-6.57	102.86	110.55
1	F	155	SER	CB-CA-C	-6.35	98.47	110.67
1	E	102	ARG	CG-CD-NE	-6.11	98.57	112.00
1	H	194	ASN	CB-CA-C	-5.88	105.18	110.71
1	J	67	THR	CB-CA-C	-5.81	100.07	110.70
1	G	18	ARG	NE-CZ-NH1	-5.77	115.73	121.50
1	F	17	ARG	CG-CD-NE	5.71	124.57	112.00
1	G	243	LEU	CA-CB-CG	5.62	135.97	116.30
1	B	5	ARG	CB-CA-C	5.47	116.74	108.86
1	B	44	MET	CG-SD-CE	-5.47	88.87	100.90
1	F	87	ILE	N-CA-CB	5.32	117.77	110.54
1	F	184	ARG	NE-CZ-NH1	-5.27	116.23	121.50
1	D	5	ARG	NE-CZ-NH2	5.16	123.85	119.20
1	J	243	LEU	CA-CB-CG	5.16	134.35	116.30
1	J	259	MET	CG-SD-CE	-5.15	89.57	100.90
1	D	100	CYS	N-CA-C	5.07	116.44	108.23
1	E	87	ILE	N-CA-C	5.06	115.78	110.62
1	G	89	SER	CB-CA-C	-5.04	102.97	110.88
1	G	87	ILE	N-CA-CB	5.02	117.36	110.54

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	64	GLY	Peptide
1	B	64	GLY	Peptide
1	C	64	GLY	Peptide
1	D	64	GLY	Peptide
1	E	64	GLY	Peptide
1	F	64	GLY	Peptide
1	G	64	GLY	Peptide
1	H	64	GLY	Peptide
1	I	64	GLY	Peptide
1	J	64	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2569	0	2484	41	0
1	B	2545	0	2453	27	0
1	C	2552	0	2464	24	0
1	D	2564	0	2488	22	0
1	E	2556	0	2475	29	0
1	F	2548	0	2462	33	0
1	G	2552	0	2464	43	0
1	H	2538	0	2435	23	0
1	I	2548	0	2462	33	0
1	J	2559	0	2470	26	0
2	A	48	0	25	2	0
2	B	48	0	25	3	0
2	C	48	0	25	0	0
2	D	48	0	25	2	0
2	E	48	0	25	2	0
2	F	48	0	25	3	0
2	G	48	0	24	1	0
2	H	48	0	25	4	0
2	I	48	0	25	4	0
2	J	48	0	25	3	0
3	A	10	0	4	0	0
3	B	10	0	4	3	0
3	C	10	0	4	4	0
3	D	10	0	4	1	0
3	E	10	0	4	2	0
3	F	10	0	4	3	0
3	G	10	0	4	1	0
3	H	10	0	4	2	0
3	I	10	0	4	2	0
3	J	10	0	4	2	0
4	A	12	0	16	2	0
4	B	18	0	24	0	0
4	C	18	0	24	0	0
4	D	18	0	24	0	0
4	E	18	0	24	0	0
4	F	6	0	8	0	0
4	G	18	0	24	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	12	0	16	2	0
4	I	12	0	16	1	0
4	J	18	0	24	0	0
5	A	5	0	0	0	0
5	J	5	0	0	0	0
6	B	12	0	12	0	0
6	C	12	0	12	0	0
6	D	12	0	12	0	0
6	I	12	0	12	0	0
6	J	12	0	12	0	0
7	A	223	0	0	9	0
7	B	131	0	0	3	0
7	C	225	0	0	7	0
7	D	272	0	0	4	0
7	E	262	0	0	7	0
7	F	214	0	0	9	0
7	G	257	0	0	9	0
7	H	159	0	0	2	0
7	I	164	0	0	9	0
7	J	202	0	0	8	0
All	All	28440	0	25206	306	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (306) 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:E:100:CYS:SG	7:E:2088:HOH:O	1.95	1.23
1:C:100:CYS:SG	7:C:2071:HOH:O	2.05	1.10
1:F:44:MET:SD	7:F:2025:HOH:O	2.10	1.08
1:A:100:CYS:SG	7:A:2061:HOH:O	2.10	1.06
1:I:13:MET:HG2	7:I:2008:HOH:O	1.61	0.99
1:E:100:CYS:CB	7:E:2088:HOH:O	2.10	0.95
1:C:100:CYS:CB	7:C:2071:HOH:O	2.18	0.90
1:I:14:GLU:OE1	1:I:18:ARG:HG2	1.75	0.85
1:J:212:GLY:HA3	7:J:2132:HOH:O	1.76	0.85
1:H:87:ILE:HD11	1:H:120:THR:HG23	1.59	0.84
1:E:64:GLY:O	1:E:65:ASP:HB2	1.76	0.84
1:I:13:MET:HE2	3:I:360:TLA:O41	1.79	0.82
1:D:118:GLU:HG2	7:D:2104:HOH:O	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:LEU:O	1:D:184[A]:ARG:HG2	1.81	0.81
1:J:13:MET:HE2	3:J:360:TLA:O41	1.82	0.79
1:A:29:ARG:NH2	1:F:33:GLU:OE2	2.13	0.79
1:D:245:GLU:OE1	7:D:2181:HOH:O	1.99	0.79
1:I:82:LEU:HD22	1:I:87:ILE:HD11	1.64	0.78
1:E:274:GLN:HE21	1:E:277:ARG:HG3	1.50	0.77
1:B:154:LYS:NZ	7:B:2055:HOH:O	2.17	0.77
1:C:61:LEU:O	1:C:100:CYS:HB2	1.86	0.75
1:H:178:GLU:OE2	7:H:2080:HOH:O	2.04	0.75
1:I:46:CYS:HB3	7:I:2009:HOH:O	1.87	0.75
1:A:102:ARG:O	7:A:2061:HOH:O	2.05	0.74
1:A:309[B]:GLU:OE1	7:A:2198:HOH:O	2.04	0.73
1:E:100:CYS:HB3	7:E:2088:HOH:O	1.82	0.72
1:A:18[B]:ARG:HD3	1:A:286:SER:HB2	1.70	0.72
1:C:13:MET:HE2	3:C:360:TLA:O41	1.87	0.72
1:H:305:PRO:O	1:H:309[A]:GLU:HG3	1.90	0.71
1:G:305:PRO:O	1:G:309[A]:GLU:HG3	1.91	0.70
2:H:350:NAP:H4N	3:H:360:TLA:O11	1.91	0.70
1:I:75:ASN:OD1	1:I:80:LYS:NZ	2.24	0.70
1:D:61:LEU:O	1:D:100:CYS:HB2	1.91	0.69
1:F:13:MET:HE2	3:F:360:TLA:O41	1.92	0.69
2:B:350:NAP:H4N	3:B:360:TLA:O11	1.93	0.69
1:F:274:GLN:NE2	1:F:277:ARG:HD2	2.08	0.68
1:I:13:MET:CG	7:I:2008:HOH:O	2.31	0.68
1:J:210:LYS:CD	7:J:2130:HOH:O	2.42	0.67
1:G:239:GLU:HB3	1:G:317:MET:HE1	1.74	0.67
1:D:82:LEU:HD22	1:D:87:ILE:HD11	1.76	0.67
1:I:239:GLU:OE2	7:I:2124:HOH:O	2.13	0.66
1:E:66:CYS:HA	7:E:2054:HOH:O	1.95	0.66
1:F:153:CYS:HB2	1:F:160:LEU:HD22	1.78	0.65
1:H:64:GLY:O	1:H:65:ASP:HB2	1.95	0.65
1:E:61:LEU:O	1:E:100:CYS:HB2	1.97	0.65
1:F:212:GLY:HA3	7:F:2132:HOH:O	1.97	0.64
1:J:64:GLY:O	1:J:65:ASP:HB2	1.97	0.64
1:G:292:GLU:HG3	7:G:2206:HOH:O	1.97	0.64
1:D:153:CYS:HB2	1:D:160:LEU:HD22	1.79	0.64
1:A:82:LEU:HD22	1:A:87:ILE:HD11	1.80	0.64
1:H:66:CYS:O	1:H:69:LYS:NZ	2.31	0.63
1:J:210:LYS:HD2	7:J:2130:HOH:O	1.99	0.63
1:B:61:LEU:O	1:B:100:CYS:HB2	1.99	0.63
1:B:184:ARG:NH1	7:B:2064:HOH:O	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:153:CYS:HB2	1:E:160:LEU:HD22	1.81	0.63
1:B:294:ASN:O	1:B:298:THR:HG23	1.99	0.62
1:C:274:GLN:HE21	1:C:277:ARG:HG3	1.64	0.62
1:H:231:ARG:HD2	4:H:361:GOL:O2	1.99	0.62
1:J:129:GLN:HG3	7:J:2089:HOH:O	1.99	0.62
1:C:205:TYR:HB2	7:C:2132:HOH:O	2.00	0.61
1:C:312:ASP:OD1	7:C:2192:HOH:O	2.16	0.61
1:F:153:CYS:CB	1:F:160:LEU:HD22	2.31	0.61
1:D:64:GLY:O	1:D:65:ASP:HB2	2.01	0.61
1:F:44:MET:HG2	7:F:2025:HOH:O	2.00	0.61
1:H:61:LEU:O	1:H:100:CYS:HB2	2.00	0.61
1:A:184[B]:ARG:NH1	1:A:277:ARG:HH11	1.99	0.60
1:I:18:ARG:HG3	1:I:286:SER:HB2	1.83	0.60
1:D:157:GLY:HA2	7:D:2118:HOH:O	2.00	0.60
1:B:13:MET:HE2	3:B:360:TLA:O41	2.02	0.60
1:E:13:MET:HE3	2:E:350:NAP:H3D	1.83	0.59
1:E:13:MET:HE2	3:E:360:TLA:O41	2.03	0.59
1:G:294:ASN:O	1:G:298:THR:HG23	2.03	0.58
1:B:153:CYS:CB	1:B:160:LEU:HD22	2.33	0.58
1:E:274:GLN:NE2	1:E:277:ARG:HD2	2.19	0.58
1:D:13:MET:HE2	3:D:360:TLA:O41	2.03	0.58
1:C:294:ASN:O	1:C:298:THR:HG23	2.04	0.58
1:I:80:LYS:HE2	7:I:2042:HOH:O	2.02	0.58
1:A:231:ARG:HH11	4:A:361:GOL:H32	1.68	0.58
1:A:239:GLU:CB	1:A:317:MET:HE1	2.34	0.57
1:B:274:GLN:NE2	1:B:277:ARG:HD2	2.19	0.57
1:A:153:CYS:HB2	1:A:160:LEU:CD2	2.33	0.57
1:G:77:TRP:O	1:G:80:LYS:HE3	2.05	0.57
1:D:294:ASN:O	1:D:298:THR:HG23	2.05	0.57
1:H:165:GLN:OE1	2:H:350:NAP:H2N	2.04	0.57
1:I:77:TRP:O	1:I:80:LYS:HE3	2.05	0.57
1:B:153:CYS:HB2	1:B:160:LEU:HD22	1.86	0.56
1:G:165:GLN:OE1	2:G:350:NAP:H2N	2.06	0.56
1:F:44:MET:CG	7:F:2025:HOH:O	2.42	0.56
1:G:240:ALA:HB1	1:G:314:ALA:HB1	1.87	0.56
1:E:294:ASN:O	1:E:298:THR:HG23	2.06	0.56
1:B:165:GLN:OE1	2:B:350:NAP:H2N	2.05	0.55
1:G:34:ARG:HD3	7:G:2028:HOH:O	2.07	0.55
1:G:13:MET:HE2	3:G:360:TLA:O41	2.07	0.55
1:D:13:MET:HE3	2:D:350:NAP:H3D	1.89	0.55
1:E:288:LEU:O	1:E:292:GLU:HG3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:165:GLN:OE1	2:J:350:NAP:H2N	2.07	0.54
1:F:126:GLN:O	1:F:130:GLU:HG3	2.07	0.54
1:A:184[B]:ARG:HH11	1:A:277:ARG:NH1	2.05	0.54
1:G:18:ARG:HD2	7:G:2198:HOH:O	2.07	0.54
1:I:64:GLY:O	1:I:65:ASP:HB2	2.06	0.54
1:I:184:ARG:NH1	7:I:2102:HOH:O	2.40	0.54
1:J:19:MET:HE3	1:J:287:SER:C	2.33	0.54
1:A:294:ASN:O	1:A:298:THR:HG23	2.07	0.54
1:B:274:GLN:HE22	1:B:277:ARG:HD2	1.73	0.54
1:A:206:LYS:HE2	1:A:209:ASP:OD1	2.08	0.54
1:D:165:GLN:OE1	2:D:350:NAP:H2N	2.08	0.53
1:G:305:PRO:O	1:G:309[A]:GLU:CG	2.56	0.53
4:G:364:GOL:H31	1:J:226:GLU:HB3	1.91	0.53
1:H:176:GLU:HA	1:H:180:LEU:HD22	1.90	0.53
1:I:294:ASN:O	1:I:298:THR:HG23	2.08	0.53
1:A:239:GLU:HB3	1:A:317:MET:HE1	1.89	0.53
1:F:157:GLY:HA2	7:F:2102:HOH:O	2.08	0.53
1:G:246:LYS:NZ	7:G:2164:HOH:O	2.43	0.52
1:A:12:THR:HG21	1:A:54:LEU:HD11	1.91	0.52
1:D:240:ALA:HB1	1:D:314:ALA:HB1	1.91	0.52
1:A:29:ARG:HH21	1:F:33:GLU:CD	2.12	0.52
1:E:87:ILE:CD1	1:E:120:THR:HG23	2.40	0.52
1:G:64:GLY:O	1:G:65:ASP:HB2	2.10	0.52
1:H:143:SER:HB3	1:H:179:LEU:HA	1.92	0.52
1:H:64:GLY:HA3	7:H:2048:HOH:O	2.09	0.51
1:A:245:GLU:OE1	7:A:2145:HOH:O	2.19	0.51
1:G:130:GLU:OE1	1:G:132:LYS:HE2	2.10	0.51
1:E:33:GLU:HG3	7:E:2020:HOH:O	2.11	0.51
1:I:153:CYS:HB3	1:I:160:LEU:HD22	1.92	0.51
1:F:126:GLN:HB2	7:F:2089:HOH:O	2.10	0.51
1:I:18:ARG:HD3	7:I:2013:HOH:O	2.10	0.51
1:B:277:ARG:HD3	7:B:2064:HOH:O	2.11	0.51
1:A:184[B]:ARG:NH1	1:A:277:ARG:NH1	2.58	0.50
1:G:86:SER:CB	4:G:364:GOL:O2	2.60	0.50
1:A:63:SER:O	1:A:63:SER:OG	2.23	0.50
1:F:118:GLU:H	1:F:118:GLU:CD	2.20	0.50
1:G:75:ASN:CG	1:G:80:LYS:HZ1	2.19	0.50
1:J:13:MET:HE3	2:J:350:NAP:H3D	1.93	0.50
2:J:350:NAP:H4N	3:J:360:TLA:O11	2.11	0.50
1:G:18:ARG:HH12	1:G:217:GLY:HA2	1.76	0.49
1:G:19:MET:HE1	1:G:27:SER:OG	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:19:MET:HE3	1:J:287:SER:CA	2.42	0.49
1:D:152:LEU:O	1:D:156:ASN:ND2	2.33	0.49
1:F:87:ILE:HD11	1:F:123:ALA:HB3	1.94	0.49
1:C:38:GLU:HG2	1:C:69:LYS:HB2	1.94	0.49
1:H:294:ASN:O	1:H:298:THR:HG23	2.11	0.49
1:G:64:GLY:N	7:G:2049:HOH:O	2.45	0.49
1:G:214:GLN:N	1:G:215:PRO:CD	2.74	0.49
1:A:277:ARG:NE	7:A:2172:HOH:O	2.45	0.49
1:F:240:ALA:HB1	1:F:314:ALA:HB1	1.95	0.49
1:A:153:CYS:HB2	1:A:160:LEU:HD22	1.94	0.49
1:E:236:HIS:CD2	7:E:2182:HOH:O	2.65	0.49
1:F:64:GLY:CA	7:F:2041:HOH:O	2.60	0.49
1:H:297:ALA:HA	1:H:300:GLU:OE2	2.13	0.49
1:G:213:LYS:HB3	1:G:215:PRO:HD3	1.94	0.49
1:G:277:ARG:NE	7:G:2195:HOH:O	2.44	0.48
1:E:239:GLU:HB3	1:E:317:MET:HE1	1.95	0.48
1:I:126:GLN:HG3	7:I:2076:HOH:O	2.11	0.48
1:B:174:GLN:OE1	1:B:324:ASN:HA	2.13	0.48
1:J:61:LEU:O	1:J:100:CYS:HB2	2.13	0.48
1:B:176:GLU:HA	1:B:180:LEU:HD22	1.95	0.48
1:I:153:CYS:CB	1:I:160:LEU:HD22	2.42	0.48
1:D:153:CYS:CB	1:D:160:LEU:HD22	2.44	0.48
1:C:274:GLN:NE2	1:C:277:ARG:HD2	2.29	0.48
1:E:165:GLN:OE1	2:E:350:NAP:H2N	2.13	0.47
1:E:240:ALA:HB1	1:E:314:ALA:HB1	1.95	0.47
1:I:239:GLU:HB3	1:I:317:MET:HE1	1.95	0.47
1:D:63:SER:O	1:D:64:GLY:C	2.58	0.47
1:E:34:ARG:NH1	1:E:299:GLU:OE1	2.47	0.47
1:F:294:ASN:O	1:F:298:THR:HG23	2.13	0.47
1:A:165:GLN:OE1	2:A:350:NAP:H2N	2.14	0.47
1:C:82:LEU:HB3	1:C:87:ILE:HD11	1.97	0.47
1:J:49:GLN:NE2	7:J:2035:HOH:O	2.46	0.47
1:F:239:GLU:CB	1:F:317:MET:HE1	2.45	0.47
1:B:43:PHE:CZ	1:F:223:ASN:HA	2.49	0.47
1:G:176:GLU:HA	1:G:180:LEU:HD22	1.95	0.47
1:E:153:CYS:CB	1:E:160:LEU:HD22	2.44	0.47
3:F:360:TLA:O1	3:F:360:TLA:O3	2.33	0.47
1:G:80:LYS:HG2	4:G:364:GOL:H2	1.97	0.47
1:I:13:MET:HE3	2:I:350:NAP:H6N	1.96	0.47
1:G:144:TRP:HA	1:H:144:TRP:HA	1.97	0.46
1:H:231:ARG:CD	4:H:361:GOL:O2	2.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:350:NAP:H52A	2:H:350:NAP:H8A	1.97	0.46
1:J:118[B]:GLU:HG3	1:J:152:LEU:HD13	1.97	0.46
1:F:176:GLU:HA	1:F:180:LEU:HD22	1.97	0.46
1:G:61:LEU:O	1:G:100:CYS:HB2	2.15	0.46
1:I:61:LEU:O	1:I:100:CYS:HB2	2.16	0.46
1:A:214:GLN:N	1:A:215:PRO:CD	2.78	0.46
1:J:49:GLN:HG3	7:J:2004:HOH:O	2.15	0.46
1:C:208:GLU:HG2	7:C:2136:HOH:O	2.15	0.46
1:F:64:GLY:O	1:F:65:ASP:HB2	2.15	0.46
1:H:87:ILE:HG21	1:H:87:ILE:HD13	1.57	0.46
1:J:294:ASN:O	1:J:298:THR:HG23	2.16	0.46
1:A:214:GLN:N	1:A:215:PRO:HD3	2.31	0.46
1:J:210:LYS:HD3	7:J:2130:HOH:O	2.09	0.46
1:B:63:SER:O	1:B:64:GLY:C	2.60	0.45
1:G:118:GLU:HG2	7:G:2086:HOH:O	2.16	0.45
1:A:239:GLU:HB2	1:A:317:MET:HE1	1.98	0.45
1:A:317:MET:HE2	1:A:317:MET:HB3	1.80	0.45
1:I:13:MET:CE	2:I:350:NAP:C6N	2.94	0.45
1:A:210:LYS:HE2	7:A:2120:HOH:O	2.15	0.45
1:E:128:HIS:HD2	1:E:129:GLN:HE21	1.64	0.45
1:B:297:ALA:HA	1:B:300:GLU:OE2	2.17	0.45
1:H:174:GLN:OE1	1:H:324:ASN:HA	2.17	0.45
1:J:317:MET:HE2	1:J:317:MET:HB3	1.86	0.45
1:B:240:ALA:O	1:B:243:LEU:HB3	2.17	0.45
1:G:63:SER:O	1:G:64:GLY:C	2.59	0.45
1:J:240:ALA:HB1	1:J:314:ALA:HB1	1.99	0.45
1:A:202:THR:OG1	1:A:204:LYS:HG2	2.16	0.44
1:G:38:GLU:HG2	1:G:69:LYS:HB2	1.99	0.44
4:I:362:GOL:H11	7:J:2097:HOH:O	2.17	0.44
1:C:224:TRP:CH2	3:C:360:TLA:H2	2.53	0.44
1:E:239:GLU:OE2	7:E:2182:HOH:O	2.21	0.44
1:G:12:THR:HG21	1:G:54:LEU:HD11	1.99	0.44
1:E:174:GLN:OE1	1:E:324:ASN:HA	2.18	0.44
1:F:13:MET:O	1:F:13:MET:HG2	2.18	0.44
1:G:309[B]:GLU:HG3	1:G:313:GLN:OE1	2.17	0.44
1:C:44:MET:CE	3:C:360:TLA:H3	2.47	0.44
1:D:18:ARG:HD3	1:D:286:SER:HB2	2.00	0.44
1:F:282:ILE:HG22	2:F:350:NAP:H4D	1.99	0.44
1:I:75:ASN:CG	1:I:80:LYS:NZ	2.76	0.44
2:B:350:NAP:H4N	3:B:360:TLA:C1	2.48	0.44
1:I:240:ALA:HB1	1:I:314:ALA:HB1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:CYS:HB2	7:A:2061:HOH:O	2.18	0.44
1:G:174:GLN:OE1	1:G:324:ASN:HA	2.17	0.43
1:G:207:TYR:OH	1:G:210:LYS:NZ	2.50	0.43
1:E:224:TRP:CZ3	3:E:360:TLA:H2	2.54	0.43
1:I:317:MET:HE2	1:I:317:MET:HB3	1.86	0.43
1:J:86:SER:O	1:J:90:GLN:HG3	2.18	0.43
1:A:231:ARG:HH11	4:A:361:GOL:C3	2.29	0.43
1:E:100:CYS:SG	1:E:102:ARG:O	2.77	0.43
1:G:245:GLU:OE1	7:G:2163:HOH:O	2.21	0.43
1:C:63:SER:O	1:C:64:GLY:C	2.62	0.43
1:F:44:MET:CE	1:F:224:TRP:NE1	2.82	0.43
1:G:118:GLU:CD	1:G:118:GLU:H	2.27	0.43
1:H:248:LEU:HD22	1:H:257:PRO:HG2	2.01	0.43
1:J:63:SER:O	1:J:64:GLY:C	2.62	0.43
1:I:277:ARG:NH1	7:I:2134:HOH:O	2.50	0.43
1:A:18[B]:ARG:HD3	1:A:286:SER:CB	2.45	0.43
1:I:297:ALA:HA	1:I:300:GLU:OE2	2.19	0.43
1:D:128:HIS:HD2	1:D:133:PHE:O	2.02	0.42
1:H:63:SER:O	1:H:64:GLY:C	2.61	0.42
1:I:224:TRP:CH2	3:I:360:TLA:H2	2.55	0.42
1:J:285:MET:HG3	1:J:291:LEU:HB2	2.01	0.42
1:A:11:GLY:HA3	2:A:350:NAP:H4D	2.02	0.42
1:G:86:SER:HA	4:G:364:GOL:O2	2.19	0.42
1:E:63:SER:O	1:E:65:ASP:HB3	2.19	0.42
1:F:29:ARG:NH2	7:F:2014:HOH:O	2.51	0.42
1:A:143:SER:HB3	1:A:179:LEU:HA	2.02	0.42
1:B:76:PRO:HB3	1:B:112:ASP:HB2	1.99	0.42
1:C:180:LEU:HB2	1:C:181:PRO:HD3	2.02	0.42
1:C:240:ALA:HB1	1:C:314:ALA:HB1	2.02	0.42
1:G:76:PRO:HB3	1:G:112:ASP:HB2	2.01	0.42
1:G:236:HIS:HB2	1:G:321:GLU:OE2	2.19	0.42
1:C:18:ARG:NH2	7:C:2011:HOH:O	2.53	0.42
1:G:126:GLN:HE21	1:G:126:GLN:HB2	1.68	0.42
1:A:121:LEU:HD11	1:A:149:ILE:HG23	2.02	0.42
1:B:285:MET:HG3	1:B:291:LEU:HB2	2.01	0.42
1:F:63:SER:O	1:F:64:GLY:C	2.62	0.42
1:B:237:HIS:HA	1:B:318:VAL:HG11	2.01	0.42
1:B:239:GLU:HB2	1:B:317:MET:HE1	2.01	0.42
1:C:19:MET:HE1	1:C:27:SER:OG	2.20	0.42
1:G:272:GLN:NE2	7:G:2190:HOH:O	2.47	0.42
1:J:297:ALA:HA	1:J:300:GLU:OE2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:178:GLU:C	1:G:181:PRO:HD2	2.45	0.42
1:H:83:LYS:NZ	1:H:119:GLU:OE1	2.48	0.42
2:H:350:NAP:H4N	3:H:360:TLA:C1	2.48	0.42
1:I:239:GLU:CB	1:I:317:MET:HE1	2.50	0.42
1:B:153:CYS:HB3	1:B:160:LEU:HD22	1.99	0.41
1:D:62:GLY:HA2	7:D:2088:HOH:O	2.20	0.41
1:D:288:LEU:O	1:D:292:GLU:HG3	2.20	0.41
1:G:121:LEU:HD23	1:G:121:LEU:HA	1.81	0.41
1:H:274:GLN:NE2	1:H:277:ARG:HD2	2.35	0.41
1:I:103:VAL:O	1:I:133:PHE:HA	2.21	0.41
1:A:100:CYS:CB	7:A:2061:HOH:O	2.57	0.41
1:A:194:ASN:N	1:A:195:PRO:CD	2.83	0.41
1:B:64:GLY:O	1:B:65:ASP:HB2	2.21	0.41
1:B:239:GLU:CB	1:B:317:MET:HE1	2.51	0.41
1:C:170:ALA:HB1	1:C:311:PHE:CD1	2.55	0.41
1:E:87:ILE:HD12	1:E:120:THR:HG23	2.02	0.41
1:F:62:GLY:HA2	7:F:2073:HOH:O	2.20	0.41
1:A:153:CYS:CB	1:A:160:LEU:CD2	2.98	0.41
1:C:224:TRP:CZ3	3:C:360:TLA:H2	2.56	0.41
1:D:28:VAL:O	1:D:32:LEU:HG	2.20	0.41
1:H:63:SER:O	1:H:66:CYS:HB2	2.20	0.41
1:I:174:GLN:OE1	1:I:324:ASN:HA	2.20	0.41
1:B:63:SER:O	1:B:63:SER:OG	2.32	0.41
1:B:207:TYR:CZ	1:B:210:LYS:HE3	2.56	0.41
1:F:87:ILE:HD13	1:F:87:ILE:HG21	1.72	0.41
1:G:18:ARG:NH1	1:G:217:GLY:HA2	2.35	0.41
1:A:234:LYS:HE3	7:A:2133:HOH:O	2.20	0.41
1:D:264:LEU:O	1:D:267:MET:HB2	2.20	0.41
1:H:153:CYS:HB2	1:H:160:LEU:HD22	2.03	0.41
1:I:194:ASN:ND2	2:I:350:NAP:O2N	2.53	0.41
1:C:153:CYS:HB3	1:C:160:LEU:HD22	2.03	0.40
1:F:184:ARG:HG3	1:F:277:ARG:CZ	2.51	0.40
1:I:165:GLN:OE1	2:I:350:NAP:H2N	2.20	0.40
1:A:63:SER:O	1:A:64:GLY:C	2.63	0.40
1:A:195:PRO:HG3	1:A:282:ILE:O	2.22	0.40
1:C:100:CYS:CA	7:C:2071:HOH:O	2.61	0.40
1:E:63:SER:O	1:E:64:GLY:C	2.64	0.40
1:F:66:CYS:O	1:F:69:LYS:NZ	2.53	0.40
1:B:272:GLN:HE21	1:B:272:GLN:HB3	1.65	0.40
1:F:165:GLN:OE1	2:F:350:NAP:H2N	2.21	0.40
1:J:7:ALA:HB3	1:J:280:ALA:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LEU:O	1:A:100:CYS:HB2	2.21	0.40
1:C:248:LEU:HD22	1:C:257:PRO:HG2	2.03	0.40
1:F:44:MET:CE	1:F:224:TRP:HE1	2.34	0.40
2:F:350:NAP:H4N	3:F:360:TLA:O11	2.22	0.40
1:J:14:GLU:OE1	1:J:18:ARG:HB2	2.21	0.40
1:J:87:ILE:HD11	1:J:123:ALA:HB3	2.04	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	326/338 (96%)	320 (98%)	4 (1%)	2 (1%)	21	27
1	B	322/338 (95%)	314 (98%)	6 (2%)	2 (1%)	21	27
1	C	323/338 (96%)	314 (97%)	7 (2%)	2 (1%)	21	27
1	D	324/338 (96%)	317 (98%)	5 (2%)	2 (1%)	21	27
1	E	323/338 (96%)	316 (98%)	6 (2%)	1 (0%)	36	46
1	F	322/338 (95%)	312 (97%)	8 (2%)	2 (1%)	21	27
1	G	323/338 (96%)	316 (98%)	5 (2%)	2 (1%)	21	27
1	H	323/338 (96%)	316 (98%)	5 (2%)	2 (1%)	21	27
1	I	322/338 (95%)	314 (98%)	6 (2%)	2 (1%)	21	27
1	J	324/338 (96%)	313 (97%)	8 (2%)	3 (1%)	14	17
All	All	3232/3380 (96%)	3152 (98%)	60 (2%)	20 (1%)	21	27

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	ASP

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Mol	Chain	Res	Type
1	B	65	ASP
1	C	65	ASP
1	D	65	ASP
1	E	65	ASP
1	F	65	ASP
1	G	65	ASP
1	H	65	ASP
1	I	65	ASP
1	J	4	LEU
1	J	65	ASP
1	G	64	GLY
1	I	64	GLY
1	J	64	GLY
1	B	64	GLY
1	A	64	GLY
1	C	64	GLY
1	F	64	GLY
1	H	64	GLY
1	D	64	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	269/276 (98%)	259 (96%)	10 (4%)	30	45
1	B	265/276 (96%)	247 (93%)	18 (7%)	14	20
1	C	267/276 (97%)	253 (95%)	14 (5%)	21	31
1	D	268/276 (97%)	257 (96%)	11 (4%)	27	41
1	E	267/276 (97%)	254 (95%)	13 (5%)	22	34
1	F	266/276 (96%)	249 (94%)	17 (6%)	16	23
1	G	267/276 (97%)	253 (95%)	14 (5%)	21	31
1	H	264/276 (96%)	248 (94%)	16 (6%)	17	24
1	I	266/276 (96%)	250 (94%)	16 (6%)	17	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	267/276 (97%)	256 (96%)	11 (4%)	27	41
All	All	2666/2760 (97%)	2526 (95%)	140 (5%)	21	30

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

Mol	Chain	Res	Type
1	A	4	LEU
1	A	67	THR
1	A	154	LYS
1	A	160	LEU
1	A	180	LEU
1	A	200	LEU
1	A	208	GLU
1	A	243	LEU
1	A	261	SER
1	A	305	PRO
1	B	5	ARG
1	B	10	LEU
1	B	18	ARG
1	B	22	SER
1	B	52	ASN
1	B	69	LYS
1	B	81	SER
1	B	118	GLU
1	B	160	LEU
1	B	162	THR
1	B	180	LEU
1	B	200	LEU
1	B	208	GLU
1	B	210	LYS
1	B	243	LEU
1	B	254	THR
1	B	261	SER
1	B	285	MET
1	C	4	LEU
1	C	17	ARG
1	C	18	ARG
1	C	52	ASN
1	C	96	LYS
1	C	100	CYS
1	C	117	VAL
1	C	200	LEU

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Mol	Chain	Res	Type
1	C	208	GLU
1	C	211	ASP
1	C	243	LEU
1	C	249	GLN
1	C	254	THR
1	C	285	MET
1	D	33	GLU
1	D	44	MET
1	D	65	ASP
1	D	100	CYS
1	D	118	GLU
1	D	160	LEU
1	D	184[A]	ARG
1	D	184[B]	ARG
1	D	208	GLU
1	D	216	VAL
1	D	243	LEU
1	E	4	LEU
1	E	17	ARG
1	E	18	ARG
1	E	44	MET
1	E	100	CYS
1	E	160	LEU
1	E	180	LEU
1	E	184	ARG
1	E	208	GLU
1	E	216	VAL
1	E	243	LEU
1	E	285	MET
1	E	309	GLU
1	F	4	LEU
1	F	5	ARG
1	F	17	ARG
1	F	44	MET
1	F	65	ASP
1	F	67	THR
1	F	100	CYS
1	F	117	VAL
1	F	118	GLU
1	F	155	SER
1	F	160	LEU
1	F	180	LEU

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Mol	Chain	Res	Type
1	F	208	GLU
1	F	216	VAL
1	F	243	LEU
1	F	261	SER
1	F	274	GLN
1	G	4	LEU
1	G	18	ARG
1	G	44	MET
1	G	59	LEU
1	G	67	THR
1	G	126	GLN
1	G	154	LYS
1	G	160	LEU
1	G	180	LEU
1	G	208	GLU
1	G	231	ARG
1	G	293	GLN
1	G	309[A]	GLU
1	G	309[B]	GLU
1	H	4	LEU
1	H	44	MET
1	H	100	CYS
1	H	117	VAL
1	H	129	GLN
1	H	154	LYS
1	H	160	LEU
1	H	162	THR
1	H	180	LEU
1	H	184	ARG
1	H	208	GLU
1	H	213	LYS
1	H	231	ARG
1	H	243	LEU
1	H	261	SER
1	H	285	MET
1	I	18	ARG
1	I	22	SER
1	I	44	MET
1	I	67	THR
1	I	117	VAL
1	I	118	GLU
1	I	126	GLN

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Mol	Chain	Res	Type
1	I	129	GLN
1	I	160	LEU
1	I	180	LEU
1	I	206	LYS
1	I	243	LEU
1	I	258	ARG
1	I	261	SER
1	I	285	MET
1	I	299	GLU
1	J	17	ARG
1	J	18	ARG
1	J	22	SER
1	J	44	MET
1	J	65	ASP
1	J	117	VAL
1	J	160	LEU
1	J	180	LEU
1	J	208	GLU
1	J	285	MET
1	J	299	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	52	ASN
1	A	128	HIS
1	A	129	GLN
1	A	185	HIS
1	A	274	GLN
1	A	313	GLN
1	B	126	GLN
1	B	129	GLN
1	B	272	GLN
1	B	274	GLN
1	B	313	GLN
1	C	36	HIS
1	C	129	GLN
1	C	140	ASN
1	C	274	GLN
1	C	293	GLN
1	D	49	GLN

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Mol	Chain	Res	Type
1	D	52	ASN
1	D	128	HIS
1	D	129	GLN
1	D	274	GLN
1	E	49	GLN
1	E	52	ASN
1	E	129	GLN
1	E	140	ASN
1	E	236	HIS
1	E	274	GLN
1	F	49	GLN
1	F	128	HIS
1	F	129	GLN
1	F	272	GLN
1	F	274	GLN
1	F	293	GLN
1	F	313	GLN
1	G	49	GLN
1	G	52	ASN
1	G	126	GLN
1	G	129	GLN
1	G	236	HIS
1	H	49	GLN
1	H	52	ASN
1	H	129	GLN
1	H	140	ASN
1	H	236	HIS
1	H	272	GLN
1	H	274	GLN
1	I	49	GLN
1	I	52	ASN
1	I	129	GLN
1	I	272	GLN
1	I	293	GLN
1	J	49	GLN
1	J	52	ASN
1	J	126	GLN
1	J	129	GLN
1	J	269	HIS
1	J	272	GLN
1	J	274	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 ⓘ

52 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	$\# Z > 2$
4	GOL	G	363	-	5,5,5	0.64	0	5,5,5	1.24	1 (20%)
4	GOL	B	362	-	5,5,5	0.81	0	5,5,5	1.35	1 (20%)
2	NAP	J	350	-	50,52,52	1.86	8 (16%)	71,80,80	1.68	15 (21%)
4	GOL	D	362	-	5,5,5	0.56	0	5,5,5	0.82	0
4	GOL	F	361	-	5,5,5	0.76	0	5,5,5	1.59	2 (40%)
3	TLA	C	360	-	9,9,9	1.67	2 (22%)	12,12,12	1.73	4 (33%)
4	GOL	C	361	-	5,5,5	0.71	0	5,5,5	1.42	0
4	GOL	I	362	-	5,5,5	0.73	0	5,5,5	1.45	1 (20%)
2	NAP	B	350	-	50,52,52	1.84	10 (20%)	71,80,80	1.79	16 (22%)
4	GOL	D	361	-	5,5,5	0.65	0	5,5,5	0.38	0
4	GOL	G	364	-	5,5,5	1.02	0	5,5,5	1.65	2 (40%)
4	GOL	H	361	-	5,5,5	0.44	0	5,5,5	0.63	0
3	TLA	H	360	-	9,9,9	1.69	3 (33%)	12,12,12	0.80	0
3	TLA	F	360	-	9,9,9	1.03	1 (11%)	12,12,12	1.93	3 (25%)
6	MES	J	368	-	12,12,12	1.79	3 (25%)	15,16,16	2.38	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PO4	J	367	-	4,4,4	1.01	0	6,6,6	0.63	0
2	NAP	G	350	-	50,52,52	1.94	12 (24%)	71,80,80	1.58	15 (21%)
4	GOL	J	363	-	5,5,5	0.46	0	5,5,5	1.11	0
3	TLA	I	360	-	9,9,9	1.86	2 (22%)	12,12,12	1.51	2 (16%)
4	GOL	J	366	-	5,5,5	0.94	0	5,5,5	0.97	0
2	NAP	F	350	-	50,52,52	1.95	6 (12%)	71,80,80	1.61	16 (22%)
4	GOL	H	362	-	5,5,5	0.76	0	5,5,5	1.13	0
3	TLA	G	360	-	9,9,9	1.79	5 (55%)	12,12,12	1.16	1 (8%)
6	MES	B	364	-	12,12,12	2.10	1 (8%)	15,16,16	3.10	10 (66%)
6	MES	D	364	-	12,12,12	1.87	1 (8%)	15,16,16	2.77	7 (46%)
4	GOL	B	363	-	5,5,5	0.73	0	5,5,5	0.98	0
4	GOL	C	363	-	5,5,5	0.86	0	5,5,5	1.45	1 (20%)
4	GOL	G	362	-	5,5,5	0.67	0	5,5,5	1.32	1 (20%)
2	NAP	H	350	-	50,52,52	2.05	9 (18%)	71,80,80	2.02	22 (30%)
4	GOL	E	362	-	5,5,5	0.69	0	5,5,5	0.69	0
4	GOL	I	361	-	5,5,5	0.56	0	5,5,5	0.91	0
5	PO4	A	364	-	4,4,4	0.82	0	6,6,6	2.48	3 (50%)
4	GOL	E	363	-	5,5,5	0.82	0	5,5,5	1.00	0
3	TLA	D	360	-	9,9,9	1.91	3 (33%)	12,12,12	1.98	4 (33%)
4	GOL	J	364	-	5,5,5	0.59	0	5,5,5	0.76	0
2	NAP	D	350	-	50,52,52	1.79	7 (14%)	71,80,80	1.50	11 (15%)
6	MES	C	364	-	12,12,12	2.11	1 (8%)	15,16,16	2.41	6 (40%)
2	NAP	C	350	-	50,52,52	1.91	7 (14%)	71,80,80	1.54	13 (18%)
3	TLA	J	360	-	9,9,9	1.69	3 (33%)	12,12,12	0.92	1 (8%)
3	TLA	A	360	-	9,9,9	1.18	1 (11%)	12,12,12	1.69	4 (33%)
4	GOL	A	361	-	5,5,5	0.56	0	5,5,5	0.74	0
6	MES	I	363	-	12,12,12	2.13	3 (25%)	15,16,16	2.56	5 (33%)
4	GOL	D	363	-	5,5,5	1.52	0	5,5,5	1.82	1 (20%)
2	NAP	I	350	-	50,52,52	1.80	5 (10%)	71,80,80	1.67	15 (21%)
4	GOL	B	361	-	5,5,5	0.56	0	5,5,5	0.57	0
2	NAP	A	350	-	50,52,52	1.87	9 (18%)	71,80,80	1.57	14 (19%)
4	GOL	E	361	-	5,5,5	0.59	0	5,5,5	0.97	0
2	NAP	E	350	-	50,52,52	2.07	5 (10%)	71,80,80	1.66	13 (18%)
4	GOL	A	363	-	5,5,5	0.87	0	5,5,5	0.96	0
4	GOL	C	362	-	5,5,5	0.58	0	5,5,5	1.22	1 (20%)
3	TLA	B	360	-	9,9,9	2.18	2 (22%)	12,12,12	1.24	2 (16%)
3	TLA	E	360	-	9,9,9	1.70	3 (33%)	12,12,12	1.32	1 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	G	363	-	-	2/4/4/4	-
4	GOL	B	362	-	-	2/4/4/4	-
2	NAP	J	350	-	-	4/35/67/67	0/5/5/5
4	GOL	D	362	-	-	0/4/4/4	-
4	GOL	F	361	-	-	2/4/4/4	-
3	TLA	C	360	-	-	6/12/12/12	-
4	GOL	C	361	-	-	1/4/4/4	-
4	GOL	I	362	-	-	2/4/4/4	-
2	NAP	B	350	-	-	3/35/67/67	0/5/5/5
4	GOL	D	361	-	-	0/4/4/4	-
4	GOL	G	364	-	-	4/4/4/4	-
4	GOL	H	361	-	-	2/4/4/4	-
3	TLA	H	360	-	-	4/12/12/12	-
3	TLA	F	360	-	-	6/12/12/12	-
6	MES	J	368	-	-	4/6/14/14	0/1/1/1
2	NAP	G	350	-	-	5/35/67/67	0/5/5/5
4	GOL	J	363	-	-	0/4/4/4	-
3	TLA	I	360	-	-	6/12/12/12	-
4	GOL	J	366	-	-	3/4/4/4	-
2	NAP	F	350	-	-	4/35/67/67	0/5/5/5
4	GOL	H	362	-	-	3/4/4/4	-
3	TLA	G	360	-	-	6/12/12/12	-
6	MES	B	364	-	-	4/6/14/14	0/1/1/1
6	MES	D	364	-	-	4/6/14/14	0/1/1/1
4	GOL	B	363	-	-	0/4/4/4	-
4	GOL	C	363	-	-	4/4/4/4	-
4	GOL	G	362	-	-	4/4/4/4	-
2	NAP	H	350	-	-	4/35/67/67	0/5/5/5
4	GOL	E	362	-	-	2/4/4/4	-
4	GOL	I	361	-	-	2/4/4/4	-
4	GOL	E	363	-	-	0/4/4/4	-
3	TLA	D	360	-	-	6/12/12/12	-
4	GOL	J	364	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	D	350	-	-	1/35/67/67	0/5/5/5
6	MES	C	364	-	-	4/6/14/14	0/1/1/1
2	NAP	C	350	-	-	2/35/67/67	0/5/5/5
3	TLA	J	360	-	-	4/12/12/12	-
3	TLA	A	360	-	-	6/12/12/12	-
4	GOL	A	361	-	-	2/4/4/4	-
6	MES	I	363	-	-	4/6/14/14	0/1/1/1
4	GOL	D	363	-	-	4/4/4/4	-
2	NAP	I	350	-	-	3/35/67/67	0/5/5/5
4	GOL	B	361	-	-	0/4/4/4	-
2	NAP	A	350	-	-	1/35/67/67	0/5/5/5
4	GOL	E	361	-	-	3/4/4/4	-
2	NAP	E	350	-	-	5/35/67/67	0/5/5/5
4	GOL	A	363	-	-	0/4/4/4	-
4	GOL	C	362	-	-	0/4/4/4	-
3	TLA	B	360	-	-	4/12/12/12	-
3	TLA	E	360	-	-	6/12/12/12	-

All (112) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	350	NAP	O7N-C7N	9.24	1.41	1.24
2	A	350	NAP	O7N-C7N	8.95	1.40	1.24
2	H	350	NAP	O7N-C7N	8.91	1.40	1.24
2	D	350	NAP	O7N-C7N	8.51	1.40	1.24
2	E	350	NAP	O7N-C7N	7.91	1.38	1.24
2	B	350	NAP	O7N-C7N	7.77	1.38	1.24
2	I	350	NAP	O7N-C7N	7.50	1.38	1.24
2	J	350	NAP	O7N-C7N	7.39	1.37	1.24
2	G	350	NAP	O7N-C7N	7.31	1.37	1.24
2	C	350	NAP	O7N-C7N	6.88	1.36	1.24
6	C	364	MES	C8-S	-6.77	1.68	1.77
2	J	350	NAP	PN-O3	6.69	1.66	1.59
6	B	364	MES	C8-S	-6.66	1.68	1.77
2	E	350	NAP	PN-O3	6.28	1.66	1.59
6	I	363	MES	C8-S	-5.94	1.69	1.77
2	C	350	NAP	PA-O3	5.63	1.65	1.59
6	D	364	MES	C8-S	-5.58	1.69	1.77
2	F	350	NAP	PN-O3	5.38	1.65	1.59
2	C	350	NAP	PN-O3	5.36	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	350	NAP	PN-O3	5.28	1.65	1.59
2	E	350	NAP	PA-O3	5.28	1.65	1.59
6	J	368	MES	C8-S	-4.99	1.70	1.77
3	B	360	TLA	O3-C3	4.63	1.51	1.42
2	I	350	NAP	PN-O3	4.55	1.64	1.59
2	G	350	NAP	C2A-N1A	4.39	1.41	1.33
2	I	350	NAP	C2A-N1A	4.31	1.41	1.33
2	C	350	NAP	O4D-C1D	4.15	1.46	1.40
2	G	350	NAP	O4D-C1D	4.12	1.46	1.40
2	D	350	NAP	PN-O3	4.10	1.63	1.59
2	I	350	NAP	C2A-N3A	4.07	1.41	1.33
2	H	350	NAP	C2A-N3A	3.99	1.41	1.33
2	H	350	NAP	PA-O3	3.93	1.63	1.59
2	J	350	NAP	C2A-N1A	3.84	1.40	1.33
2	F	350	NAP	C2A-N1A	3.74	1.40	1.33
2	E	350	NAP	C2A-N1A	3.69	1.40	1.33
3	I	360	TLA	O3-C3	3.67	1.49	1.42
2	B	350	NAP	O4D-C1D	3.55	1.45	1.40
2	C	350	NAP	C2A-N1A	3.50	1.40	1.33
2	B	350	NAP	PA-O3	3.47	1.63	1.59
2	E	350	NAP	O4D-C1D	3.37	1.45	1.40
2	G	350	NAP	PA-O3	3.33	1.63	1.59
3	E	360	TLA	C3-C4	-3.27	1.48	1.52
2	H	350	NAP	C2N-N1N	3.24	1.38	1.35
2	A	350	NAP	O4D-C1D	3.15	1.45	1.40
3	J	360	TLA	O1-C1	3.14	1.31	1.22
3	D	360	TLA	O4I-C4	-3.13	1.20	1.30
2	B	350	NAP	C8A-N7A	3.09	1.37	1.31
2	I	350	NAP	C8A-N7A	3.08	1.37	1.31
2	F	350	NAP	C2A-N3A	3.07	1.39	1.33
2	A	350	NAP	C5A-N7A	-3.07	1.33	1.39
2	G	350	NAP	C2A-N3A	3.06	1.39	1.33
2	G	350	NAP	C3N-C7N	-3.04	1.46	1.50
2	F	350	NAP	O4D-C1D	3.04	1.44	1.40
2	A	350	NAP	C2A-N1A	3.02	1.39	1.33
3	H	360	TLA	O3-C3	2.96	1.48	1.42
2	G	350	NAP	C4A-N3A	2.95	1.39	1.34
3	I	360	TLA	O1-C1	2.92	1.30	1.22
2	B	350	NAP	C2N-N1N	2.92	1.38	1.35
2	J	350	NAP	PA-O3	2.91	1.62	1.59
2	D	350	NAP	PA-O3	2.84	1.62	1.59
2	G	350	NAP	O4B-C4B	-2.78	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	360	TLA	C2-C1	-2.76	1.48	1.52
3	C	360	TLA	O3-C3	2.73	1.47	1.42
2	A	350	NAP	C2N-N1N	2.71	1.38	1.35
2	G	350	NAP	PN-O3	2.70	1.62	1.59
2	H	350	NAP	C8A-N7A	2.70	1.36	1.31
3	B	360	TLA	O4-C4	2.69	1.30	1.22
2	A	350	NAP	PA-O3	2.61	1.62	1.59
2	J	350	NAP	C2A-N3A	2.54	1.38	1.33
2	H	350	NAP	C2A-N1A	2.53	1.38	1.33
2	C	350	NAP	C8A-N7A	2.53	1.36	1.31
2	G	350	NAP	O3B-C3B	-2.50	1.36	1.43
2	B	350	NAP	C3D-C4D	2.45	1.59	1.53
2	B	350	NAP	C8A-N9A	2.45	1.41	1.37
6	I	363	MES	O2S-S	2.41	1.51	1.45
6	I	363	MES	O1S-S	2.39	1.51	1.45
3	G	360	TLA	C2-C1	-2.39	1.49	1.52
3	D	360	TLA	O2-C2	2.39	1.46	1.42
3	G	360	TLA	O11-C1	-2.37	1.23	1.30
3	A	360	TLA	O41-C4	-2.36	1.23	1.30
3	G	360	TLA	C3-C4	-2.35	1.49	1.52
2	C	350	NAP	P2B-O2B	2.35	1.63	1.59
6	J	368	MES	O1S-S	2.31	1.51	1.45
2	D	350	NAP	C2A-N1A	2.29	1.38	1.33
3	H	360	TLA	C2-C1	-2.27	1.49	1.52
2	B	350	NAP	PN-O3	2.27	1.61	1.59
2	A	350	NAP	PN-O2N	-2.26	1.44	1.55
3	E	360	TLA	O41-C4	-2.26	1.23	1.30
2	A	350	NAP	C2A-N3A	2.24	1.37	1.33
2	J	350	NAP	O4D-C1D	2.23	1.43	1.40
2	B	350	NAP	C2A-N1A	2.22	1.37	1.33
2	J	350	NAP	C3N-C7N	-2.22	1.47	1.50
2	F	350	NAP	PA-O3	2.21	1.61	1.59
2	D	350	NAP	P2B-O2B	2.20	1.63	1.59
6	J	368	MES	O2S-S	2.20	1.51	1.45
2	A	350	NAP	O4B-C4B	-2.19	1.40	1.45
3	F	360	TLA	O4-C4	2.18	1.28	1.22
2	D	350	NAP	O4B-C4B	-2.14	1.40	1.45
2	J	350	NAP	C8A-N7A	2.13	1.35	1.31
2	B	350	NAP	C2N-C3N	2.12	1.42	1.39
2	D	350	NAP	PA-O2A	-2.09	1.45	1.55
2	G	350	NAP	C2N-N1N	2.09	1.37	1.35
3	G	360	TLA	O3-C3	2.08	1.46	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	350	NAP	O5D-C5D	-2.08	1.36	1.44
3	E	360	TLA	O11-C1	-2.08	1.24	1.30
3	D	360	TLA	O3-C3	2.07	1.46	1.42
3	G	360	TLA	O41-C4	-2.05	1.24	1.30
2	H	350	NAP	O2B-C2B	-2.04	1.37	1.44
2	G	350	NAP	O2B-C2B	-2.03	1.37	1.44
3	J	360	TLA	O4-C4	2.03	1.28	1.22
3	H	360	TLA	O4-C4	2.03	1.28	1.22
3	J	360	TLA	O41-C4	-2.03	1.24	1.30

All (219) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	368	MES	C5-N4-C3	7.31	124.58	108.84
6	D	364	MES	C5-N4-C3	7.28	124.52	108.84
2	B	350	NAP	N3A-C2A-N1A	-7.20	117.69	128.58
2	E	350	NAP	N3A-C2A-N1A	-7.15	117.76	128.58
6	B	364	MES	C5-N4-C3	6.60	123.05	108.84
6	I	363	MES	C5-N4-C3	6.59	123.03	108.84
2	J	350	NAP	N3A-C2A-N1A	-6.15	119.27	128.58
2	F	350	NAP	N3A-C2A-N1A	-5.81	119.78	128.58
2	D	350	NAP	N3A-C2A-N1A	-5.48	120.29	128.58
6	B	364	MES	O1S-S-C8	5.33	114.78	106.73
2	H	350	NAP	O7N-C7N-C3N	-5.18	113.27	119.60
2	E	350	NAP	C2A-N1A-C6A	4.96	126.88	118.73
2	C	350	NAP	N3A-C2A-N1A	-4.93	121.12	128.58
2	H	350	NAP	C5A-C4A-N3A	-4.92	119.95	126.72
2	H	350	NAP	N9A-C8A-N7A	-4.70	107.27	113.94
2	G	350	NAP	N3A-C2A-N1A	-4.67	121.51	128.58
6	B	364	MES	O2S-S-C8	4.60	113.69	106.73
2	H	350	NAP	N3A-C2A-N1A	-4.55	121.70	128.58
2	A	350	NAP	N3A-C2A-N1A	-4.53	121.73	128.58
6	C	364	MES	C5-N4-C3	4.48	118.49	108.84
5	A	364	PO4	O4-P-O3	4.46	121.80	107.91
6	I	363	MES	C2-C3-N4	-4.40	103.43	110.12
6	C	364	MES	O3S-S-C8	4.21	114.23	106.00
2	I	350	NAP	C5A-C4A-N3A	-4.19	120.95	126.72
2	I	350	NAP	C5N-C4N-C3N	-4.19	116.25	120.36
2	D	350	NAP	C5A-C4A-N3A	-4.17	120.97	126.72
2	A	350	NAP	C5A-C4A-N3A	-4.16	121.00	126.72
6	C	364	MES	C7-N4-C5	4.07	122.08	111.24
2	J	350	NAP	C5N-C4N-C3N	-4.03	116.41	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	350	NAP	C2N-C3N-C4N	3.95	122.86	118.26
2	I	350	NAP	N3A-C2A-N1A	-3.92	122.65	128.58
3	F	360	TLA	O11-C1-C2	3.91	124.19	113.31
2	H	350	NAP	O2X-P2B-O2B	3.88	120.96	105.85
4	D	363	GOL	O1-C1-C2	3.87	127.80	110.38
2	I	350	NAP	C2N-C3N-C4N	3.85	122.74	118.26
6	D	364	MES	O2S-S-C8	3.82	112.50	106.73
2	B	350	NAP	C5N-C4N-C3N	-3.77	116.66	120.36
2	H	350	NAP	C5N-C4N-C3N	-3.76	116.67	120.36
2	G	350	NAP	C2N-C3N-C4N	3.73	122.60	118.26
2	J	350	NAP	N9A-C8A-N7A	-3.71	108.68	113.94
2	F	350	NAP	N9A-C8A-N7A	-3.68	108.71	113.94
3	D	360	TLA	O2-C2-C1	-3.65	102.90	110.69
2	B	350	NAP	O2B-P2B-O1X	-3.61	96.47	109.33
2	H	350	NAP	C5A-N7A-C8A	3.56	109.05	103.45
2	H	350	NAP	N3A-C4A-N9A	3.51	133.13	127.17
2	I	350	NAP	O7N-C7N-N7N	-3.49	117.57	122.62
2	B	350	NAP	C2A-N3A-C4A	3.47	120.31	111.83
2	D	350	NAP	C2A-N3A-C4A	3.45	120.27	111.83
3	C	360	TLA	O41-C4-O4	-3.45	116.25	124.08
2	C	350	NAP	O2X-P2B-O2B	3.37	118.97	105.85
3	D	360	TLA	O3-C3-C2	3.34	116.97	110.17
2	B	350	NAP	O3D-C3D-C4D	3.34	120.67	111.08
2	A	350	NAP	N3A-C4A-N9A	3.29	132.75	127.17
2	G	350	NAP	C5A-C4A-N3A	-3.27	122.22	126.72
2	C	350	NAP	C6N-N1N-C2N	-3.25	119.11	121.88
2	I	350	NAP	O7N-C7N-C3N	3.25	123.57	119.60
2	B	350	NAP	O2A-PA-O3	-3.24	98.53	107.27
6	D	364	MES	C2-C3-N4	3.19	114.97	110.12
6	I	363	MES	C7-N4-C3	3.18	119.71	111.24
3	I	360	TLA	O3-C3-C2	3.16	116.59	110.17
2	A	350	NAP	C5A-N7A-C8A	3.12	108.36	103.45
2	B	350	NAP	O3B-C3B-C2B	-3.12	102.46	111.19
2	G	350	NAP	C5N-C4N-C3N	-3.10	117.32	120.36
6	B	364	MES	O1-C2-C3	3.09	118.43	111.77
6	B	364	MES	C7-N4-C3	3.08	119.45	111.24
2	A	350	NAP	N9A-C8A-N7A	-3.04	109.62	113.94
6	C	364	MES	C7-N4-C3	3.01	119.26	111.24
2	E	350	NAP	C4D-O4D-C1D	-3.01	107.17	109.92
2	G	350	NAP	C6N-N1N-C2N	-3.01	119.32	121.88
2	A	350	NAP	P2B-O2B-C2B	3.00	131.45	123.43
2	I	350	NAP	N3A-C4A-N9A	2.99	132.25	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	363	MES	O3S-S-C8	2.98	111.84	106.00
2	F	350	NAP	C5A-C4A-N3A	-2.97	122.62	126.72
2	E	350	NAP	C6N-N1N-C2N	-2.97	119.35	121.88
2	B	350	NAP	C2A-N1A-C6A	2.97	123.60	118.73
5	A	364	PO4	O3-P-O1	-2.96	100.47	110.95
2	F	350	NAP	C5A-N7A-C8A	2.96	108.10	103.45
2	C	350	NAP	O3D-C3D-C4D	2.94	119.53	111.08
2	B	350	NAP	O2X-P2B-O2B	2.93	117.27	105.85
2	B	350	NAP	C5A-C4A-N3A	-2.93	122.69	126.72
3	A	360	TLA	O41-C4-C3	2.92	121.44	113.31
2	F	350	NAP	C2N-C3N-C4N	2.92	121.65	118.26
2	C	350	NAP	N9A-C8A-N7A	-2.91	109.81	113.94
2	J	350	NAP	O7N-C7N-C3N	2.90	123.15	119.60
2	A	350	NAP	C2N-C3N-C4N	2.89	121.62	118.26
2	H	350	NAP	O2N-PN-O3	2.89	115.09	107.27
2	A	350	NAP	C4D-O4D-C1D	2.88	112.56	109.92
2	G	350	NAP	O7N-C7N-C3N	-2.88	116.08	119.60
3	F	360	TLA	C2-C3-C4	2.87	116.19	109.82
2	I	350	NAP	N9A-C8A-N7A	-2.87	109.86	113.94
2	G	350	NAP	N3A-C4A-N9A	2.84	131.99	127.17
3	C	360	TLA	O41-C4-C3	2.83	121.17	113.31
2	I	350	NAP	O3D-C3D-C4D	2.82	119.18	111.08
2	A	350	NAP	C6N-N1N-C2N	-2.81	119.48	121.88
2	A	350	NAP	C2A-N3A-C4A	2.81	118.69	111.83
2	H	350	NAP	O2A-PA-O3	-2.81	99.68	107.27
2	H	350	NAP	C2A-N3A-C4A	2.81	118.69	111.83
2	I	350	NAP	C6N-N1N-C2N	-2.78	119.51	121.88
2	F	350	NAP	C4A-C5A-N7A	-2.77	107.42	110.58
6	D	364	MES	O3S-S-C8	2.76	111.41	106.00
2	I	350	NAP	O2N-PN-O3	2.75	114.70	107.27
2	H	350	NAP	O2B-P2B-O1X	-2.71	99.69	109.33
2	G	350	NAP	C5A-N7A-C8A	2.70	107.69	103.45
2	J	350	NAP	C5A-N7A-C8A	2.70	107.69	103.45
2	F	350	NAP	O2X-P2B-O2B	2.68	116.31	105.85
2	J	350	NAP	C2A-N3A-C4A	2.67	118.35	111.83
3	B	360	TLA	O2-C2-C1	-2.67	104.99	110.69
2	E	350	NAP	O4D-C4D-C3D	2.67	110.44	105.15
2	H	350	NAP	O7N-C7N-N7N	2.66	126.46	122.62
3	A	360	TLA	C3-C2-C1	2.64	115.67	109.82
6	D	364	MES	O3S-S-O1S	-2.63	104.81	111.40
6	D	364	MES	C7-N4-C3	2.62	118.23	111.24
2	J	350	NAP	C4A-N9A-C8A	2.61	108.48	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	350	NAP	C5N-C4N-C3N	-2.61	117.80	120.36
2	F	350	NAP	C2A-N3A-C4A	2.59	118.15	111.83
2	I	350	NAP	C6A-C5A-C4A	2.58	120.71	117.18
2	J	350	NAP	C6N-N1N-C2N	-2.58	119.68	121.88
6	J	368	MES	C7-N4-C5	2.58	118.11	111.24
2	D	350	NAP	O3-PN-O1N	-2.57	102.98	110.70
3	I	360	TLA	O4-C4-C3	-2.57	114.78	121.62
2	B	350	NAP	N9A-C8A-N7A	-2.56	110.30	113.94
2	H	350	NAP	P2B-O2B-C2B	2.55	130.25	123.43
2	H	350	NAP	C4A-N9A-C8A	2.54	108.41	105.74
2	H	350	NAP	C6N-C5N-C4N	2.54	123.11	119.45
2	H	350	NAP	O3D-C3D-C4D	2.52	118.33	111.08
2	D	350	NAP	O3D-C3D-C4D	2.52	118.32	111.08
2	G	350	NAP	O2B-P2B-O1X	-2.52	100.37	109.33
2	J	350	NAP	C5A-C4A-N3A	-2.51	123.26	126.72
2	J	350	NAP	C2A-N1A-C6A	2.50	122.84	118.73
4	F	361	GOL	O1-C1-C2	2.50	121.65	110.38
2	G	350	NAP	C6A-C5A-C4A	2.50	120.59	117.18
2	F	350	NAP	O5D-PN-O1N	-2.50	99.03	108.94
3	A	360	TLA	O41-C4-O4	-2.50	118.41	124.08
2	H	350	NAP	C5A-C6A-N6A	-2.49	117.11	123.29
2	I	350	NAP	O2D-C2D-C3D	-2.48	103.88	111.82
4	C	362	GOL	O1-C1-C2	2.47	121.50	110.38
2	E	350	NAP	C2A-N3A-C4A	2.47	117.86	111.83
2	E	350	NAP	N9A-C8A-N7A	-2.45	110.46	113.94
2	C	350	NAP	C2A-N1A-C6A	2.44	122.74	118.73
2	H	350	NAP	O3B-C3B-C2B	-2.44	104.36	111.19
2	C	350	NAP	O7N-C7N-C3N	-2.42	116.64	119.60
2	D	350	NAP	N3A-C4A-N9A	2.41	131.27	127.17
2	I	350	NAP	C5A-N7A-C8A	2.41	107.24	103.45
4	F	361	GOL	C3-C2-C1	2.41	120.63	111.80
2	G	350	NAP	O2X-P2B-O2B	2.41	115.23	105.85
2	G	350	NAP	N9A-C8A-N7A	-2.40	110.53	113.94
2	E	350	NAP	O3D-C3D-C4D	2.40	117.97	111.08
2	F	350	NAP	O2N-PN-O1N	2.38	123.53	112.44
3	D	360	TLA	O41-C4-O4	-2.38	118.68	124.08
2	J	350	NAP	C2B-C3B-C4B	-2.37	96.89	101.99
3	D	360	TLA	O3-C3-C4	-2.37	105.63	110.69
4	B	362	GOL	O1-C1-C2	2.36	121.00	110.38
2	A	350	NAP	C5N-C4N-C3N	-2.35	118.05	120.36
2	C	350	NAP	C5A-N7A-C8A	2.35	107.15	103.45
6	B	364	MES	C7-N4-C5	2.35	117.49	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	350	NAP	C6A-C5A-C4A	2.33	120.36	117.18
4	I	362	GOL	O1-C1-C2	2.33	120.84	110.38
2	B	350	NAP	C6N-C5N-C4N	2.32	122.80	119.45
2	J	350	NAP	O4B-C1B-C2B	-2.32	102.59	106.59
3	J	360	TLA	C2-C3-C4	2.32	114.95	109.82
6	B	364	MES	C6-C5-N4	-2.31	106.61	110.12
2	G	350	NAP	O7N-C7N-N7N	2.30	125.94	122.62
2	B	350	NAP	C6N-N1N-C2N	-2.29	119.92	121.88
2	J	350	NAP	O7N-C7N-N7N	-2.29	119.30	122.62
6	J	368	MES	C7-N4-C3	2.28	117.31	111.24
2	E	350	NAP	O5D-C5D-C4D	2.27	116.73	108.99
2	G	350	NAP	O2N-PN-O1N	2.26	122.97	112.44
6	I	363	MES	C7-N4-C5	2.26	117.25	111.24
6	C	364	MES	O3S-S-O1S	-2.24	105.78	111.40
2	F	350	NAP	C2A-N1A-C6A	2.24	122.41	118.73
6	D	364	MES	C7-N4-C5	2.24	117.20	111.24
2	H	350	NAP	C6A-C5A-C4A	2.23	120.22	117.18
2	E	350	NAP	O2N-PN-O3	2.23	113.29	107.27
2	E	350	NAP	C2B-C1B-N9A	-2.21	110.12	113.75
6	C	364	MES	C6-O1-C2	2.21	117.02	109.88
3	C	360	TLA	C2-C3-C4	2.20	114.70	109.82
4	G	362	GOL	O3-C3-C2	2.19	120.25	110.38
4	G	364	GOL	O3-C3-C2	2.19	120.25	110.38
2	B	350	NAP	N3A-C4A-N9A	2.19	130.89	127.17
3	G	360	TLA	O41-C4-C3	2.19	119.39	113.31
2	I	350	NAP	C2A-N3A-C4A	2.18	117.16	111.83
2	D	350	NAP	C4D-O4D-C1D	-2.18	107.93	109.92
2	H	350	NAP	O5B-PA-O1A	-2.17	100.35	108.94
2	J	350	NAP	O4B-C4B-C3B	2.16	109.45	105.15
2	B	350	NAP	PA-O5B-C5B	-2.16	108.95	121.35
6	B	364	MES	O3S-S-O1S	-2.16	106.00	111.40
2	C	350	NAP	C2A-N3A-C4A	2.16	117.10	111.83
2	F	350	NAP	C5A-C4A-N9A	2.15	108.15	105.81
4	G	363	GOL	C3-C2-C1	2.14	119.66	111.80
6	J	368	MES	O3S-S-C8	2.14	110.19	106.00
2	E	350	NAP	O4B-C1B-N9A	2.13	112.17	108.09
4	G	364	GOL	O1-C1-C2	2.12	119.94	110.38
3	B	360	TLA	O2-C2-C3	2.12	114.48	110.17
2	C	350	NAP	O2A-PA-O3	-2.11	101.56	107.27
3	F	360	TLA	O11-C1-O1	-2.11	119.29	124.08
2	E	350	NAP	N6A-C6A-N1A	2.11	123.07	118.38
2	F	350	NAP	O2A-PA-O3	-2.10	101.58	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	364	PO4	O4-P-O1	-2.10	103.51	110.95
6	J	368	MES	C2-C3-N4	2.10	113.31	110.12
6	B	364	MES	C6-O1-C2	2.10	116.67	109.88
4	C	363	GOL	O2-C2-C3	-2.09	100.50	109.18
3	C	360	TLA	O3-C3-C4	2.09	115.17	110.69
2	D	350	NAP	N9A-C8A-N7A	-2.08	110.98	113.94
2	C	350	NAP	O2B-P2B-O1X	-2.08	101.94	109.33
2	A	350	NAP	C2B-C1B-N9A	-2.07	110.34	113.75
2	C	350	NAP	C4A-C5A-N7A	-2.07	108.22	110.58
3	A	360	TLA	O11-C1-C2	2.07	119.05	113.31
2	B	350	NAP	O2N-PN-O3	2.06	112.83	107.27
2	D	350	NAP	C6A-C5A-C4A	2.05	119.98	117.18
6	B	364	MES	O1-C6-C5	-2.05	107.36	111.77
2	G	350	NAP	O3X-P2B-O2X	2.05	115.47	107.80
3	E	360	TLA	O41-C4-O4	-2.04	119.44	124.08
2	C	350	NAP	C5A-C4A-N3A	-2.04	123.90	126.72
2	H	350	NAP	C3N-C7N-N7N	2.03	120.24	117.74
2	A	350	NAP	O5D-C5D-C4D	2.03	115.89	108.99
2	D	350	NAP	O4D-C4D-C3D	2.02	109.17	105.15
2	F	350	NAP	C6A-C5A-C4A	2.02	119.94	117.18
2	D	350	NAP	O5D-C5D-C4D	2.02	115.87	108.99
2	F	350	NAP	C4A-N9A-C1B	-2.01	121.92	126.63

There are no chirality outliers.

All (150) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	350	NAP	O4D-C1D-N1N-C2N
2	B	350	NAP	O4D-C1D-N1N-C6N
2	E	350	NAP	O4D-C1D-N1N-C6N
2	G	350	NAP	O4D-C1D-N1N-C6N
2	H	350	NAP	O4D-C1D-N1N-C6N
2	I	350	NAP	O4D-C1D-N1N-C6N
2	J	350	NAP	PN-O3-PA-O5B
2	J	350	NAP	O4D-C1D-N1N-C6N
4	B	362	GOL	O1-C1-C2-C3
4	C	363	GOL	O1-C1-C2-O2
4	C	363	GOL	O1-C1-C2-C3
4	C	363	GOL	C1-C2-C3-O3
4	D	363	GOL	C1-C2-C3-O3
4	E	362	GOL	O1-C1-C2-C3
4	F	361	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	G	362	GOL	O1-C1-C2-C3
4	G	364	GOL	C1-C2-C3-O3
4	I	362	GOL	C1-C2-C3-O3
4	J	366	GOL	C1-C2-C3-O3
6	B	364	MES	C7-C8-S-O2S
6	B	364	MES	C7-C8-S-O3S
6	D	364	MES	C7-C8-S-O2S
6	D	364	MES	C7-C8-S-O3S
6	I	363	MES	C7-C8-S-O2S
6	J	368	MES	C7-C8-S-O2S
6	J	368	MES	C7-C8-S-O3S
3	A	360	TLA	O1-C1-C2-C3
3	A	360	TLA	O11-C1-C2-C3
3	C	360	TLA	O1-C1-C2-C3
3	C	360	TLA	O11-C1-C2-C3
3	G	360	TLA	O11-C1-C2-C3
3	I	360	TLA	O11-C1-C2-C3
3	D	360	TLA	O1-C1-C2-C3
3	E	360	TLA	O1-C1-C2-C3
3	G	360	TLA	O1-C1-C2-C3
3	I	360	TLA	O1-C1-C2-C3
4	D	363	GOL	O1-C1-C2-O2
4	G	362	GOL	O1-C1-C2-O2
4	I	361	GOL	O1-C1-C2-O2
6	C	364	MES	C7-C8-S-O3S
3	D	360	TLA	O11-C1-C2-C3
3	C	360	TLA	O1-C1-C2-O2
3	G	360	TLA	O1-C1-C2-O2
3	I	360	TLA	O1-C1-C2-O2
3	E	360	TLA	O11-C1-C2-C3
4	A	361	GOL	C1-C2-C3-O3
4	D	363	GOL	O1-C1-C2-C3
4	G	362	GOL	C1-C2-C3-O3
4	G	363	GOL	C1-C2-C3-O3
4	G	364	GOL	O1-C1-C2-C3
4	H	361	GOL	O1-C1-C2-C3
4	I	361	GOL	O1-C1-C2-C3
4	J	364	GOL	O1-C1-C2-C3
4	J	366	GOL	O1-C1-C2-C3
3	A	360	TLA	O11-C1-C2-O2
3	C	360	TLA	O11-C1-C2-O2
3	G	360	TLA	O11-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	F	360	TLA	O1-C1-C2-C3
3	J	360	TLA	O1-C1-C2-C3
4	A	361	GOL	O2-C2-C3-O3
4	B	362	GOL	O1-C1-C2-O2
4	C	363	GOL	O2-C2-C3-O3
4	F	361	GOL	O1-C1-C2-O2
4	G	364	GOL	O2-C2-C3-O3
4	J	364	GOL	O1-C1-C2-O2
3	J	360	TLA	O11-C1-C2-C3
6	I	363	MES	C7-C8-S-O3S
3	D	360	TLA	O1-C1-C2-O2
3	I	360	TLA	O11-C1-C2-O2
3	F	360	TLA	O11-C1-C2-C3
3	E	360	TLA	O1-C1-C2-O2
4	D	363	GOL	O2-C2-C3-O3
4	I	362	GOL	O2-C2-C3-O3
3	H	360	TLA	C1-C2-C3-C4
2	C	350	NAP	C2B-O2B-P2B-O1X
2	J	350	NAP	C2B-O2B-P2B-O1X
3	B	360	TLA	C1-C2-C3-C4
6	C	364	MES	C8-C7-N4-C3
6	I	363	MES	C8-C7-N4-C3
3	A	360	TLA	O1-C1-C2-O2
3	B	360	TLA	O1-C1-C2-C3
3	J	360	TLA	C1-C2-C3-C4
4	E	361	GOL	O2-C2-C3-O3
3	H	360	TLA	O1-C1-C2-C3
3	D	360	TLA	C1-C2-C3-C4
3	B	360	TLA	O11-C1-C2-C3
3	A	360	TLA	C1-C2-C3-C4
3	C	360	TLA	C1-C2-C3-C4
3	E	360	TLA	C1-C2-C3-C4
3	F	360	TLA	C1-C2-C3-C4
3	G	360	TLA	C1-C2-C3-C4
3	I	360	TLA	C1-C2-C3-C4
2	A	350	NAP	PN-O3-PA-O5B
2	B	350	NAP	PN-O3-PA-O5B
2	C	350	NAP	PN-O3-PA-O5B
2	D	350	NAP	PN-O3-PA-O5B
2	E	350	NAP	PN-O3-PA-O5B
2	G	350	NAP	PN-O3-PA-O5B
2	H	350	NAP	PN-O3-PA-O5B

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Mol	Chain	Res	Type	Atoms
2	I	350	NAP	PN-O3-PA-O5B
3	D	360	TLA	O11-C1-C2-O2
4	G	363	GOL	O2-C2-C3-O3
4	H	361	GOL	O1-C1-C2-O2
4	J	366	GOL	O1-C1-C2-O2
6	B	364	MES	C7-C8-S-O1S
6	C	364	MES	C7-C8-S-O1S
6	C	364	MES	C7-C8-S-O2S
6	D	364	MES	C7-C8-S-O1S
6	I	363	MES	C7-C8-S-O1S
6	J	368	MES	C7-C8-S-O1S
3	H	360	TLA	O11-C1-C2-C3
4	C	361	GOL	O1-C1-C2-C3
4	E	361	GOL	O1-C1-C2-C3
3	F	360	TLA	O1-C1-C2-O2
3	A	360	TLA	O2-C2-C3-O3
3	B	360	TLA	O2-C2-C3-O3
3	C	360	TLA	O2-C2-C3-O3
3	E	360	TLA	O2-C2-C3-O3
3	F	360	TLA	O2-C2-C3-O3
3	G	360	TLA	O2-C2-C3-O3
3	H	360	TLA	O2-C2-C3-O3
3	I	360	TLA	O2-C2-C3-O3
3	J	360	TLA	O2-C2-C3-O3
4	G	362	GOL	O2-C2-C3-O3
3	D	360	TLA	O2-C2-C3-O3
2	E	350	NAP	C2B-O2B-P2B-O1X
2	F	350	NAP	C2B-O2B-P2B-O1X
2	H	350	NAP	C2B-O2B-P2B-O1X
4	E	362	GOL	O1-C1-C2-O2
4	G	364	GOL	O1-C1-C2-O2
6	B	364	MES	C8-C7-N4-C5
6	D	364	MES	C8-C7-N4-C5
6	J	368	MES	C8-C7-N4-C5
3	E	360	TLA	O11-C1-C2-O2
4	H	362	GOL	O1-C1-C2-C3
4	H	362	GOL	C1-C2-C3-O3
2	E	350	NAP	O4D-C1D-N1N-C2N
2	F	350	NAP	O4D-C1D-N1N-C2N
2	G	350	NAP	O4D-C1D-N1N-C2N
2	H	350	NAP	O4D-C1D-N1N-C2N
2	I	350	NAP	O4D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
2	J	350	NAP	O4D-C1D-N1N-C2N
2	G	350	NAP	C2B-O2B-P2B-O1X
2	F	350	NAP	PN-O3-PA-O5B
4	H	362	GOL	O2-C2-C3-O3
3	F	360	TLA	O11-C1-C2-O2
2	G	350	NAP	C2B-O2B-P2B-O3X
4	E	361	GOL	C1-C2-C3-O3
2	E	350	NAP	C4D-C5D-O5D-PN
2	F	350	NAP	PN-O3-PA-O2A

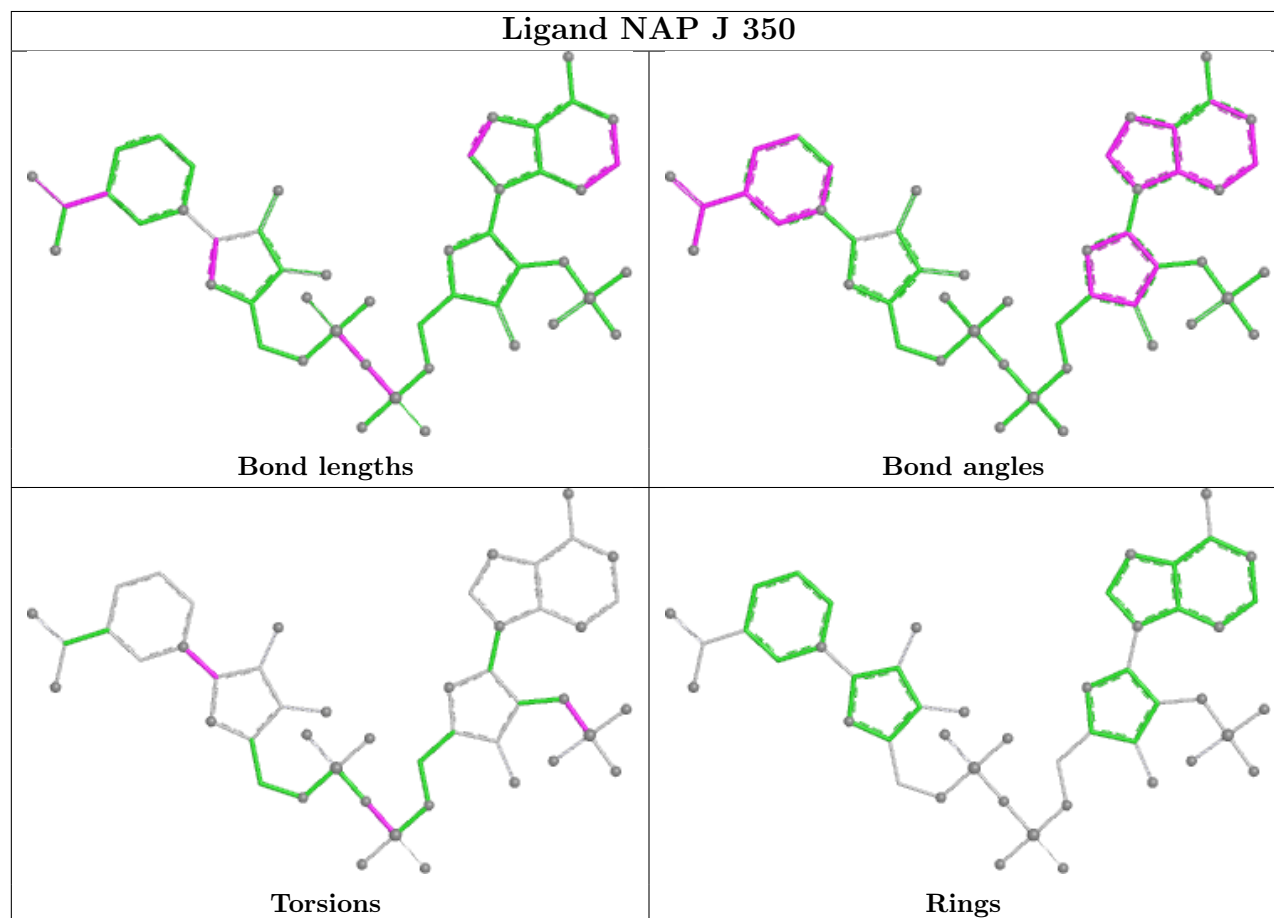
There are no ring outliers.

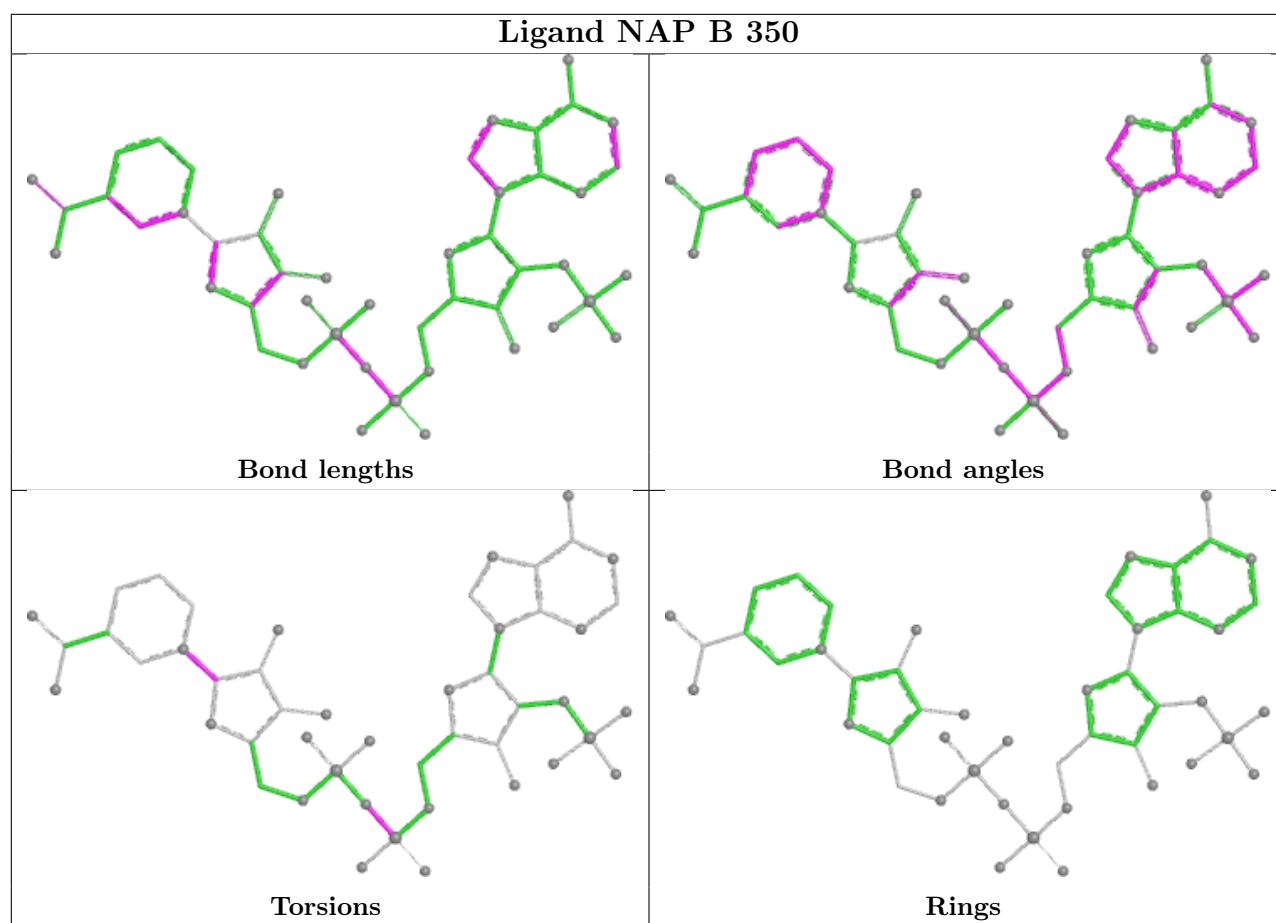
22 monomers are involved in 47 short contacts:

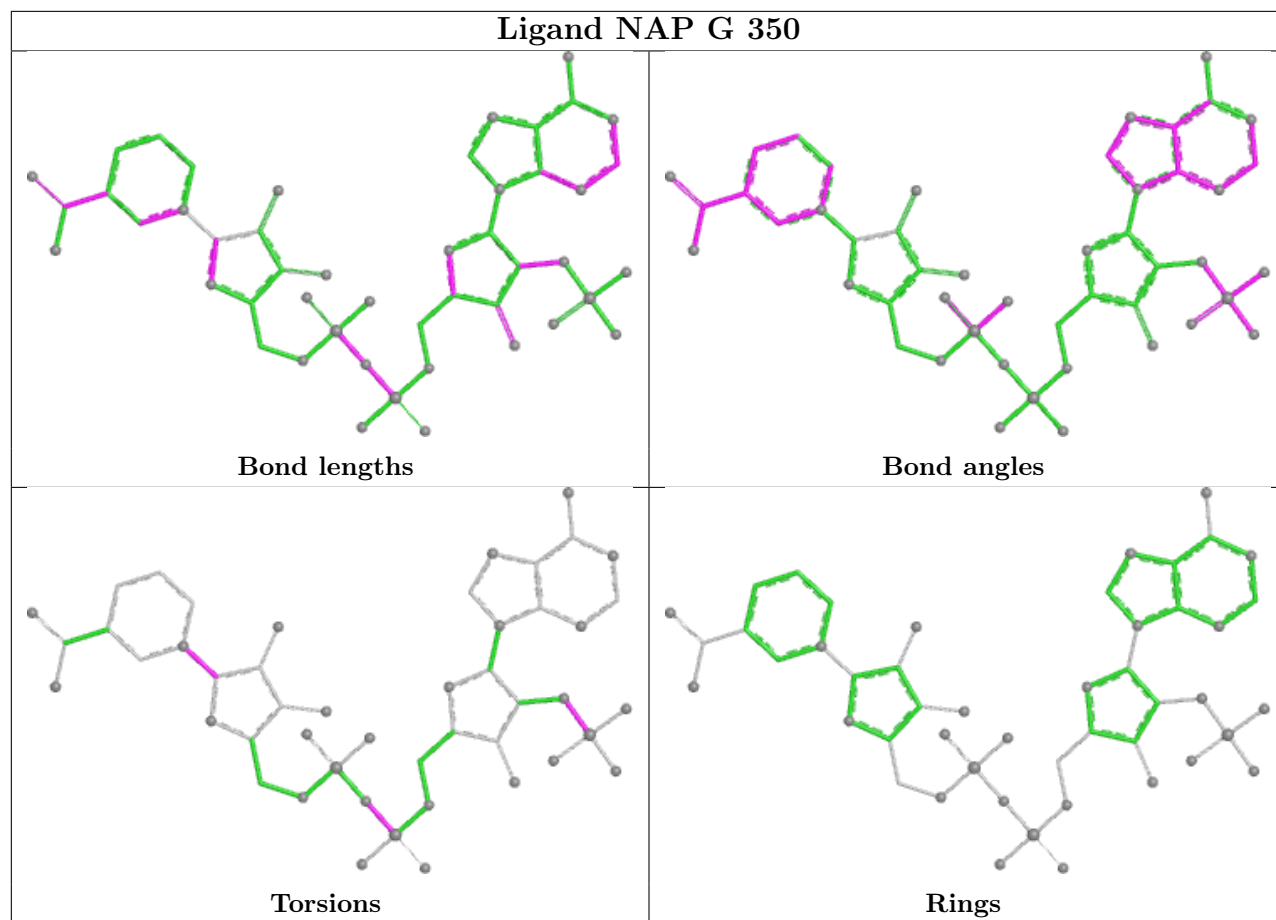
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	350	NAP	3	0
3	C	360	TLA	4	0
4	I	362	GOL	1	0
2	B	350	NAP	3	0
4	G	364	GOL	4	0
4	H	361	GOL	2	0
3	H	360	TLA	2	0
3	F	360	TLA	3	0
2	G	350	NAP	1	0
3	I	360	TLA	2	0
2	F	350	NAP	3	0
3	G	360	TLA	1	0
2	H	350	NAP	4	0
3	D	360	TLA	1	0
2	D	350	NAP	2	0
3	J	360	TLA	2	0
4	A	361	GOL	2	0
2	I	350	NAP	4	0
2	A	350	NAP	2	0
2	E	350	NAP	2	0
3	B	360	TLA	3	0
3	E	360	TLA	2	0

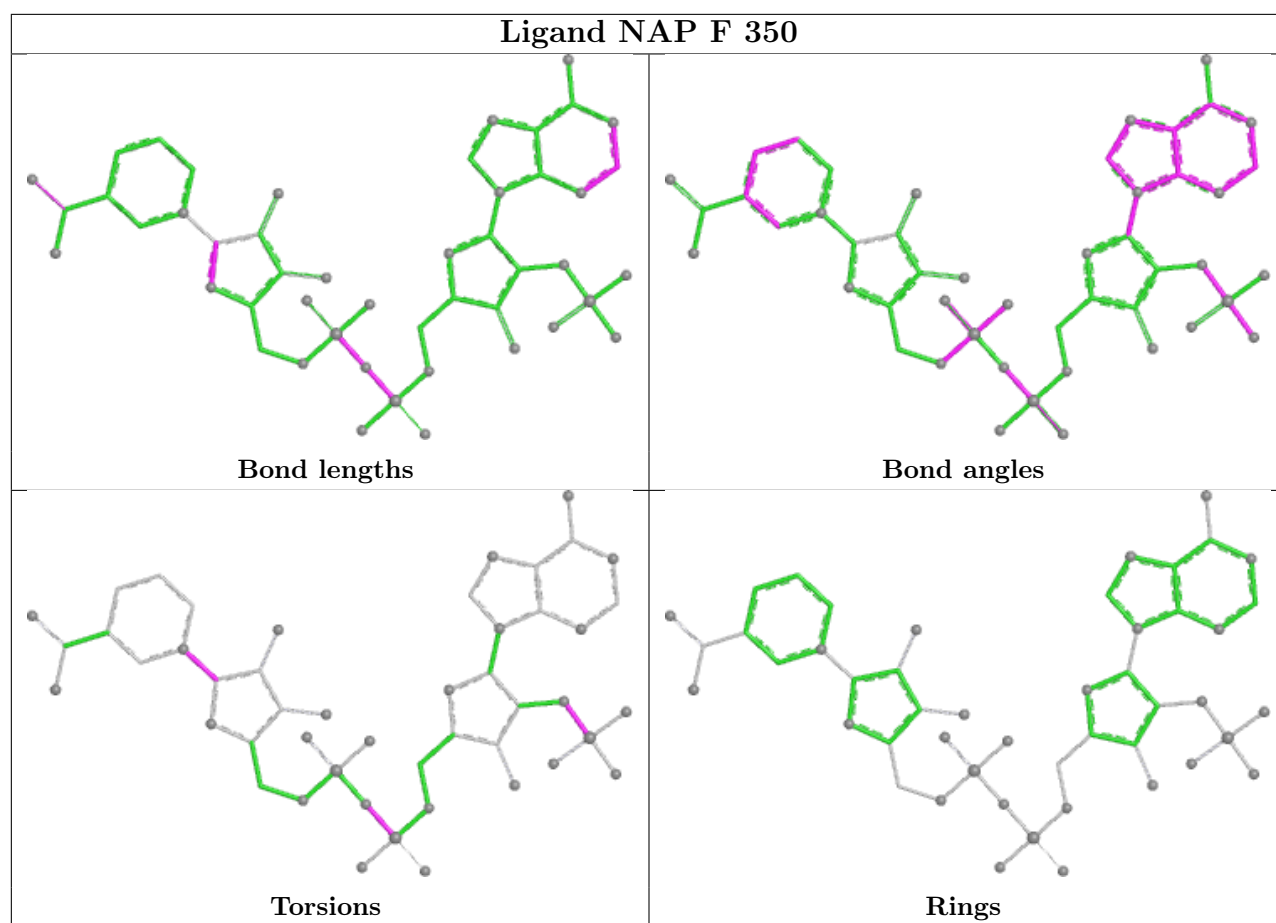
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

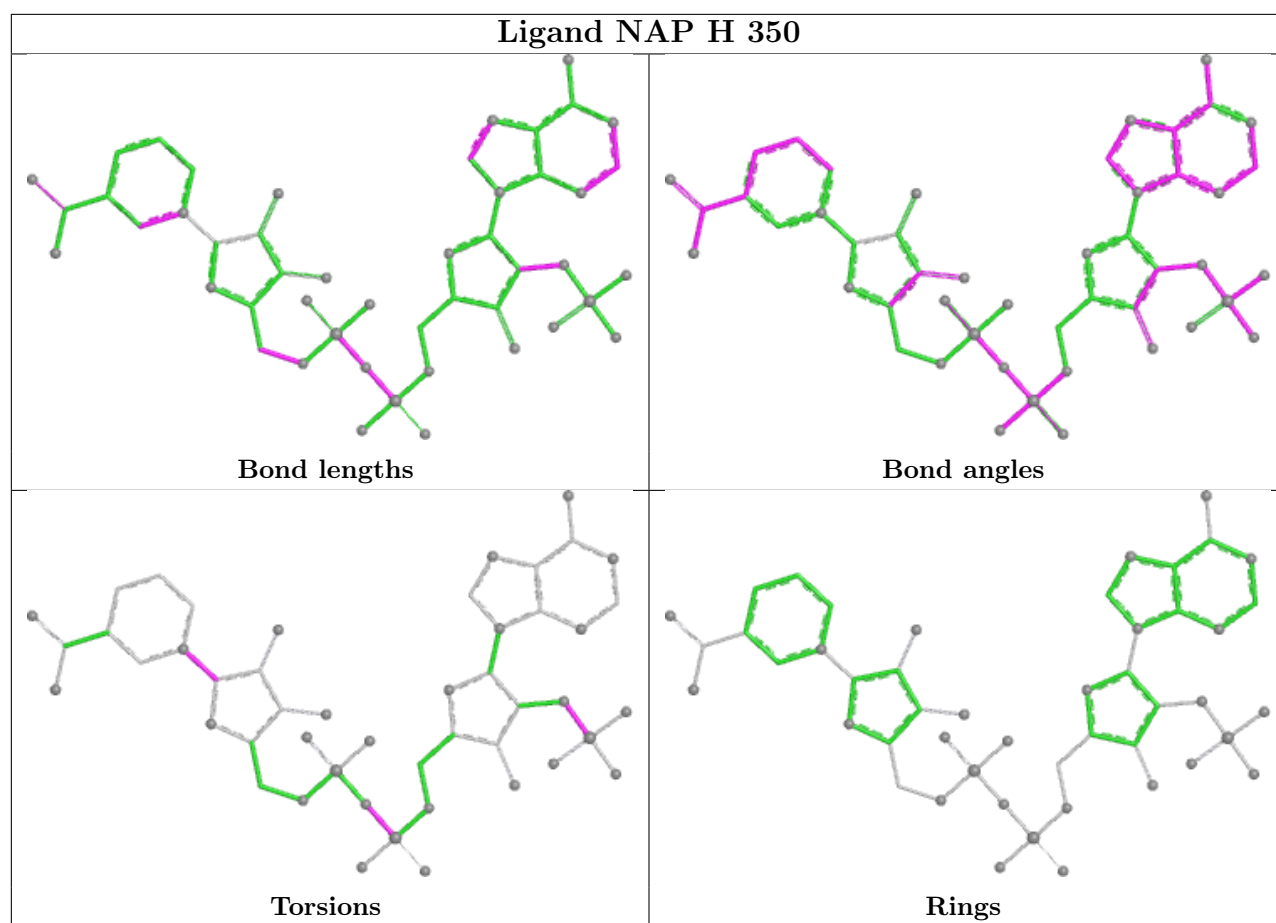
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

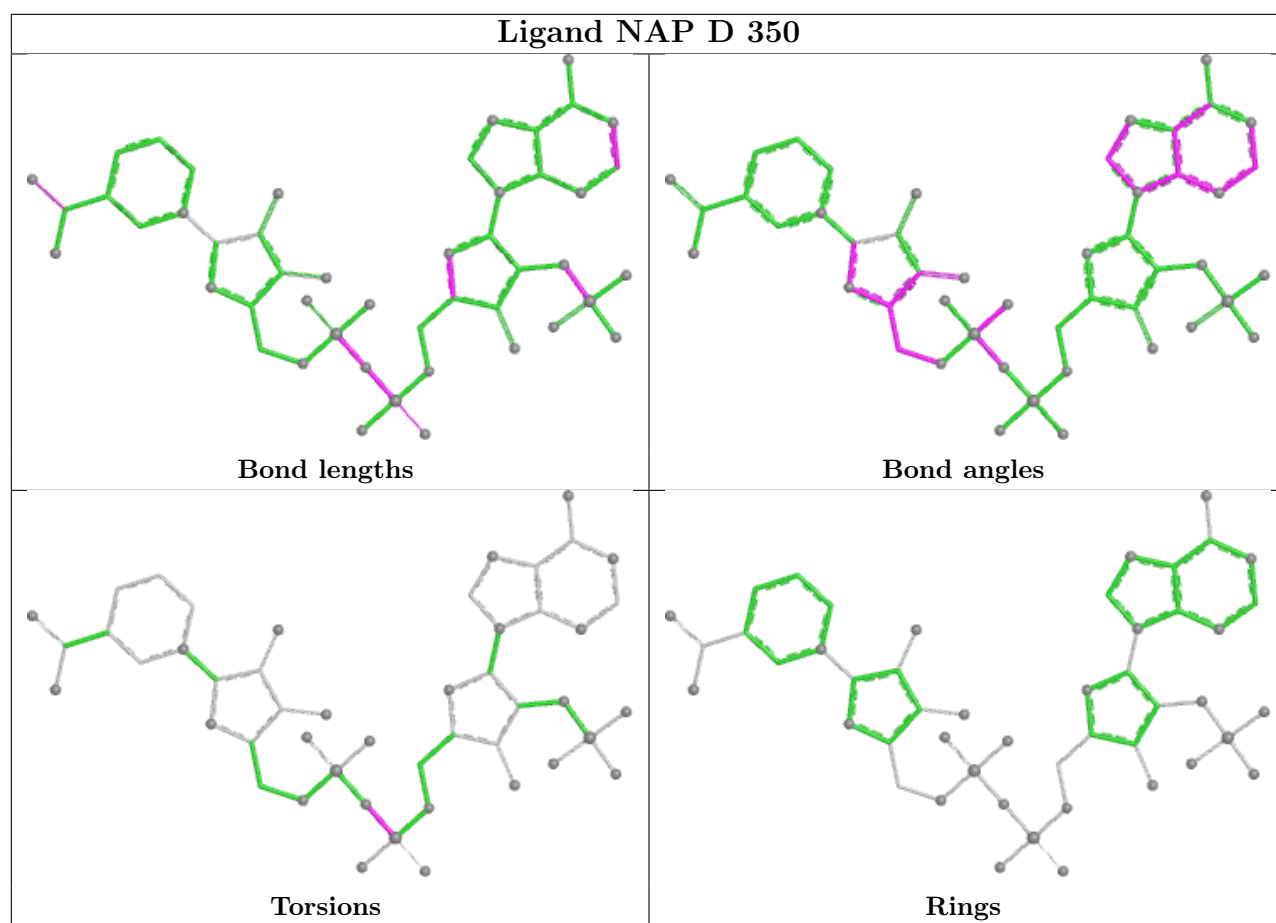


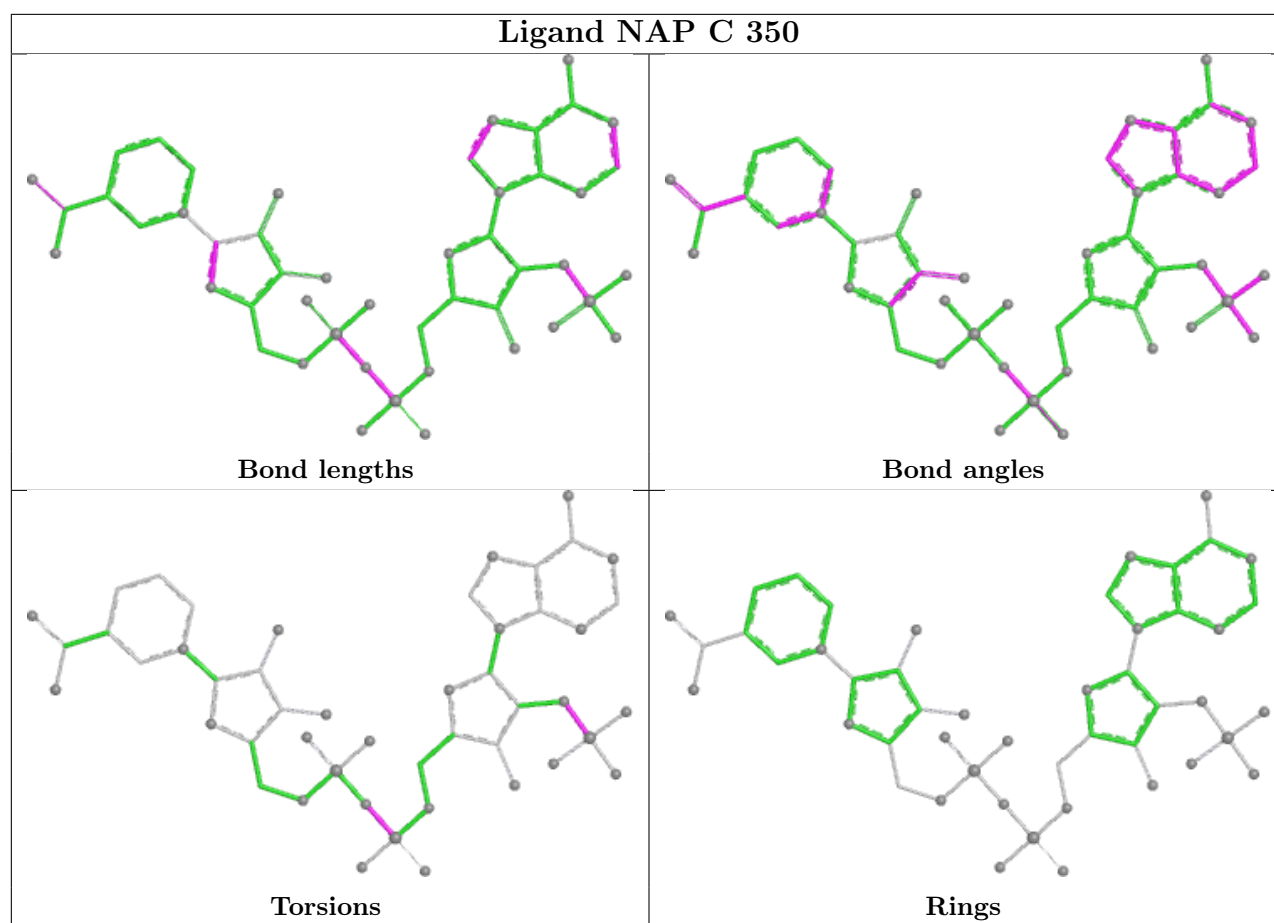


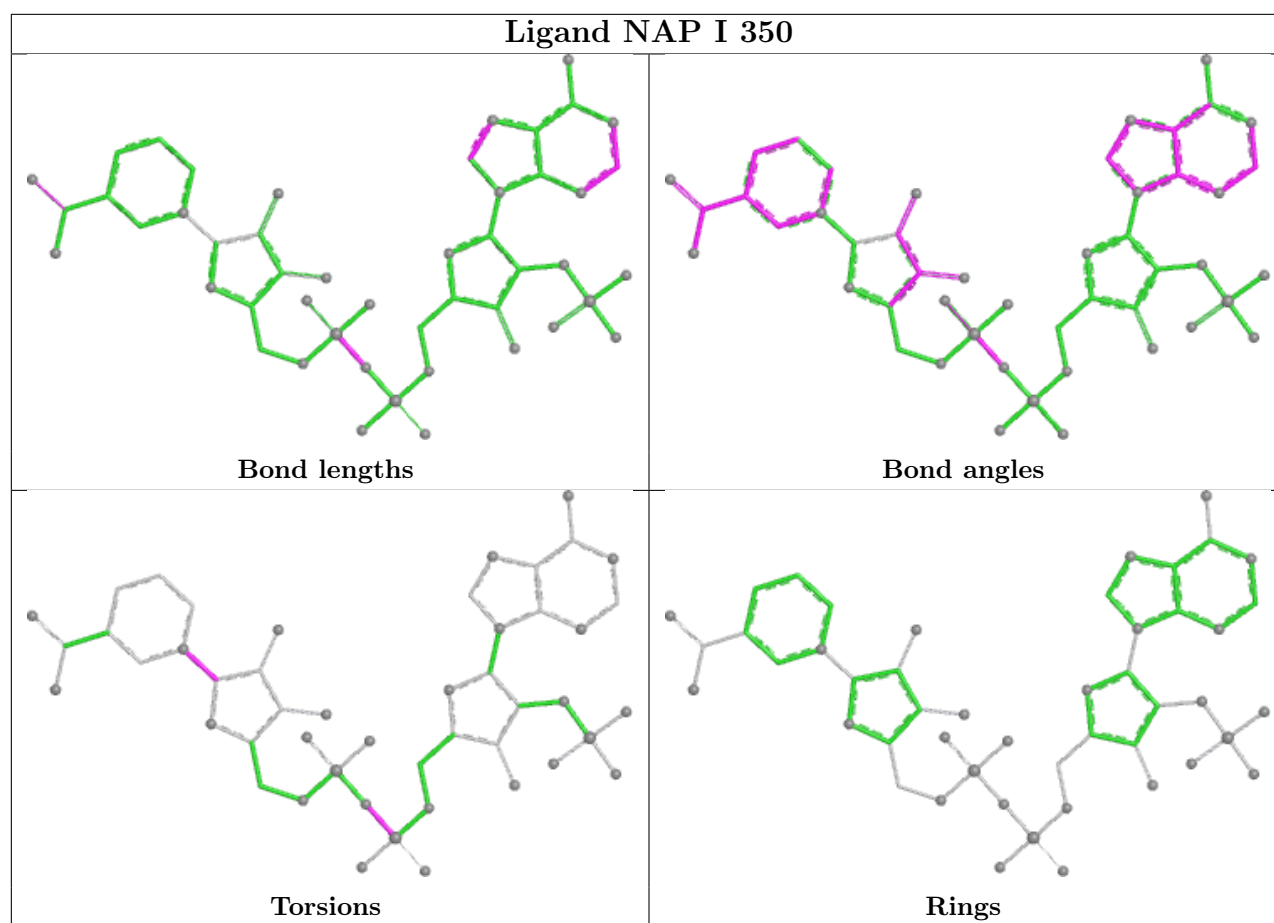


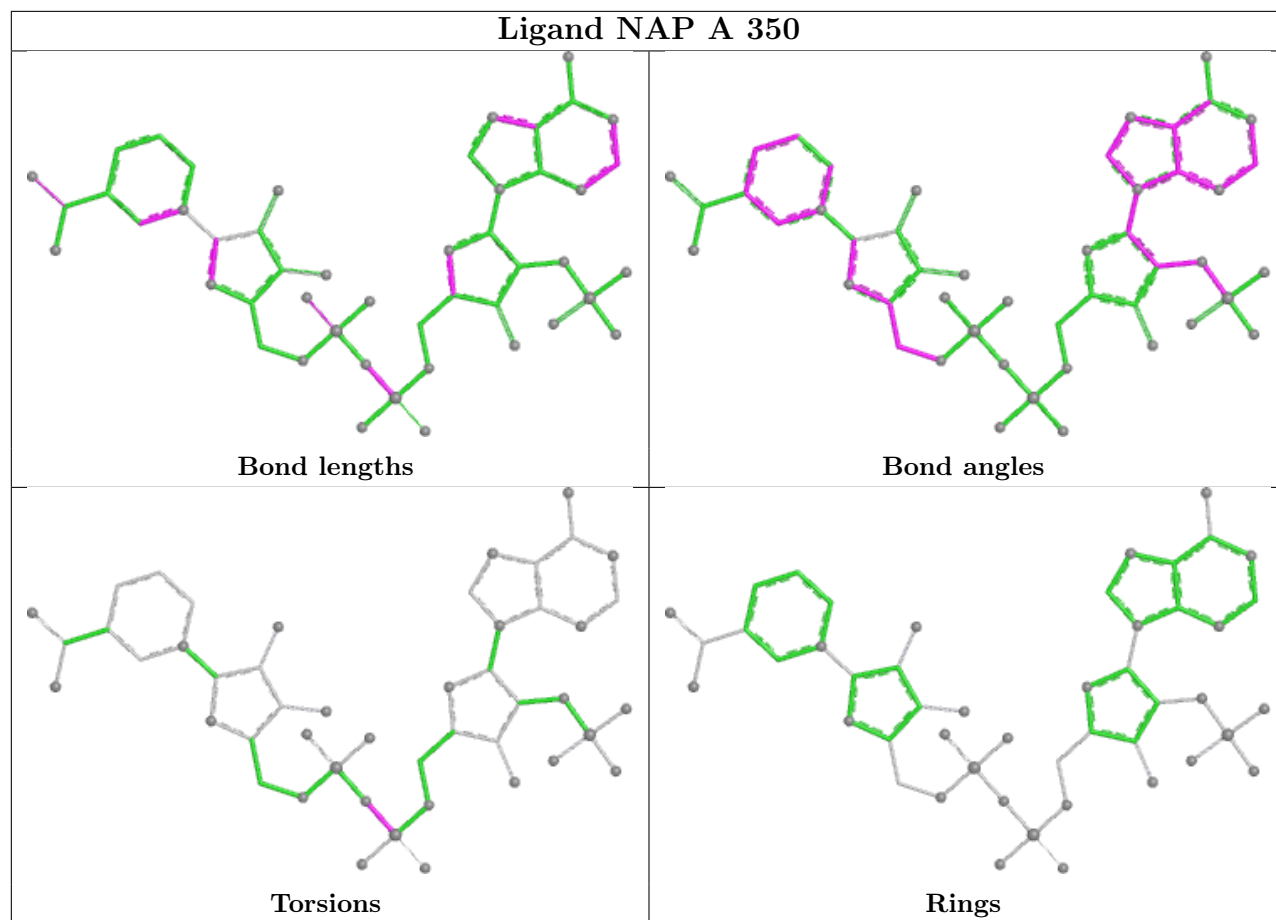


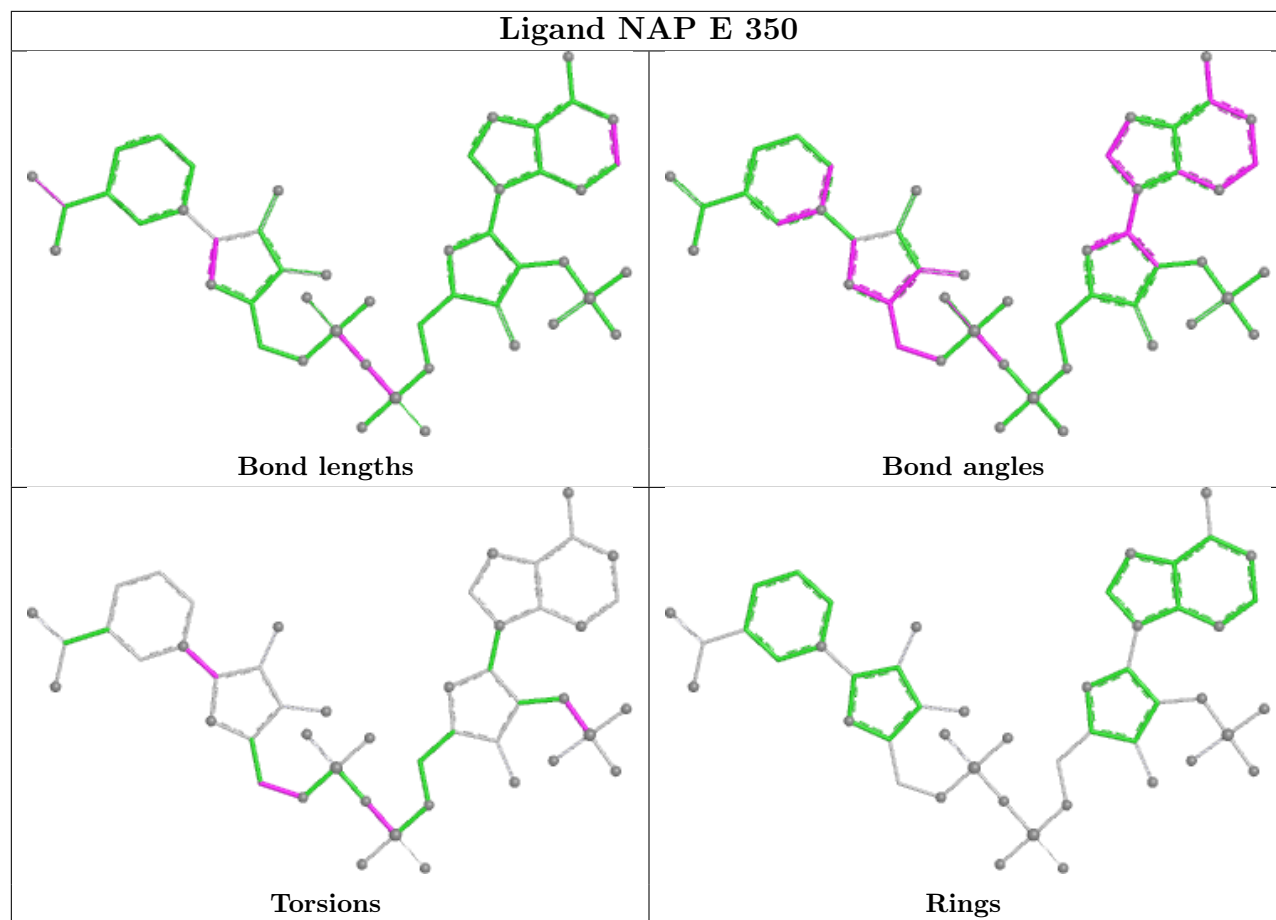












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	325/338 (96%)	-1.52	0 100 100	22, 36, 47, 72	3 (0%)
1	B	324/338 (95%)	-1.46	0 100 100	29, 36, 47, 71	0
1	C	324/338 (95%)	-1.52	0 100 100	25, 36, 47, 72	1 (0%)
1	D	324/338 (95%)	-1.53	0 100 100	19, 36, 47, 73	2 (0%)
1	E	324/338 (95%)	-1.52	0 100 100	25, 36, 47, 72	1 (0%)
1	F	324/338 (95%)	-1.51	0 100 100	30, 36, 47, 72	0
1	G	324/338 (95%)	-1.51	0 100 100	25, 36, 47, 72	1 (0%)
1	H	324/338 (95%)	-1.49	0 100 100	22, 36, 46, 71	1 (0%)
1	I	324/338 (95%)	-1.50	0 100 100	29, 36, 47, 72	0
1	J	325/338 (96%)	-1.51	0 100 100	22, 36, 47, 72	1 (0%)
All	All	3242/3380 (95%)	-1.51	0 100 100	19, 36, 47, 73	10 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

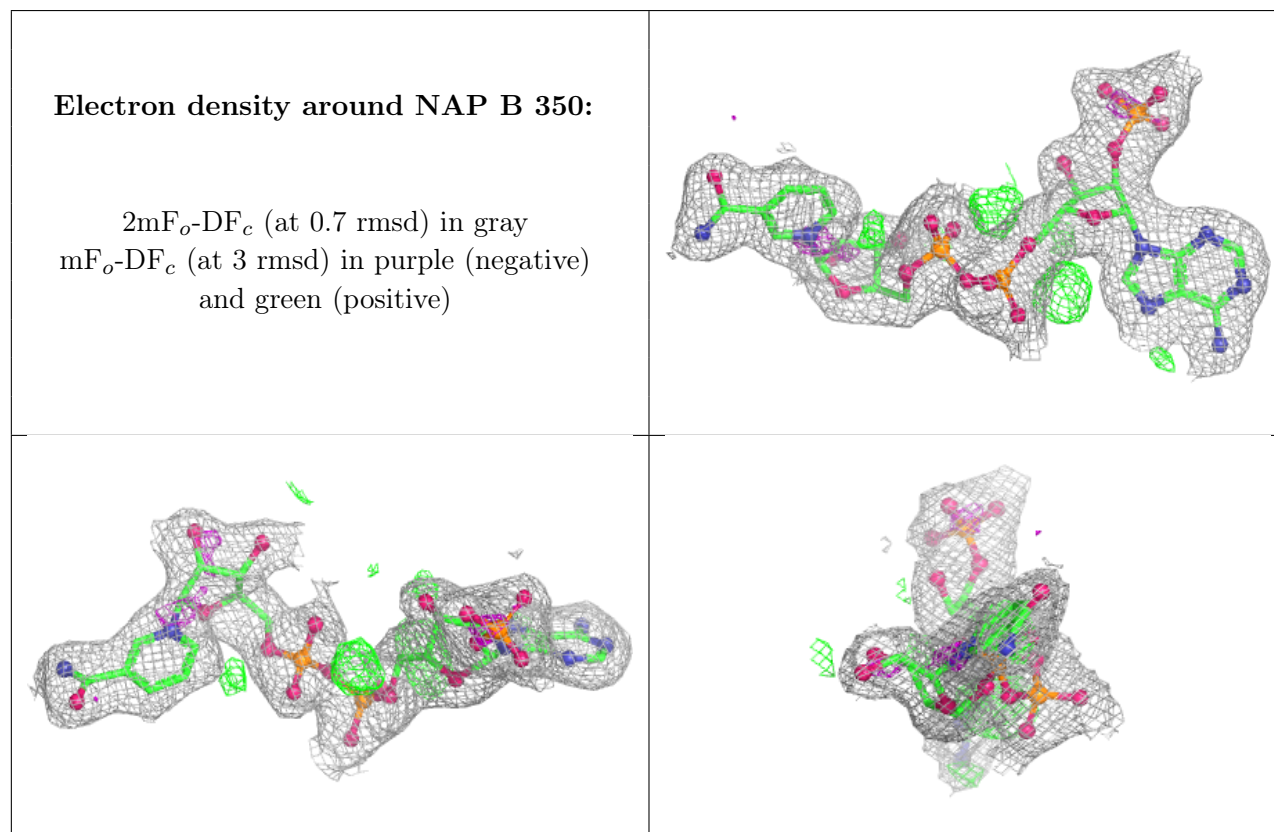
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAP	B	350	48/48	0.99	0.03	27,32,38,43	0
2	NAP	H	350	48/48	0.99	0.03	24,33,37,43	0
3	TLA	A	360	10/10	0.99	0.03	28,33,35,35	0
3	TLA	B	360	10/10	0.99	0.04	34,37,41,42	0
3	TLA	C	360	10/10	0.99	0.04	29,33,38,41	0
3	TLA	D	360	10/10	0.99	0.04	25,31,34,36	0
3	TLA	F	360	10/10	0.99	0.04	31,36,39,39	0
4	GOL	A	361	6/6	0.99	0.05	37,40,45,46	0
4	GOL	A	363	6/6	0.99	0.05	39,42,42,43	0
4	GOL	B	361	6/6	0.99	0.04	33,40,42,42	0
4	GOL	B	362	6/6	0.99	0.05	57,61,62,63	0
4	GOL	B	363	6/6	0.99	0.03	30,33,34,35	0
4	GOL	C	361	6/6	0.99	0.03	38,45,47,50	0
4	GOL	C	362	6/6	0.99	0.04	33,36,39,39	0
4	GOL	C	363	6/6	0.99	0.06	49,60,61,62	0
4	GOL	D	361	6/6	0.99	0.04	29,29,33,33	0
4	GOL	D	362	6/6	0.99	0.03	33,34,35,36	0
4	GOL	D	363	6/6	0.99	0.06	48,53,55,55	0
4	GOL	E	362	6/6	0.99	0.04	31,33,36,36	0
4	GOL	F	361	6/6	0.99	0.04	36,39,41,42	0
4	GOL	G	362	6/6	0.99	0.03	31,36,37,39	0
4	GOL	G	363	6/6	0.99	0.05	34,36,36,38	0
4	GOL	G	364	6/6	0.99	0.05	58,62,62,64	0
4	GOL	H	361	6/6	0.99	0.04	37,44,45,46	0
4	GOL	H	362	6/6	0.99	0.05	30,34,36,36	0
4	GOL	I	361	6/6	0.99	0.05	44,47,48,48	0
4	GOL	I	362	6/6	0.99	0.04	33,34,36,39	0
4	GOL	J	363	6/6	0.99	0.04	39,42,42,46	0
4	GOL	J	364	6/6	0.99	0.04	45,48,49,50	0
4	GOL	J	366	6/6	0.99	0.07	51,53,53,54	0
5	PO4	A	364	5/5	0.99	0.04	59,59,63,65	0
5	PO4	J	367	5/5	0.99	0.04	60,60,65,67	0
6	MES	B	364	12/12	0.99	0.04	50,61,65,65	0
6	MES	C	364	12/12	0.99	0.04	57,62,64,64	0
6	MES	D	364	12/12	0.99	0.05	48,62,66,67	0
6	MES	I	363	12/12	0.99	0.04	55,60,61,61	0
6	MES	J	368	12/12	0.99	0.04	53,57,59,60	0
2	NAP	J	350	48/48	1.00	0.03	23,30,35,40	0
2	NAP	C	350	48/48	1.00	0.03	23,29,35,37	0
2	NAP	D	350	48/48	1.00	0.02	20,25,32,37	0
2	NAP	E	350	48/48	1.00	0.02	20,27,31,36	0

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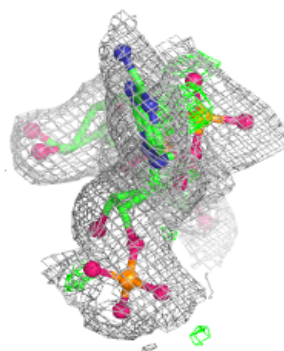
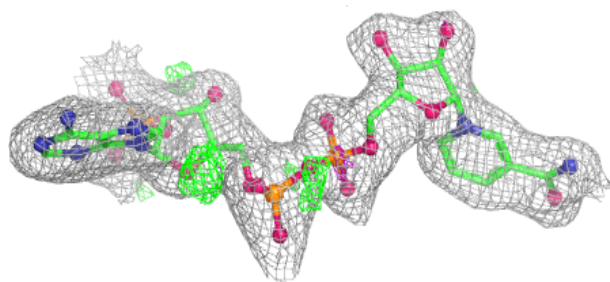
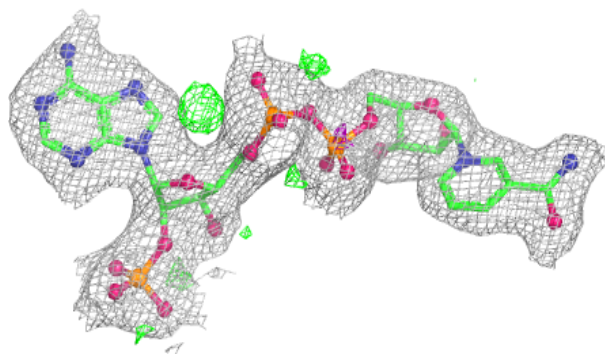
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAP	F	350	48/48	1.00	0.03	23,29,34,36	0
3	TLA	E	360	10/10	1.00	0.03	26,31,35,35	0
2	NAP	G	350	48/48	1.00	0.02	19,27,31,35	0
3	TLA	G	360	10/10	1.00	0.03	31,33,35,35	0
3	TLA	H	360	10/10	1.00	0.05	30,36,41,43	0
4	GOL	E	361	6/6	1.00	0.02	33,36,36,37	0
3	TLA	I	360	10/10	1.00	0.03	27,35,37,40	0
4	GOL	E	363	6/6	1.00	0.05	28,31,31,32	0
3	TLA	J	360	10/10	1.00	0.04	29,33,34,37	0
2	NAP	A	350	48/48	1.00	0.02	21,26,31,35	0
2	NAP	I	350	48/48	1.00	0.03	22,31,35,36	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.

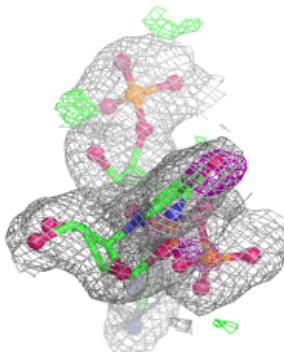
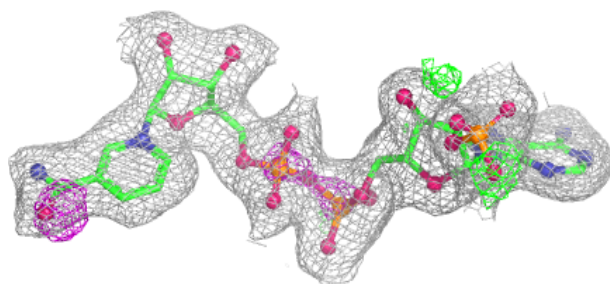
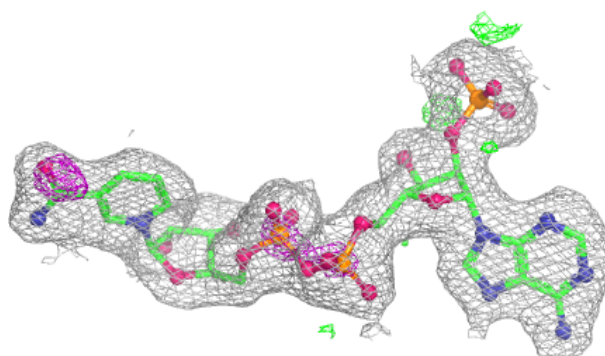


Electron density around NAP H 350:

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

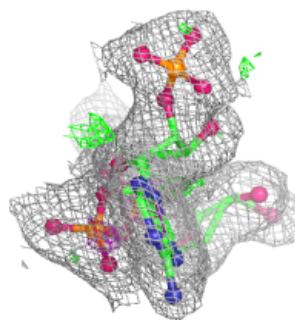
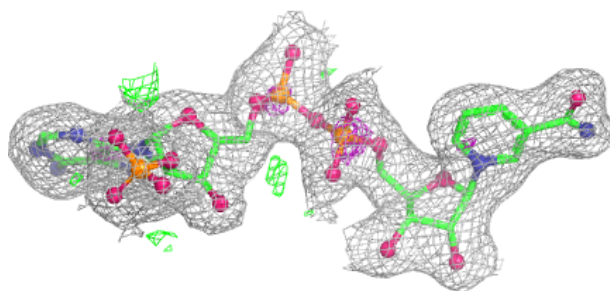
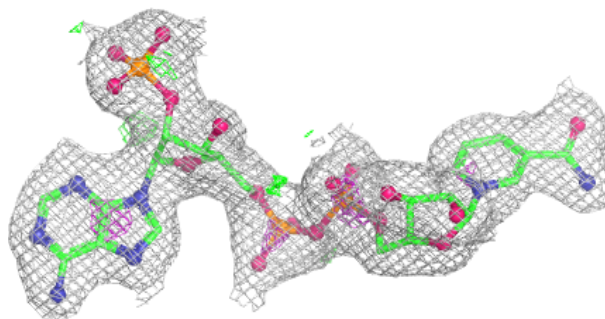
**Electron density around NAP J 350:**

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

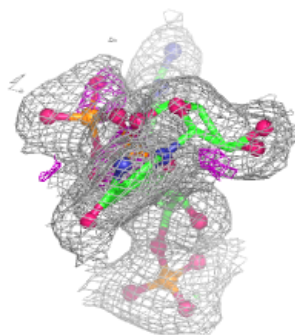
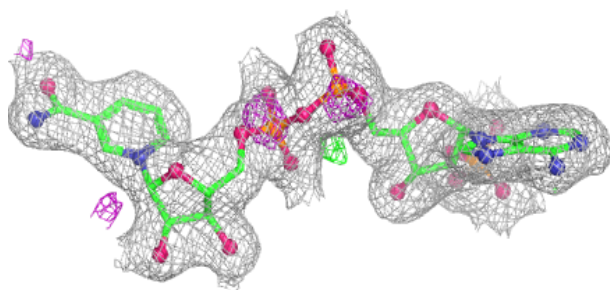
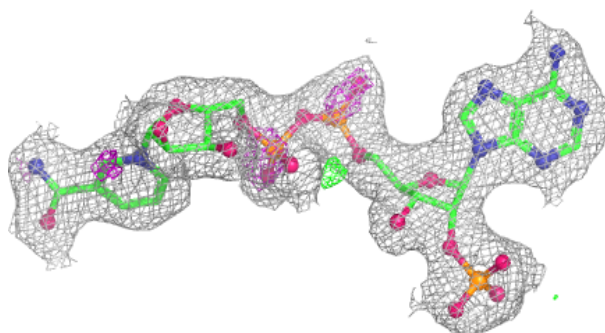


Electron density around NAP C 350:

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

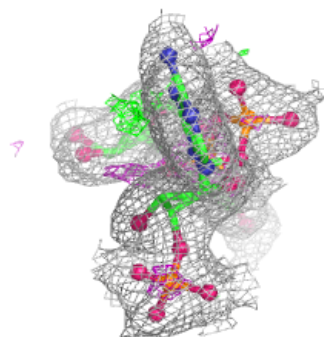
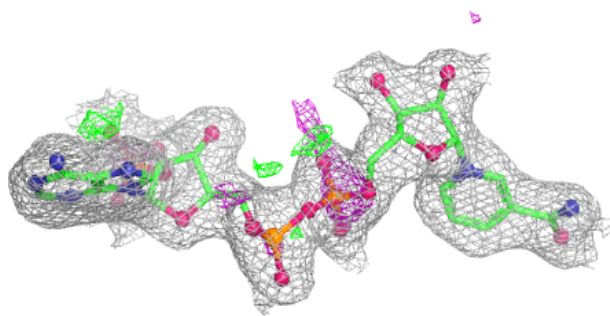
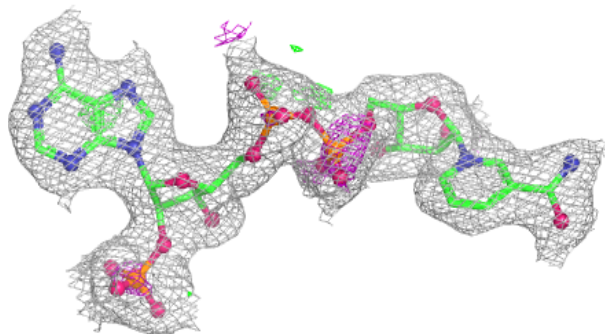
**Electron density around NAP D 350:**

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

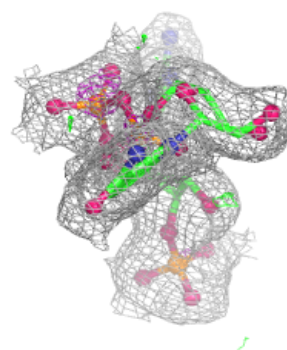
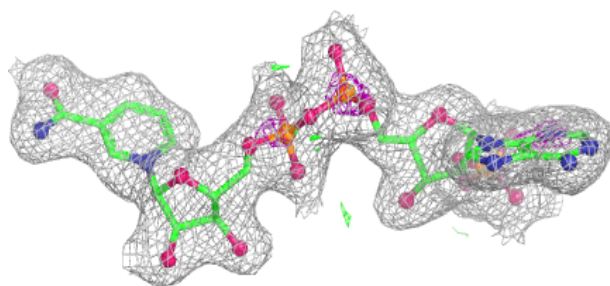
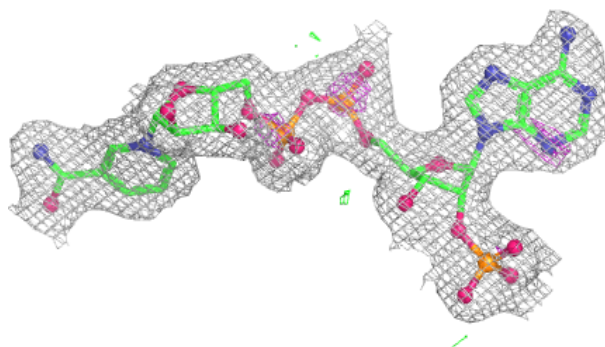


Electron density around NAP E 350:

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

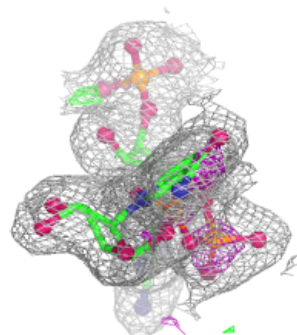
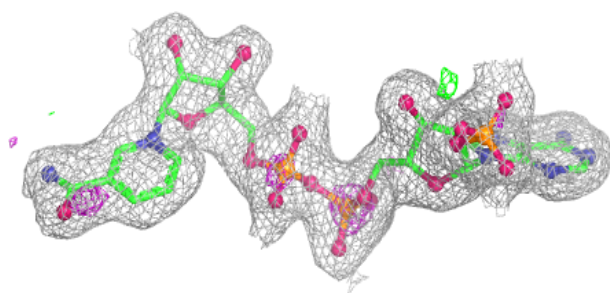
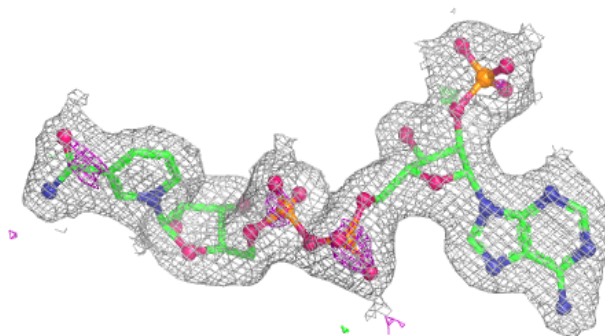
**Electron density around NAP F 350:**

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

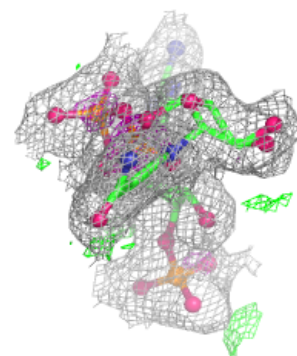
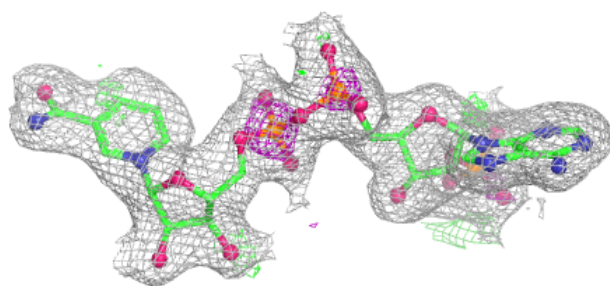
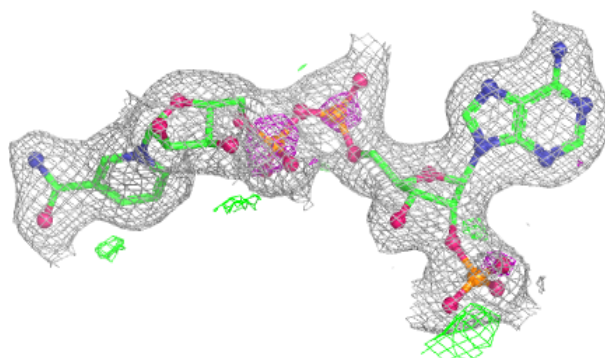


Electron density around NAP G 350:

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

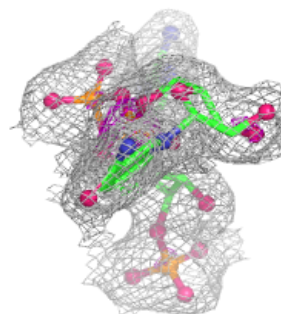
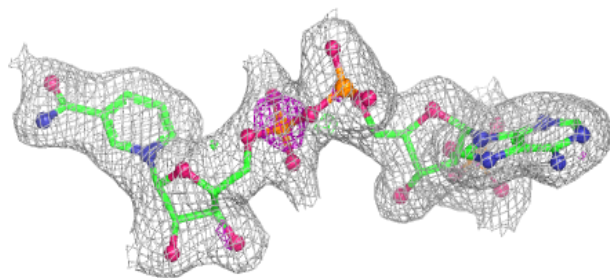
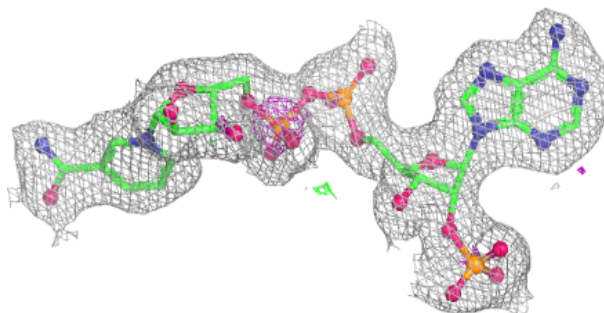
**Electron density around NAP A 350:**

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



Electron density around NAP I 350:

$2mF_o-DF_c$ (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.