



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:47 PM UTC

PDB ID : 2YAU / pdb_00002yau
Title : X-ray structure of the Leishmania infantum trypanothione reductase in complex with auranofin
Authors : Baiocco, P.; Ilari, A.; Colotti, G.
Deposited on : 2011-02-24
Resolution : 3.50 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

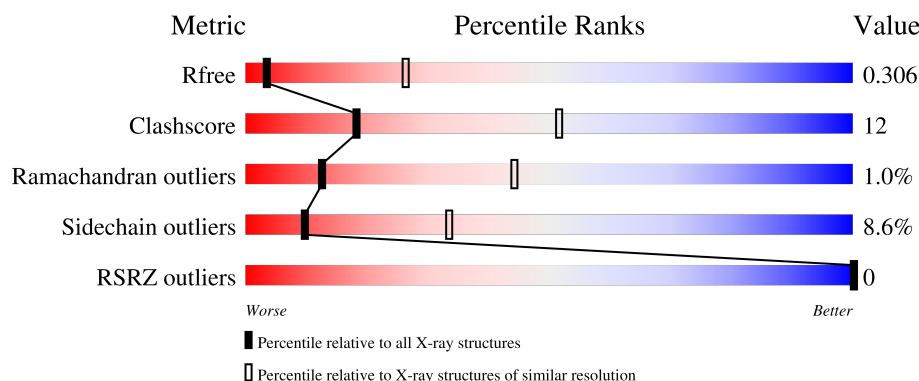
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	511	
1	B	511	

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
4	AU	B	600	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7652 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 TRYPANOTHIONE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	488	Total	C	N	O	S	0	0	0
			3694	2322	634	711	27			
1	B	488	Total	C	N	O	S	0	0	0
			3694	2322	634	711	27			

There are 40 discrepancies between the modelled and reference sequences:

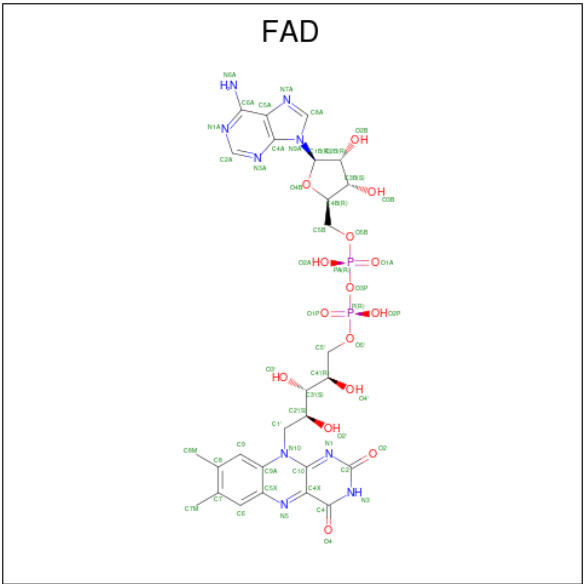
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP A4HSF7
A	-18	GLY	-	expression tag	UNP A4HSF7
A	-17	SER	-	expression tag	UNP A4HSF7
A	-16	SER	-	expression tag	UNP A4HSF7
A	-15	HIS	-	expression tag	UNP A4HSF7
A	-14	HIS	-	expression tag	UNP A4HSF7
A	-13	HIS	-	expression tag	UNP A4HSF7
A	-12	HIS	-	expression tag	UNP A4HSF7
A	-11	HIS	-	expression tag	UNP A4HSF7
A	-10	HIS	-	expression tag	UNP A4HSF7
A	-9	SER	-	expression tag	UNP A4HSF7
A	-8	SER	-	expression tag	UNP A4HSF7
A	-7	GLY	-	expression tag	UNP A4HSF7
A	-6	LEU	-	expression tag	UNP A4HSF7
A	-5	VAL	-	expression tag	UNP A4HSF7
A	-4	PRO	-	expression tag	UNP A4HSF7
A	-3	ARG	-	expression tag	UNP A4HSF7
A	-2	GLY	-	expression tag	UNP A4HSF7
A	-1	SER	-	expression tag	UNP A4HSF7
A	0	HIS	-	expression tag	UNP A4HSF7
B	-19	MET	-	expression tag	UNP A4HSF7
B	-18	GLY	-	expression tag	UNP A4HSF7
B	-17	SER	-	expression tag	UNP A4HSF7
B	-16	SER	-	expression tag	UNP A4HSF7
B	-15	HIS	-	expression tag	UNP A4HSF7

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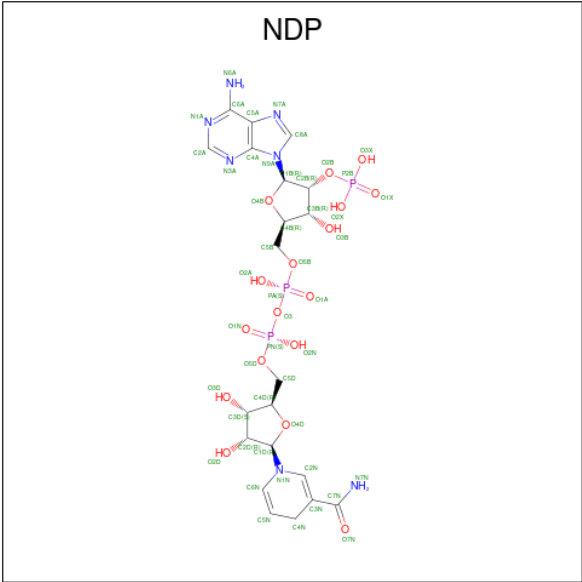
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP A4HSF7
B	-13	HIS	-	expression tag	UNP A4HSF7
B	-12	HIS	-	expression tag	UNP A4HSF7
B	-11	HIS	-	expression tag	UNP A4HSF7
B	-10	HIS	-	expression tag	UNP A4HSF7
B	-9	SER	-	expression tag	UNP A4HSF7
B	-8	SER	-	expression tag	UNP A4HSF7
B	-7	GLY	-	expression tag	UNP A4HSF7
B	-6	LEU	-	expression tag	UNP A4HSF7
B	-5	VAL	-	expression tag	UNP A4HSF7
B	-4	PRO	-	expression tag	UNP A4HSF7
B	-3	ARG	-	expression tag	UNP A4HSF7
B	-2	GLY	-	expression tag	UNP A4HSF7
B	-1	SER	-	expression tag	UNP A4HSF7
B	0	HIS	-	expression tag	UNP A4HSF7

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

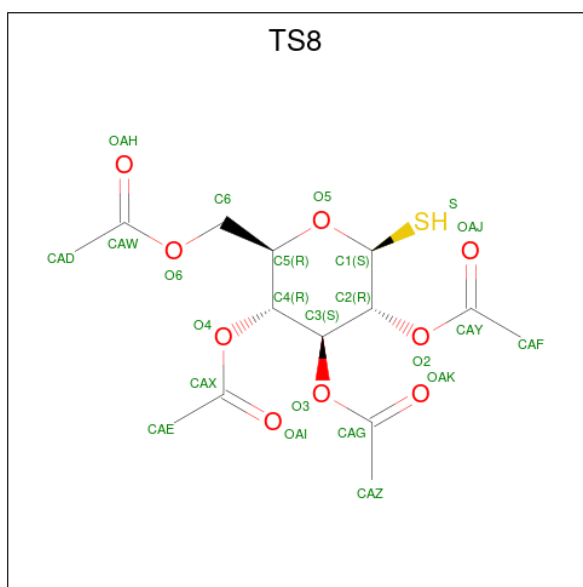


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is GOLD ION (CCD ID: AU) (formula: Au).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Au	0	0
			1	1		
4	B	1	Total	Au	0	0
			1	1		

- Molecule 5 is 2,3,4,6-tetra-O-acetyl-1-thio-beta-D-glucopyranose (CCD ID: TS8) (formula: C₁₄H₂₀O₉S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			24	14	9	1		
5	B	1	Total	C	O	S	0	0
			24	14	9	1		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		
6	B	1	Total	Cl	0	0
			1	1		

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



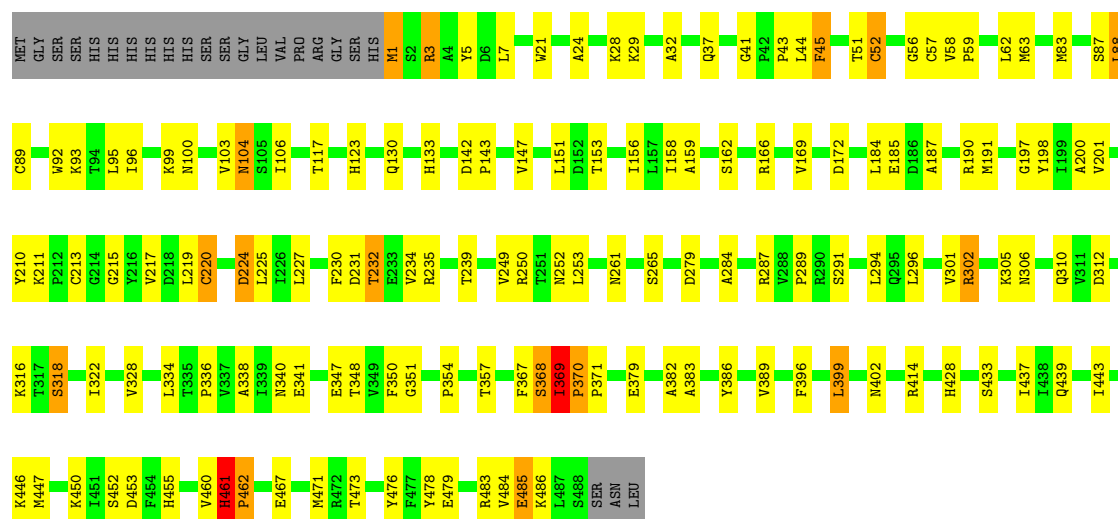
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		

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.

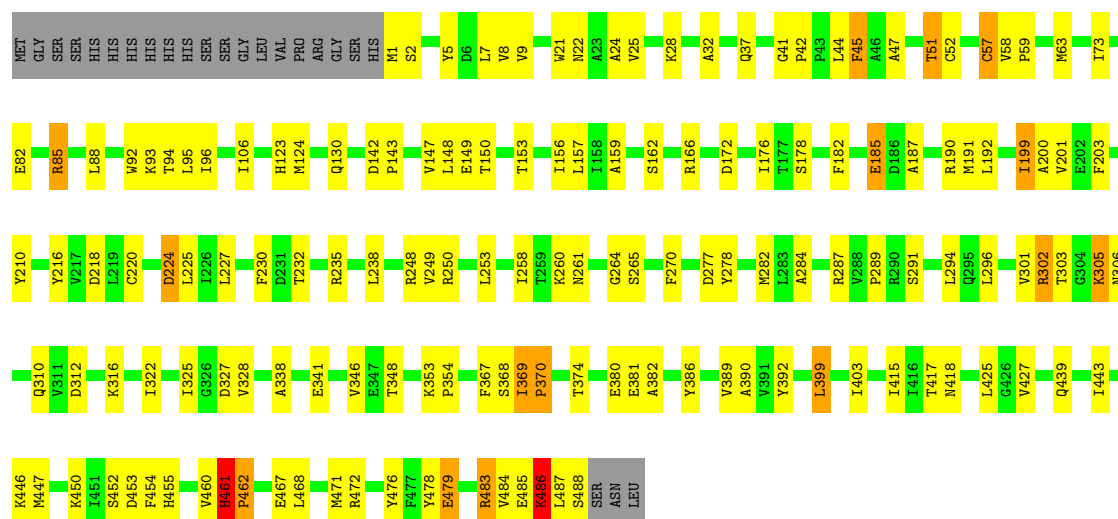
• Molecule 1: TRYPANOTHIONE REDUCTASE

Chain A: 



• Molecule 1: TRYPANOTHIONE REDUCTASE

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	103.06Å 103.06Å 191.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.50 50.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-3.50) 99.9 (50.00-3.50)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.267 , 0.319 0.259 , 0.306	Depositor DCC
R_{free} test set	1291 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	95.9	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 144.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.389 for h,-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	7652	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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: NDP, TS8, CL, SO4, FAD, AU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.58	1/3767 (0.0%)	0.88	3/5100 (0.1%)
1	B	0.58	0/3767	0.89	4/5100 (0.1%)
All	All	0.58	1/7534 (0.0%)	0.89	7/10200 (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	2
1	B	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	369	ILE	CA-CB	6.94	1.58	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	PHE	N-CA-C	5.93	117.41	111.07
1	B	42	PRO	N-CA-C	5.72	117.68	110.70
1	B	45	PHE	N-CA-C	5.61	117.08	110.97
1	B	486	LYS	N-CA-C	5.36	122.21	110.80
1	A	461	HIS	N-CA-C	5.24	121.39	109.81
1	B	461	HIS	N-CA-C	5.22	121.34	109.81
1	A	486	LYS	N-CA-C	5.17	116.14	108.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	369	ILE	Peptide
1	A	461	HIS	Peptide
1	B	461	HIS	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	3694	0	3645	90	0
1	B	3694	0	3645	95	0
2	A	53	0	31	2	0
2	B	53	0	31	2	0
3	A	48	0	26	1	0
3	B	48	0	26	2	0
4	A	1	0	0	0	0
4	B	1	0	0	2	0
5	A	24	0	20	2	0
5	B	24	0	20	3	0
6	A	1	0	0	0	0
6	B	1	0	0	1	0
7	A	5	0	0	0	0
7	B	5	0	0	0	0
All	All	7652	0	7444	179	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 12.

All (179) 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:A:3:ARG:HH12	1:A:133:HIS:CG	1.77	1.01
1:A:1:MET:SD	1:A:1:MET:N	2.30	0.99
1:B:85:ARG:HG2	1:B:85:ARG:HH11	1.29	0.98
1:B:389:VAL:HG23	1:B:478:TYR:HB2	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:PHE:CE1	1:B:462:PRO:HG2	2.10	0.86
1:B:58:VAL:HB	1:B:59:PRO:HD3	1.57	0.85
1:A:3:ARG:NH1	1:A:133:HIS:CG	2.46	0.82
1:A:479:GLU:HB2	1:A:484:VAL:HG11	1.62	0.81
1:A:162:SER:HB2	1:A:287:ARG:HB3	1.64	0.79
1:A:302:ARG:HB3	1:A:310:GLN:HB2	1.67	0.77
1:A:462:PRO:HG2	1:B:367:PHE:CE1	2.21	0.76
1:B:348:THR:HA	1:B:354:PRO:HA	1.68	0.75
1:A:348:THR:HA	1:A:354:PRO:HA	1.66	0.75
1:A:1:MET:HB2	1:A:3:ARG:HD2	1.67	0.75
1:A:291:SER:HA	1:A:294:LEU:HG	1.68	0.75
1:B:57:CYS:HG	4:B:600:AU:AU	1.41	0.74
1:B:302:ARG:HB3	1:B:310:GLN:HB2	1.69	0.73
1:A:92:TRP:CZ2	1:A:96:ILE:HD11	2.24	0.73
1:A:3:ARG:HH12	1:A:133:HIS:CD2	2.06	0.72
1:B:85:ARG:HG2	1:B:85:ARG:NH1	1.93	0.72
1:B:296:LEU:HB3	1:B:301:VAL:HB	1.73	0.69
1:B:162:SER:HB2	1:B:287:ARG:HB3	1.73	0.68
1:A:41:GLY:O	1:A:45:PHE:HA	1.94	0.68
1:A:83:MET:HE1	1:B:73:ILE:HG21	1.76	0.67
1:B:85:ARG:HH11	1:B:85:ARG:CG	2.06	0.66
1:B:199:ILE:HG13	3:B:550:NDP:O2N	1.96	0.65
1:A:29:LYS:HE3	1:A:350:PHE:HD1	1.61	0.65
1:A:383:ALA:CB	1:A:478:TYR:HD2	2.10	0.65
1:A:389:VAL:HG23	1:A:478:TYR:HB2	1.78	0.65
1:A:32:ALA:HB1	1:A:123:HIS:CD2	2.32	0.64
1:A:452:SER:HA	1:A:455:HIS:CE1	2.33	0.64
1:A:220:CYS:HB2	1:A:253:LEU:HD23	1.79	0.64
1:B:289:PRO:HB3	1:B:328:VAL:HA	1.79	0.64
1:A:92:TRP:HB2	1:A:187:ALA:HB2	1.80	0.63
1:A:201:VAL:HG12	1:A:368:SER:HB3	1.81	0.62
1:B:389:VAL:CG2	1:B:478:TYR:HB2	2.25	0.62
1:B:37:GLN:HE21	1:B:47:ALA:HB2	1.65	0.62
1:A:63:MET:HG2	1:A:95:LEU:HD21	1.80	0.62
1:B:176:ILE:O	1:B:282:MET:HA	1.99	0.62
1:A:383:ALA:HB2	1:A:478:TYR:HD2	1.65	0.62
1:B:291:SER:HA	1:B:294:LEU:HG	1.80	0.62
1:B:479:GLU:HG3	1:B:486:LYS:HG2	1.83	0.61
1:B:190:ARG:HG2	1:B:216:TYR:CE1	2.35	0.60
1:B:52:CYS:HG	4:B:600:AU:AU	1.55	0.60
1:A:52:CYS:HA	1:A:56:GLY:HA3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:HIS:HE1	5:B:650:TS8:H2	1.67	0.59
1:A:5:TYR:O	1:A:153:THR:HA	2.01	0.59
1:B:487:LEU:HG	1:B:488:SER:N	2.18	0.58
1:A:296:LEU:HB3	1:A:301:VAL:HB	1.84	0.58
1:B:452:SER:HA	1:B:455:HIS:CE1	2.38	0.58
1:B:390:ALA:HB3	1:B:417:THR:OG1	2.04	0.58
1:A:51:THR:HG21	1:A:287:ARG:NH2	2.19	0.58
1:A:21:TRP:HZ3	1:A:117:THR:HG1	1.52	0.57
1:A:219:LEU:O	1:A:250:ARG:N	2.37	0.57
1:A:24:ALA:O	1:A:28:LYS:HA	2.05	0.57
1:A:312:ASP:OD2	1:A:316:LYS:HB3	2.04	0.57
1:B:1:MET:HE3	1:B:2:SER:H	1.70	0.57
1:B:156:ILE:HB	1:B:322:ILE:HG23	1.86	0.57
1:B:199:ILE:HG22	1:B:203:PHE:HD2	1.70	0.57
1:A:92:TRP:CE2	1:A:96:ILE:HD11	2.40	0.56
1:B:41:GLY:O	1:B:45:PHE:HA	2.05	0.56
1:A:231:ASP:HB3	1:A:234:VAL:HG23	1.87	0.56
1:A:261:ASN:HB2	1:A:265:SER:O	2.06	0.56
1:A:3:ARG:NH1	1:A:133:HIS:ND1	2.53	0.56
1:A:58:VAL:HB	1:A:59:PRO:CD	2.36	0.56
1:B:382:ALA:O	1:B:386:TYR:HB2	2.05	0.56
1:A:289:PRO:HB3	1:A:328:VAL:HA	1.88	0.55
1:B:479:GLU:CG	1:B:486:LYS:HG2	2.36	0.55
1:B:312:ASP:OD2	1:B:316:LYS:HB3	2.07	0.55
1:A:224:ASP:HB3	1:A:252:ASN:HD21	1.70	0.55
1:A:305:LYS:HD2	1:A:305:LYS:H	1.72	0.55
1:B:95:LEU:HD13	1:B:210:TYR:OH	2.07	0.54
1:B:201:VAL:HG12	1:B:368:SER:HB3	1.88	0.54
1:B:305:LYS:HD2	1:B:305:LYS:H	1.71	0.54
1:B:52:CYS:SG	1:B:57:CYS:HB3	2.48	0.53
1:B:92:TRP:CZ2	1:B:96:ILE:HD11	2.43	0.53
1:A:382:ALA:O	1:A:386:TYR:HB2	2.09	0.53
1:B:483:ARG:HD3	1:B:483:ARG:H	1.74	0.53
1:B:148:LEU:HD23	1:B:149:GLU:HG3	1.91	0.52
1:A:479:GLU:HB2	1:A:484:VAL:CG1	2.37	0.52
1:B:443:ILE:O	1:B:447:MET:HB2	2.10	0.52
1:A:63:MET:HE3	1:A:92:TRP:CH2	2.45	0.52
1:A:450:LYS:O	1:A:453:ASP:HB2	2.10	0.52
1:A:433:SER:O	1:A:437:ILE:HG13	2.10	0.51
1:B:9:VAL:HG13	1:B:157:LEU:HD23	1.93	0.51
1:B:51:THR:HG21	1:B:287:ARG:NH2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:MET:HE3	1:B:192:LEU:C	2.36	0.51
1:A:1:MET:HB2	1:A:3:ARG:CD	2.39	0.50
1:B:166:ARG:NH1	1:B:172:ASP:O	2.44	0.50
1:B:199:ILE:HD12	3:B:550:NDP:O1N	2.11	0.50
1:B:418:ASN:HB2	1:B:425:LEU:HD21	1.94	0.50
1:A:347:GLU:HA	1:A:351:GLY:HA3	1.93	0.50
1:B:200:ALA:HB2	1:B:284:ALA:HB3	1.93	0.50
5:B:650:TS8:S	6:B:1489:CL:CL	3.07	0.50
1:A:58:VAL:HG13	1:B:399:LEU:HD12	1.94	0.49
1:A:200:ALA:HB2	1:A:284:ALA:HB3	1.94	0.49
1:B:32:ALA:HB1	1:B:123:HIS:CD2	2.48	0.49
5:A:650:TS8:H2	1:B:461:HIS:HE1	1.78	0.49
1:A:369:ILE:HG22	1:A:370:PRO:HD3	1.94	0.49
1:A:439:GLN:OE1	1:B:460:VAL:HG23	2.13	0.48
1:A:103:VAL:O	1:A:106:ILE:N	2.45	0.48
1:A:190:ARG:HB2	1:A:279:ASP:H	1.78	0.48
1:B:8:VAL:HG23	1:B:153:THR:HB	1.94	0.48
1:A:231:ASP:HB3	1:A:234:VAL:CG2	2.44	0.48
1:A:462:PRO:HG3	2:B:500:FAD:O4	2.13	0.48
1:A:227:LEU:HB3	1:A:230:PHE:CD1	2.49	0.48
3:A:550:NDP:H51N	3:A:550:NDP:H6N	1.95	0.48
1:B:415:ILE:HG12	1:B:427:VAL:HG22	1.96	0.48
1:A:95:LEU:HD13	1:A:210:TYR:OH	2.14	0.47
1:A:396:PHE:HB2	5:B:650:TS8:HAE	1.96	0.47
2:A:500:FAD:O4	1:B:462:PRO:HG3	2.14	0.47
1:B:227:LEU:HB3	1:B:230:PHE:CD2	2.50	0.47
1:A:156:ILE:HD12	1:A:322:ILE:HG12	1.97	0.47
1:B:392:TYR:HE2	1:B:472:ARG:O	1.98	0.47
1:B:156:ILE:HD12	1:B:322:ILE:HG12	1.97	0.47
1:B:63:MET:HE3	1:B:92:TRP:CH2	2.50	0.46
1:B:338:ALA:HA	1:B:341:GLU:HB2	1.98	0.46
1:A:159:ALA:O	2:A:500:FAD:H52A	2.15	0.46
1:A:340:ASN:HD22	1:A:357:THR:HG23	1.81	0.46
1:A:443:ILE:O	1:A:447:MET:HB2	2.14	0.46
1:B:261:ASN:HB2	1:B:265:SER:O	2.15	0.46
1:B:380:GLU:H	1:B:380:GLU:CD	2.24	0.46
1:A:32:ALA:HB1	1:A:123:HIS:NE2	2.30	0.46
1:B:224:ASP:OD1	1:B:224:ASP:N	2.46	0.46
1:B:369:ILE:HG22	1:B:370:PRO:HD3	1.98	0.46
1:A:389:VAL:HG23	1:A:478:TYR:CB	2.46	0.46
1:B:92:TRP:HB2	1:B:187:ALA:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:LYS:HA	1:B:354:PRO:HD3	1.86	0.45
1:A:232:THR:HA	1:A:235:ARG:HD3	1.99	0.45
1:B:253:LEU:HD11	1:B:270:PHE:HB3	1.98	0.45
1:A:62:LEU:HD22	1:B:403:ILE:HD12	1.98	0.45
1:A:197:GLY:O	1:A:198:TYR:C	2.60	0.45
1:B:185:GLU:CD	1:B:185:GLU:H	2.25	0.45
1:B:461:HIS:O	1:B:461:HIS:ND1	2.49	0.45
1:B:5:TYR:O	1:B:153:THR:HA	2.17	0.44
1:A:379:GLU:OE2	1:A:414:ARG:NH2	2.50	0.44
1:A:467:GLU:O	1:A:471:MET:HE2	2.18	0.44
5:A:650:TS8:H2	1:B:461:HIS:CE1	2.52	0.44
1:B:232:THR:HA	1:B:235:ARG:HD3	2.00	0.44
1:B:454:PHE:HE2	1:B:468:LEU:HD22	1.83	0.44
1:B:63:MET:HG2	1:B:95:LEU:HD21	2.00	0.43
1:A:302:ARG:HH11	1:A:318:SER:HB3	1.82	0.43
1:A:399:LEU:O	1:A:402:ASN:ND2	2.50	0.43
1:A:100:ASN:O	1:A:104:ASN:HB3	2.18	0.43
1:A:211:LYS:HD2	1:A:215:GLY:O	2.19	0.43
1:B:24:ALA:O	1:B:28:LYS:HA	2.18	0.43
1:B:467:GLU:O	1:B:471:MET:HE2	2.17	0.43
1:A:460:VAL:HG23	1:B:439:GLN:OE1	2.19	0.43
1:B:415:ILE:HG23	1:B:427:VAL:HG22	2.01	0.43
1:A:59:PRO:HB3	1:A:99:LYS:HD3	2.01	0.43
1:B:260:LYS:HE3	1:B:264:GLY:O	2.19	0.43
1:B:325:ILE:CG2	1:B:341:GLU:HB3	2.48	0.43
1:A:291:SER:HB2	1:A:296:LEU:HD21	2.01	0.42
1:A:334:LEU:HB3	1:A:336:PRO:HD2	2.00	0.42
1:B:21:TRP:CE2	1:B:25:VAL:HG21	2.54	0.42
1:B:22:ASN:HB3	1:B:346:VAL:HG11	2.02	0.42
1:B:190:ARG:HD2	1:B:277:ASP:O	2.19	0.42
1:B:450:LYS:O	1:B:453:ASP:HB2	2.20	0.42
1:A:191:MET:HB3	1:A:217:VAL:HG22	2.02	0.41
1:B:369:ILE:HD13	1:B:369:ILE:HA	1.90	0.41
1:A:383:ALA:HB2	1:A:478:TYR:CD2	2.50	0.41
1:B:192:LEU:HD22	1:B:278:TYR:CE2	2.56	0.41
1:B:218:ASP:OD1	1:B:248:ARG:HB3	2.21	0.41
1:A:88:LEU:HD23	1:B:82:GLU:O	2.19	0.41
1:B:159:ALA:O	2:B:500:FAD:H52A	2.21	0.41
1:B:479:GLU:HG3	1:B:484:VAL:HG11	2.01	0.41
1:A:484:VAL:HG22	1:A:485:GLU:N	2.36	0.41
1:A:166:ARG:NH1	1:A:172:ASP:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ASP:HB2	1:A:428:HIS:CG	2.55	0.41
1:B:59:PRO:HB2	1:B:182:PHE:CE1	2.56	0.41
1:B:190:ARG:HG2	1:B:216:TYR:CZ	2.55	0.41
1:A:158:ILE:HG22	1:A:328:VAL:HG11	2.02	0.41
1:B:142:ASP:HA	1:B:143:PRO:HD3	1.86	0.41
1:B:162:SER:HB3	1:B:327:ASP:HB3	2.02	0.41
1:B:37:GLN:HA	1:B:124:MET:HE3	2.02	0.40
1:A:89:CYS:SG	1:A:213:CYS:N	2.94	0.40
1:A:142:ASP:HA	1:A:143:PRO:HD3	1.94	0.40
1:A:338:ALA:HA	1:A:341:GLU:HB2	2.03	0.40
1:A:370:PRO:HA	1:A:371:PRO:HD3	2.01	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	486/511 (95%)	436 (90%)	45 (9%)	5 (1%)	12	44
1	B	486/511 (95%)	437 (90%)	44 (9%)	5 (1%)	12	44
All	All	972/1022 (95%)	873 (90%)	89 (9%)	10 (1%)	12	44

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	462	PRO
1	B	461	HIS
1	B	462	PRO
1	A	43	PRO
1	B	486	LYS
1	A	232	THR
1	A	370	PRO

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Mol	Chain	Res	Type
1	A	461	HIS
1	B	305	LYS
1	B	370	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	397/417 (95%)	364 (92%)	33 (8%)	10	34
1	B	397/417 (95%)	362 (91%)	35 (9%)	9	32
All	All	794/834 (95%)	726 (91%)	68 (9%)	10	33

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	ARG
1	A	7	LEU
1	A	37	GLN
1	A	44	LEU
1	A	52	CYS
1	A	57	CYS
1	A	87	SER
1	A	88	LEU
1	A	93	LYS
1	A	104	ASN
1	A	130	GLN
1	A	147	VAL
1	A	151	LEU
1	A	169	VAL
1	A	184	LEU
1	A	185	GLU
1	A	220	CYS
1	A	224	ASP
1	A	225	LEU

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Mol	Chain	Res	Type
1	A	239	THR
1	A	249	VAL
1	A	302	ARG
1	A	306	ASN
1	A	318	SER
1	A	368	SER
1	A	369	ILE
1	A	399	LEU
1	A	446	LYS
1	A	473	THR
1	A	476	TYR
1	A	483	ARG
1	A	485	GLU
1	B	7	LEU
1	B	44	LEU
1	B	51	THR
1	B	57	CYS
1	B	85	ARG
1	B	88	LEU
1	B	93	LYS
1	B	94	THR
1	B	106	ILE
1	B	130	GLN
1	B	147	VAL
1	B	150	THR
1	B	178	SER
1	B	185	GLU
1	B	199	ILE
1	B	220	CYS
1	B	224	ASP
1	B	225	LEU
1	B	238	LEU
1	B	249	VAL
1	B	250	ARG
1	B	258	ILE
1	B	302	ARG
1	B	303	THR
1	B	306	ASN
1	B	369	ILE
1	B	374	THR
1	B	381	GLU
1	B	399	LEU

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Mol	Chain	Res	Type
1	B	446	LYS
1	B	476	TYR
1	B	479	GLU
1	B	483	ARG
1	B	485	GLU
1	B	486	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	100	ASN
1	A	241	GLN
1	A	252	ASN
1	A	269	HIS
1	A	340	ASN
1	A	385	ASN
1	A	461	HIS
1	B	37	GLN
1	B	130	GLN
1	B	252	ASN
1	B	269	HIS
1	B	295	GLN
1	B	310	GLN
1	B	340	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

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	B	500	-	58,58,58	1.07	5 (8%)	85,89,89	1.63	16 (18%)
5	TS8	B	650	-	23,24,24	2.05	4 (17%)	31,33,33	2.04	9 (29%)
7	SO4	A	1490	-	4,4,4	0.24	0	6,6,6	0.16	0
2	FAD	A	500	-	58,58,58	1.05	5 (8%)	85,89,89	1.65	16 (18%)
7	SO4	B	1490	-	4,4,4	0.23	0	6,6,6	0.09	0
3	NDP	B	550	-	51,52,52	1.97	14 (27%)	71,80,80	1.70	15 (21%)
3	NDP	A	550	-	51,52,52	2.00	14 (27%)	71,80,80	1.68	12 (16%)
5	TS8	A	650	-	23,24,24	2.04	4 (17%)	31,33,33	1.98	10 (32%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	B	500	-	-	8/34/50/50	0/6/6/6
5	TS8	B	650	-	-	11/17/37/37	0/1/1/1
2	FAD	A	500	-	-	11/34/50/50	0/6/6/6
3	NDP	B	550	-	-	11/34/77/77	0/5/5/5
3	NDP	A	550	-	-	11/34/77/77	0/5/5/5
5	TS8	A	650	-	-	9/17/37/37	0/1/1/1

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	550	NDP	PA-O3	6.62	1.66	1.59
3	B	550	NDP	PA-O3	5.66	1.65	1.59
5	B	650	TS8	O2-CAY	5.60	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	650	TS8	O3-CAG	5.44	1.47	1.35
5	B	650	TS8	O3-CAG	5.38	1.47	1.35
5	A	650	TS8	O2-CAY	5.19	1.46	1.35
5	A	650	TS8	O4-CAX	5.08	1.46	1.35
3	A	550	NDP	PN-O3	5.00	1.64	1.59
5	B	650	TS8	O4-CAX	4.85	1.45	1.35
3	B	550	NDP	PN-O3	4.54	1.64	1.59
3	B	550	NDP	PN-O1N	4.20	1.65	1.50
3	B	550	NDP	PA-O1A	4.09	1.65	1.50
3	A	550	NDP	PN-O1N	3.96	1.64	1.50
3	A	550	NDP	PA-O1A	3.89	1.64	1.50
3	B	550	NDP	P2B-O1X	3.87	1.62	1.50
3	B	550	NDP	C7N-C3N	3.70	1.56	1.48
3	A	550	NDP	P2B-O1X	3.59	1.61	1.50
3	A	550	NDP	C4N-C5N	-3.41	1.40	1.49
3	B	550	NDP	C4N-C5N	-3.30	1.40	1.49
3	A	550	NDP	C5A-N7A	-3.13	1.33	1.39
2	B	500	FAD	C2A-N3A	3.11	1.39	1.33
3	B	550	NDP	C5A-N7A	-3.03	1.33	1.39
2	A	500	FAD	C4X-N5	3.01	1.37	1.30
2	B	500	FAD	C4X-N5	3.00	1.37	1.30
2	B	500	FAD	C10-N1	2.81	1.38	1.33
2	A	500	FAD	C10-N1	2.80	1.38	1.33
3	A	550	NDP	C7N-C3N	2.77	1.54	1.48
3	B	550	NDP	O4D-C1D	2.75	1.48	1.42
5	B	650	TS8	O6-CAW	2.66	1.46	1.33
3	B	550	NDP	C4N-C3N	2.62	1.55	1.50
5	A	650	TS8	O6-CAW	2.59	1.45	1.33
2	A	500	FAD	C2A-N3A	2.55	1.38	1.33
3	A	550	NDP	O4D-C1D	2.54	1.47	1.42
2	A	500	FAD	C2A-N1A	2.46	1.38	1.33
3	A	550	NDP	C4N-C3N	2.44	1.54	1.50
2	B	500	FAD	C8A-N7A	2.42	1.36	1.31
3	A	550	NDP	O4B-C1B	2.27	1.47	1.42
3	A	550	NDP	C6N-C5N	2.26	1.40	1.33
3	B	550	NDP	C6N-C5N	2.19	1.39	1.33
2	A	500	FAD	C8A-N7A	2.18	1.35	1.31
3	B	550	NDP	C8A-N9A	-2.15	1.33	1.37
3	B	550	NDP	P2B-O2X	2.14	1.62	1.54
3	A	550	NDP	P2B-O2X	2.10	1.62	1.54
3	A	550	NDP	C8A-N9A	-2.09	1.34	1.37
2	B	500	FAD	C2A-N1A	2.07	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	550	NDP	O4B-C1B	2.02	1.46	1.42

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	FAD	N3A-C2A-N1A	-5.88	119.68	128.58
2	B	500	FAD	N3A-C2A-N1A	-5.84	119.74	128.58
3	A	550	NDP	C5A-C4A-N3A	-5.62	118.98	126.72
3	B	550	NDP	C5A-C4A-N3A	-5.44	119.23	126.72
5	B	650	TS8	O3-CAG-CAZ	5.31	120.57	111.09
5	A	650	TS8	O3-CAG-CAZ	4.99	119.99	111.09
5	A	650	TS8	O4-CAX-CAE	4.90	119.82	111.09
2	B	500	FAD	C5A-C4A-N3A	-4.72	120.22	126.72
3	A	550	NDP	N3A-C2A-N1A	-4.69	121.49	128.58
3	B	550	NDP	N3A-C2A-N1A	-4.65	121.54	128.58
2	A	500	FAD	C5A-C4A-N3A	-4.53	120.48	126.72
2	B	500	FAD	N9A-C8A-N7A	-4.24	107.92	113.94
2	A	500	FAD	N9A-C8A-N7A	-4.13	108.07	113.94
5	B	650	TS8	O2-CAY-CAF	4.09	118.39	111.09
5	B	650	TS8	O4-CAX-CAE	4.05	118.31	111.09
3	A	550	NDP	N3A-C4A-N9A	3.92	133.83	127.17
3	B	550	NDP	N3A-C4A-N9A	3.90	133.79	127.17
2	B	500	FAD	C5A-N7A-C8A	3.87	109.53	103.45
3	A	550	NDP	C2A-N3A-C4A	3.71	120.89	111.83
2	A	500	FAD	C5A-N7A-C8A	3.70	109.26	103.45
3	B	550	NDP	O4D-C1D-N1N	3.67	115.09	108.08
3	B	550	NDP	C2A-N3A-C4A	3.62	120.67	111.83
2	B	500	FAD	C2A-N3A-C4A	3.54	120.48	111.83
2	A	500	FAD	C4-N3-C2	-3.49	119.44	125.64
5	B	650	TS8	C1-O5-C5	3.49	118.80	112.55
3	A	550	NDP	O4D-C1D-N1N	3.48	114.72	108.08
5	A	650	TS8	O2-CAY-CAF	3.46	117.26	111.09
2	B	500	FAD	C4-N3-C2	-3.42	119.57	125.64
3	B	550	NDP	C2B-C1B-N9A	-3.41	108.14	113.75
2	A	500	FAD	C2A-N3A-C4A	3.40	120.14	111.83
3	B	550	NDP	N9A-C8A-N7A	-3.30	109.26	113.94
3	A	550	NDP	N9A-C8A-N7A	-3.29	109.27	113.94
3	A	550	NDP	C5A-N7A-C8A	3.12	108.35	103.45
2	A	500	FAD	C4X-C4-N3	3.04	121.00	113.25
3	B	550	NDP	C5A-N7A-C8A	3.03	108.21	103.45
2	B	500	FAD	N3A-C4A-N9A	2.97	132.23	127.17
2	B	500	FAD	C4X-C4-N3	2.94	120.74	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	550	NDP	C4A-C5A-N7A	-2.93	107.23	110.58
2	B	500	FAD	C4A-C5A-N7A	-2.91	107.25	110.58
3	B	550	NDP	C4A-C5A-N7A	-2.87	107.30	110.58
2	A	500	FAD	N3A-C4A-N9A	2.84	132.00	127.17
2	A	500	FAD	O4-C4-C4X	-2.82	119.08	126.53
3	B	550	NDP	C2D-C1D-N1N	-2.78	106.47	113.31
5	A	650	TS8	O5-C5-C6	2.76	112.16	106.69
2	A	500	FAD	O4B-C1B-N9A	2.75	113.36	108.09
2	B	500	FAD	O4B-C1B-N9A	2.73	113.33	108.09
2	A	500	FAD	C4A-C5A-N7A	-2.71	107.48	110.58
5	A	650	TS8	O2-C2-C3	2.60	113.42	108.25
5	A	650	TS8	C4-O4-CAX	-2.59	113.69	117.72
2	A	500	FAD	C9A-C5X-N5	-2.58	119.71	122.45
2	B	500	FAD	C9A-C5X-N5	-2.50	119.80	122.45
2	A	500	FAD	C5A-C6A-N6A	-2.48	117.15	123.29
2	B	500	FAD	O4-C4-C4X	-2.45	120.07	126.53
3	A	550	NDP	C2B-C1B-N9A	-2.41	109.78	113.75
5	A	650	TS8	O4-CAX-OAI	-2.40	118.36	122.99
2	B	500	FAD	C4X-C10-N1	-2.40	118.71	124.59
3	B	550	NDP	C4A-N9A-C8A	2.40	108.26	105.74
5	B	650	TS8	O3-CAG-OAK	-2.40	118.36	122.99
2	B	500	FAD	C10-C4X-N5	-2.36	120.00	124.81
5	B	650	TS8	O2-C2-C3	2.33	112.88	108.25
5	B	650	TS8	C4-O4-CAX	-2.33	114.10	117.72
5	B	650	TS8	O4-CAX-OAI	-2.32	118.51	122.99
2	A	500	FAD	C4X-C10-N1	-2.32	118.91	124.59
2	B	500	FAD	C5A-C6A-N6A	-2.31	117.56	123.29
5	A	650	TS8	C1-O5-C5	2.29	116.65	112.55
3	B	550	NDP	C5B-C4B-C3B	-2.27	107.05	115.21
3	A	550	NDP	C2D-C1D-N1N	-2.26	107.75	113.31
5	A	650	TS8	O6-C6-C5	2.25	113.16	108.41
2	A	500	FAD	C6A-C5A-C4A	2.25	120.24	117.18
3	A	550	NDP	O2A-PA-O3	2.20	113.22	107.27
3	A	550	NDP	C4A-N9A-C8A	2.12	107.97	105.74
5	A	650	TS8	O3-CAG-OAK	-2.10	118.93	122.99
2	B	500	FAD	C6A-C5A-C4A	2.07	120.00	117.18
2	A	500	FAD	C10-C4X-N5	-2.06	120.59	124.81
3	B	550	NDP	O3-PN-O1N	-2.06	104.52	110.70
5	B	650	TS8	C6-O6-CAW	2.05	122.13	117.08
3	B	550	NDP	O2B-P2B-O1X	-2.04	102.06	109.33
3	B	550	NDP	O3X-P2B-O2B	2.00	113.66	105.85

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	FAD	C5'-O5'-P-O1P
2	A	500	FAD	C5'-O5'-P-O2P
2	A	500	FAD	C5'-O5'-P-O3P
2	B	500	FAD	C5'-O5'-P-O1P
2	B	500	FAD	C5'-O5'-P-O3P
3	A	550	NDP	C5D-O5D-PN-O3
3	A	550	NDP	O4D-C1D-N1N-C2N
3	B	550	NDP	C5B-O5B-PA-O1A
3	B	550	NDP	C5B-O5B-PA-O2A
3	B	550	NDP	C5D-O5D-PN-O1N
5	A	650	TS8	C1-C2-O2-CAY
5	A	650	TS8	CAZ-CAG-O3-C3
5	B	650	TS8	C1-C2-O2-CAY
5	B	650	TS8	CAZ-CAG-O3-C3
5	B	650	TS8	CAE-CAX-O4-C4
5	A	650	TS8	OAK-CAG-O3-C3
5	A	650	TS8	CAE-CAX-O4-C4
5	B	650	TS8	OAK-CAG-O3-C3
5	B	650	TS8	OAI-CAX-O4-C4
5	A	650	TS8	CAD-CAW-O6-C6
5	A	650	TS8	OAI-CAX-O4-C4
5	A	650	TS8	OAH-CAW-O6-C6
3	B	550	NDP	O4D-C1D-N1N-C2N
2	A	500	FAD	C2'-C3'-C4'-O4'
5	B	650	TS8	OAH-CAW-O6-C6
5	B	650	TS8	CAD-CAW-O6-C6
5	B	650	TS8	CAF-CAY-O2-C2
2	A	500	FAD	O3'-C3'-C4'-C5'
2	A	500	FAD	C2'-C3'-C4'-C5'
5	B	650	TS8	C3-C2-O2-CAY
5	A	650	TS8	C3-C2-O2-CAY
2	A	500	FAD	O3'-C3'-C4'-O4'
5	B	650	TS8	OAJ-CAY-O2-C2
2	A	500	FAD	PA-O3P-P-O5'
2	B	500	FAD	PA-O3P-P-O5'
3	A	550	NDP	PA-O3-PN-O5D
3	B	550	NDP	PA-O3-PN-O5D
3	B	550	NDP	C2B-O2B-P2B-O1X
3	A	550	NDP	C3B-C2B-O2B-P2B
2	B	500	FAD	C5'-O5'-P-O2P
3	A	550	NDP	C5B-O5B-PA-O2A
3	A	550	NDP	C5D-O5D-PN-O1N

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Mol	Chain	Res	Type	Atoms
3	B	550	NDP	C5B-O5B-PA-O3
3	B	550	NDP	C5D-O5D-PN-O3
5	B	650	TS8	O5-C5-C6-O6
3	A	550	NDP	C1B-C2B-O2B-P2B
3	A	550	NDP	C2N-C3N-C7N-N7N
3	B	550	NDP	C2N-C3N-C7N-N7N
3	A	550	NDP	C2B-O2B-P2B-O1X
2	A	500	FAD	PA-O3P-P-O1P
2	B	500	FAD	O2'-C2'-C3'-O3'
2	A	500	FAD	O4B-C4B-C5B-O5B
2	B	500	FAD	C1'-C2'-C3'-O3'
3	A	550	NDP	O4B-C4B-C5B-O5B
2	B	500	FAD	PA-O3P-P-O1P
3	A	550	NDP	PA-O3-PN-O1N
3	B	550	NDP	PA-O3-PN-O1N
2	A	500	FAD	O2'-C2'-C3'-O3'
2	B	500	FAD	O2'-C2'-C3'-C4'
3	B	550	NDP	C2B-O2B-P2B-O2X
5	A	650	TS8	C3-C4-O4-CAX

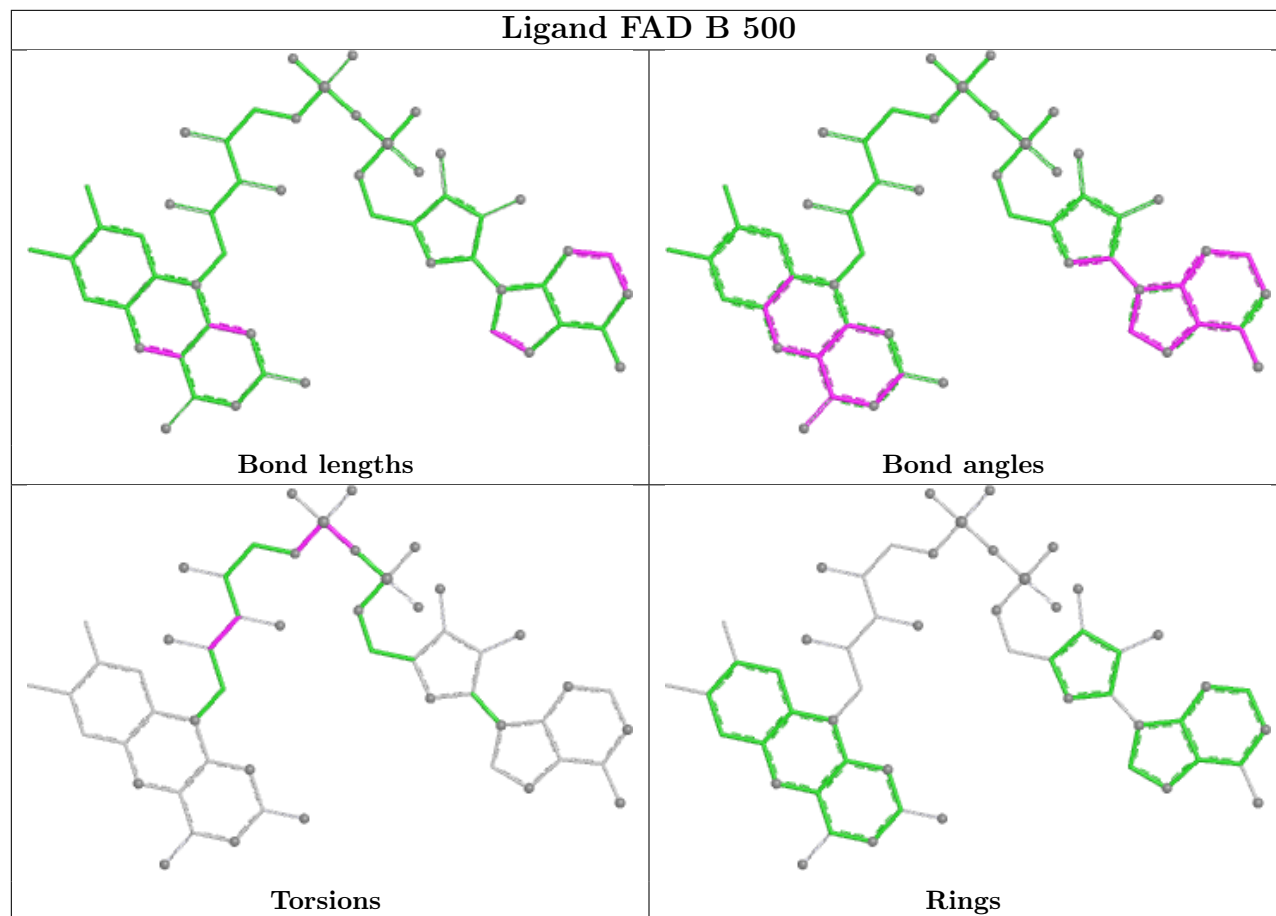
There are no ring outliers.

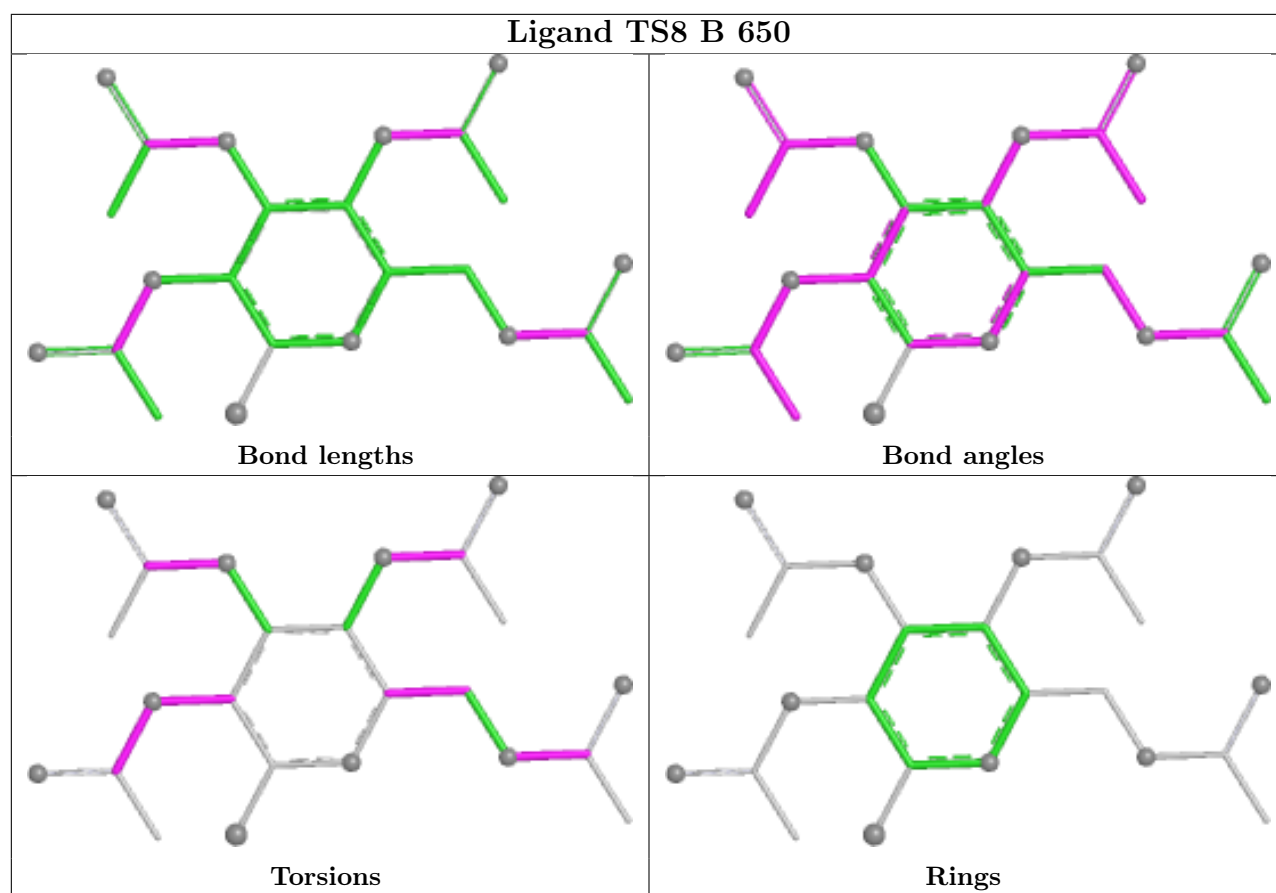
6 monomers are involved in 12 short contacts:

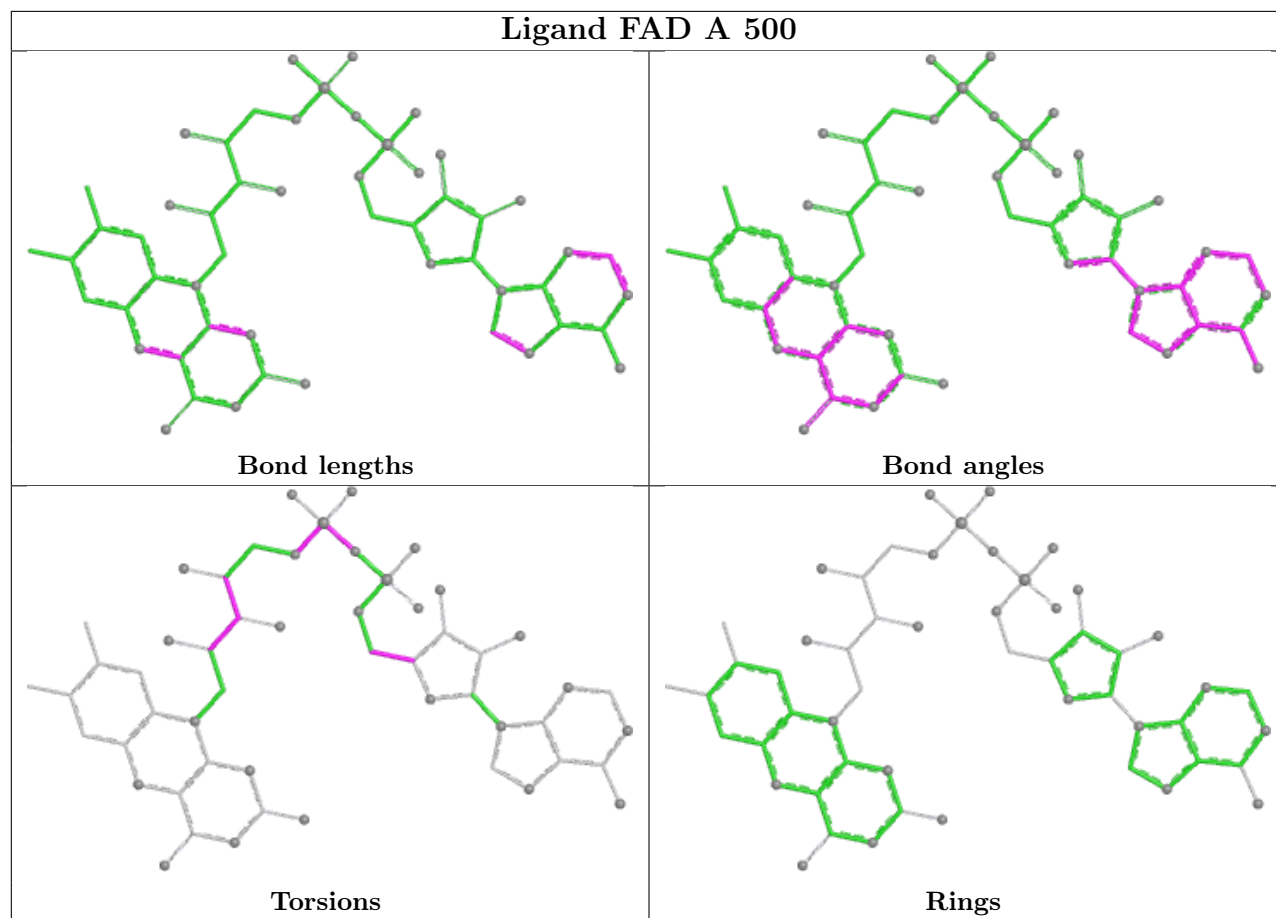
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	FAD	2	0
5	B	650	TS8	3	0
2	A	500	FAD	2	0
3	B	550	NDP	2	0
3	A	550	NDP	1	0
5	A	650	TS8	2	0

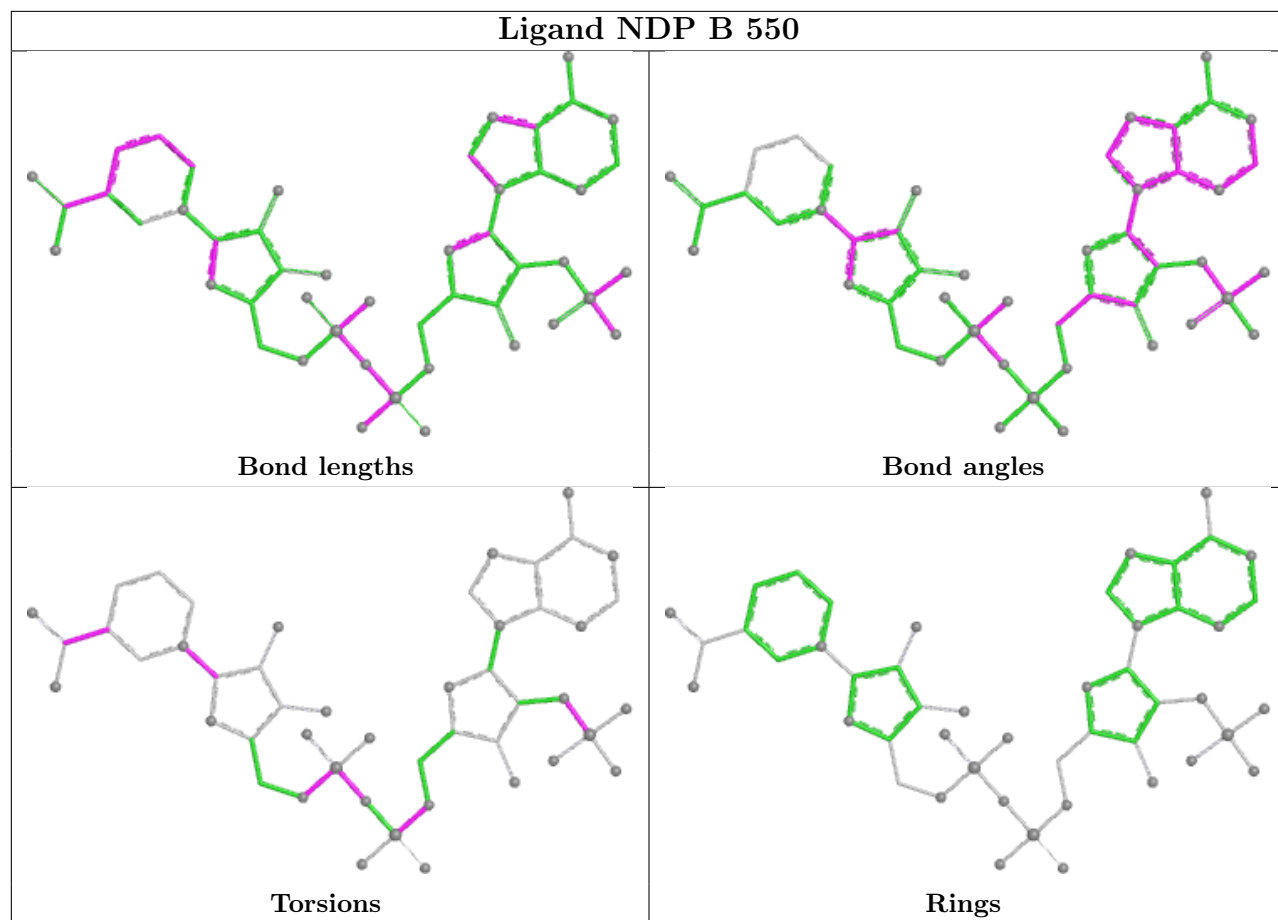
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

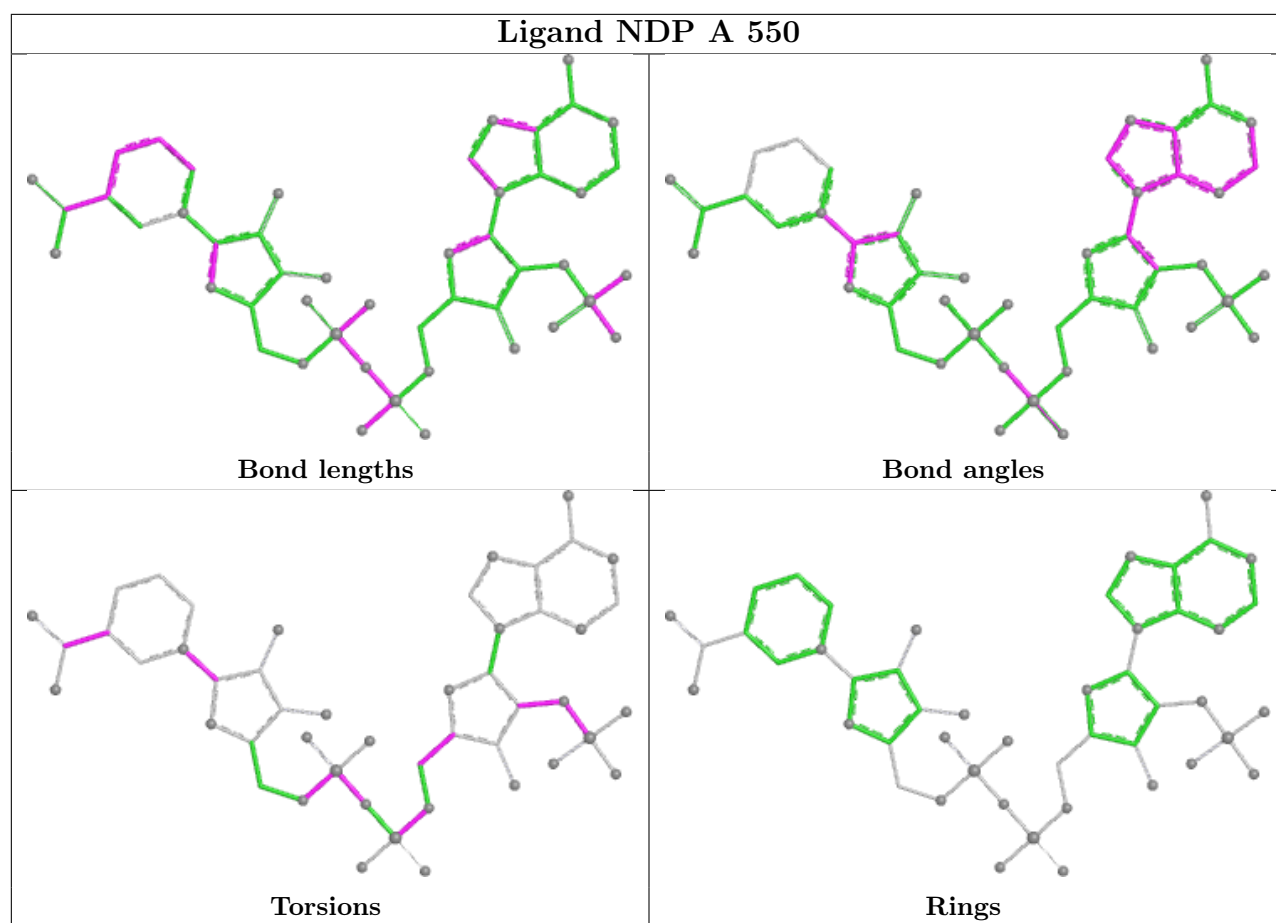
equivalents in the CSD to analyse the geometry.

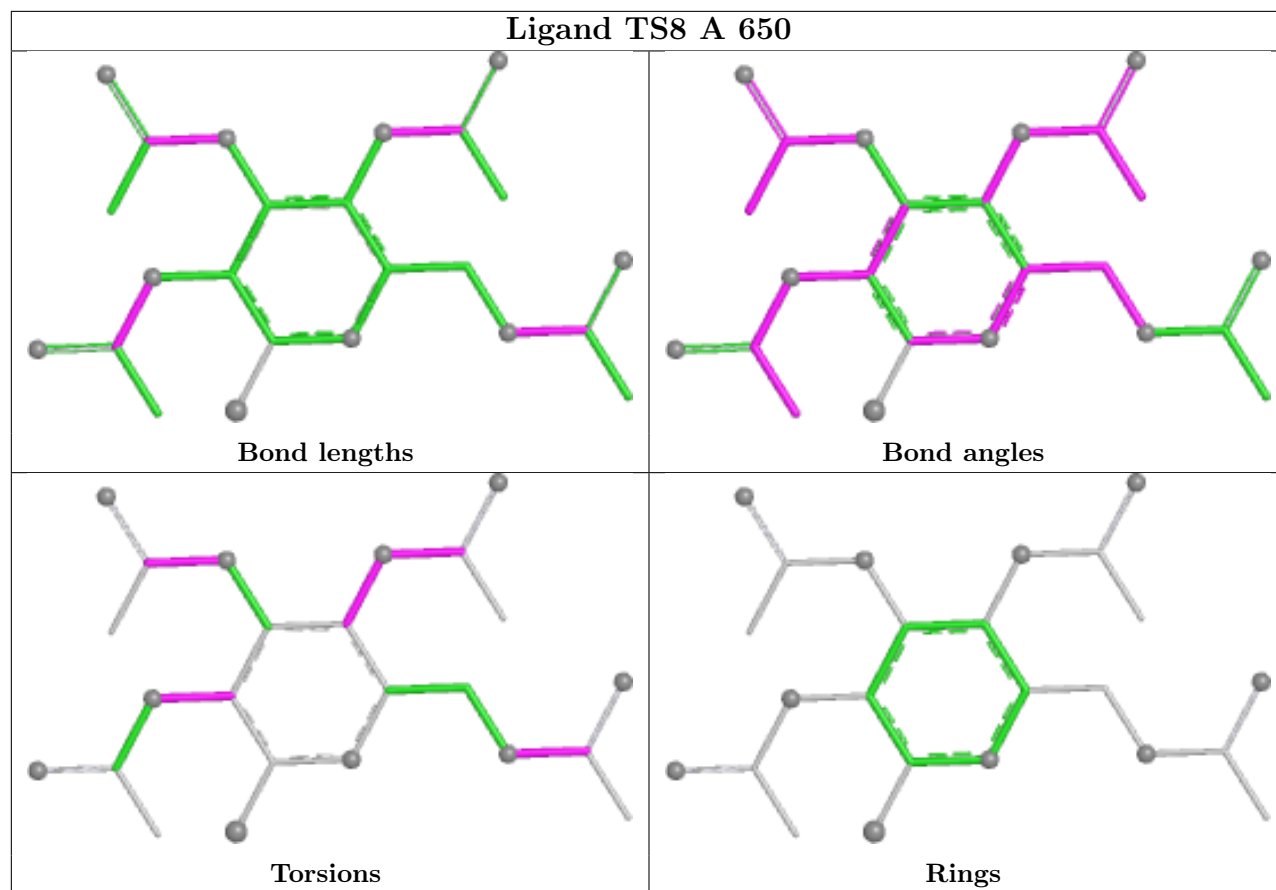












5.7 Other polymers [i](#)

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	488/511 (95%)	-0.55	0 100 100	63, 67, 69, 71	0
1	B	488/511 (95%)	-0.56	0 100 100	63, 67, 69, 71	0
All	All	976/1022 (95%)	-0.56	0 100 100	63, 67, 69, 71	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.

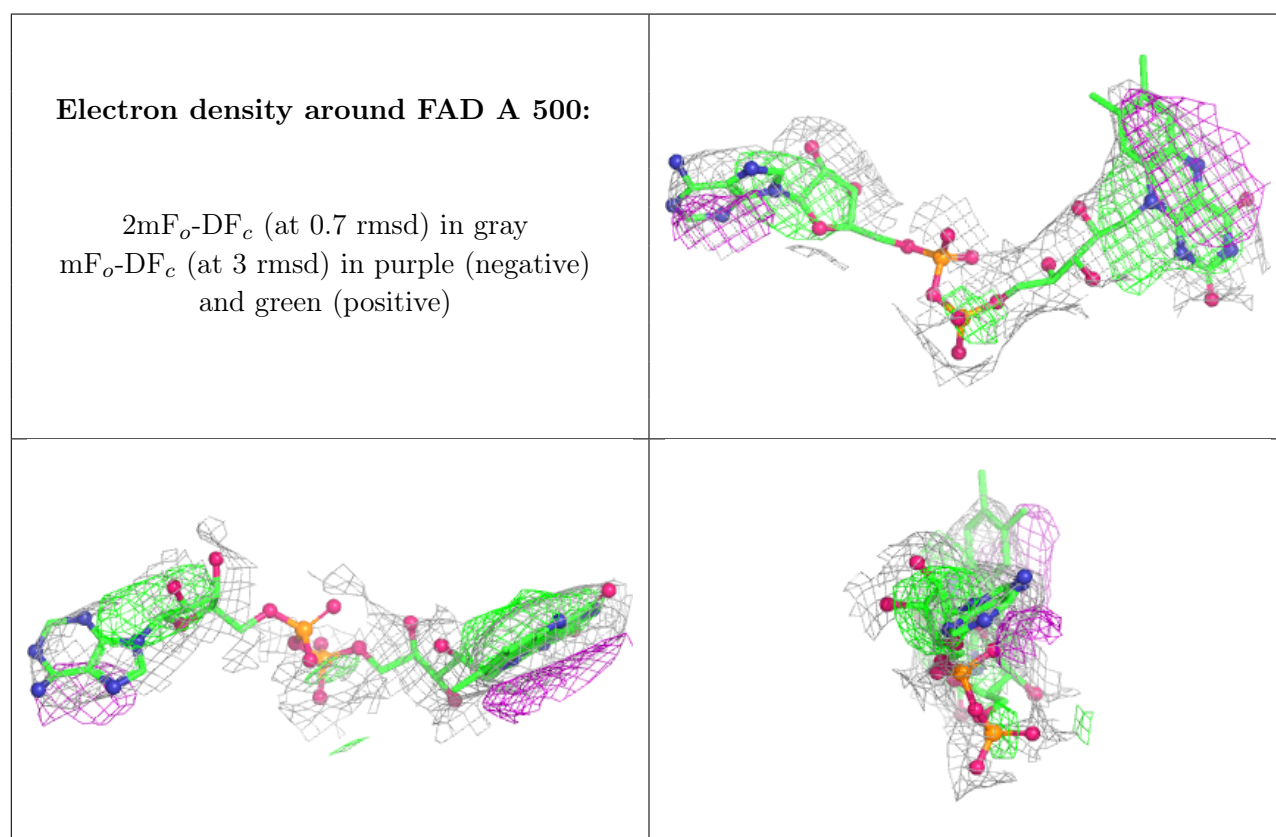
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FAD	A	500	53/53	0.97	0.11	87,90,91,92	0
2	FAD	B	500	53/53	0.97	0.12	86,89,92,92	0
3	NDP	A	550	48/48	0.97	0.09	60,60,60,60	0
3	NDP	B	550	48/48	0.97	0.09	60,60,60,60	0
5	TS8	A	650	24/24	0.97	0.11	73,76,77,78	24
7	SO4	B	1490	5/5	0.97	0.10	64,64,64,64	5
7	SO4	A	1490	5/5	0.98	0.12	59,59,59,60	5

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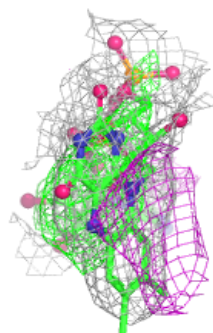
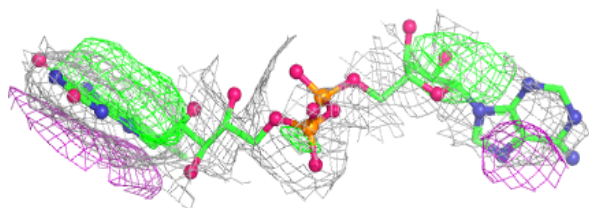
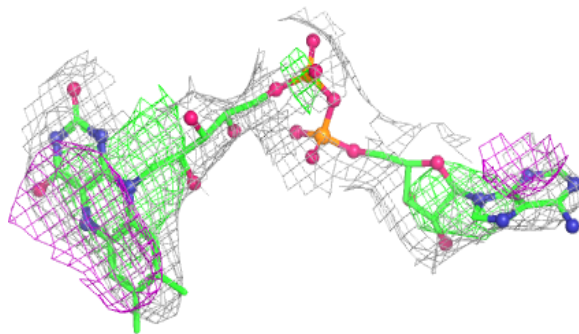
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	TS8	B	650	24/24	0.98	0.09	77,79,80,80	24
6	CL	A	1489	1/1	0.99	0.06	30,30,30,30	1
6	CL	B	1489	1/1	0.99	0.03	25,25,25,25	1
4	AU	A	600	1/1	1.00	0.02	78,78,78,78	1
4	AU	B	600	1/1	1.00	0.02	78,78,78,78	1

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.

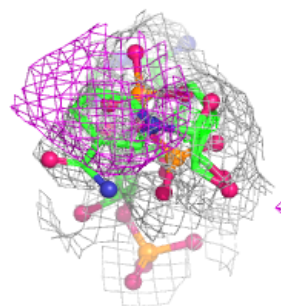
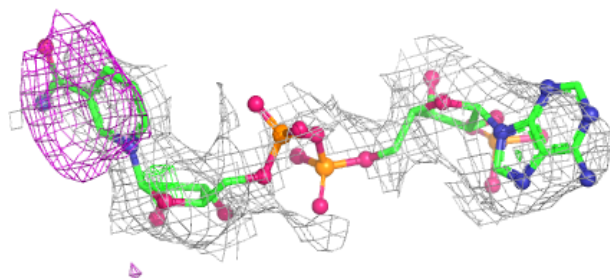
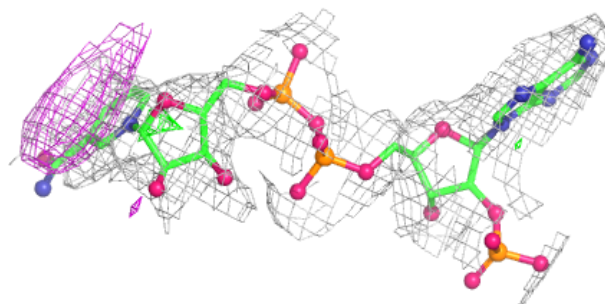


Electron density around FAD B 500:

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

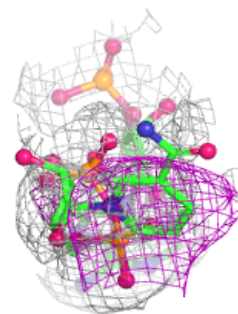
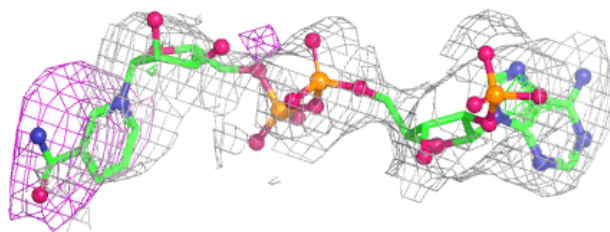
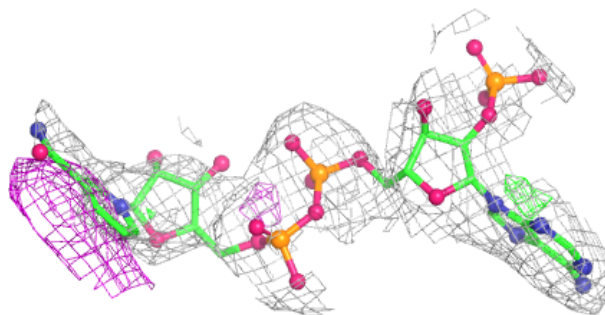
**Electron density around NDP A 550:**

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



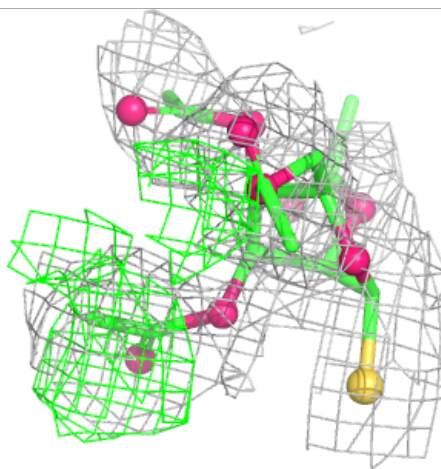
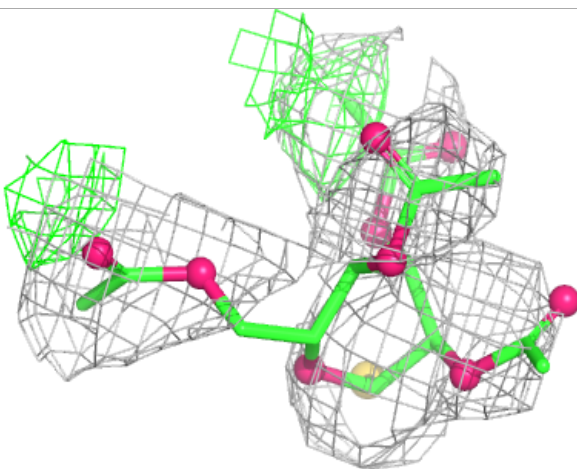
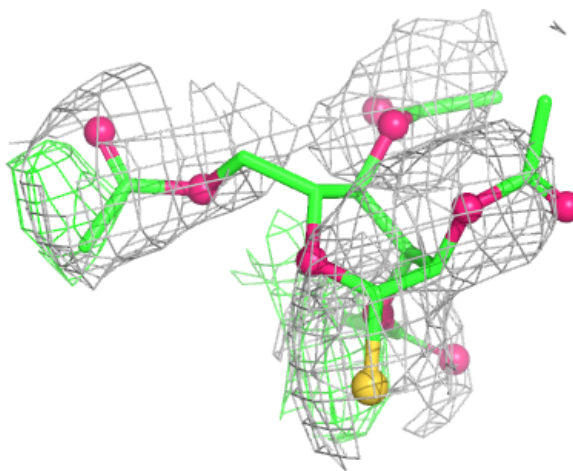
Electron density around NDP B 550:

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



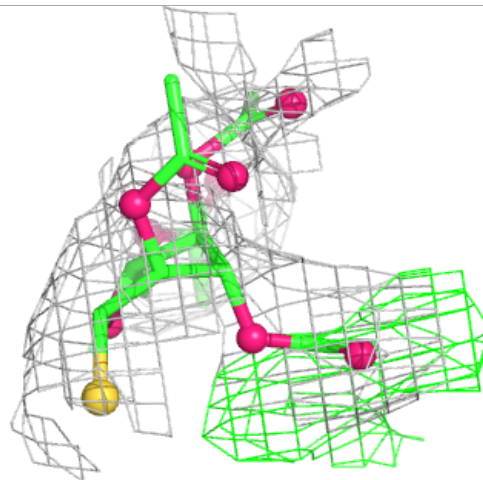
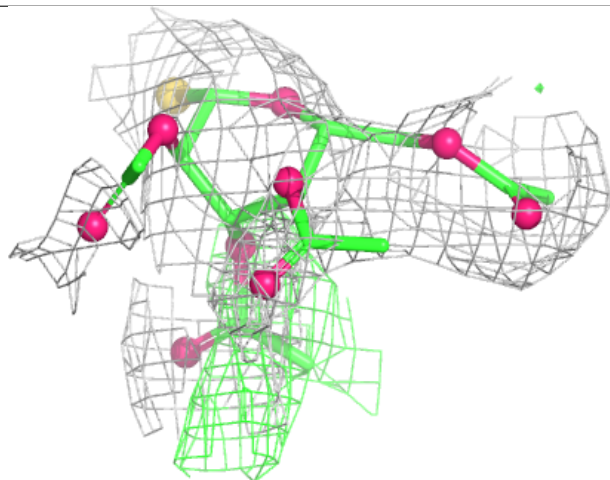
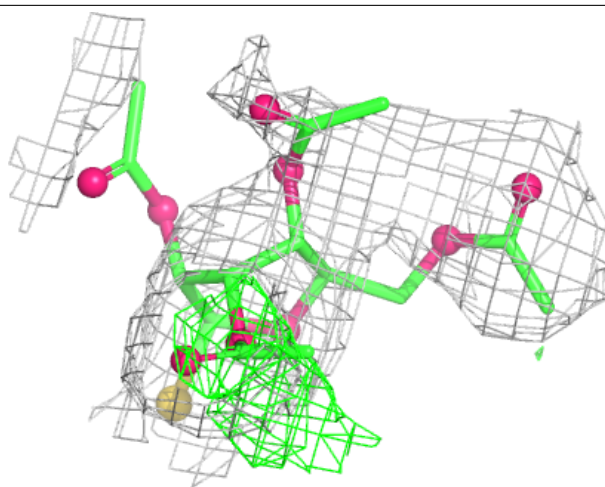
Electron density around TS8 A 650:

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



Electron density around TS8 B 650:

$2mF_o-DF_c$ (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.