



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:18 PM UTC

PDB ID : 3F4B / pdb_00003f4b
Title : Crystal structure of Plasmodium berghei Enoyl-acyl-carrier-protein reductase with TRICLOSAN
Authors : Sacchettini, J.C.; Tsai, H.-C.
Deposited on : 2008-10-31
Resolution : 2.49 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

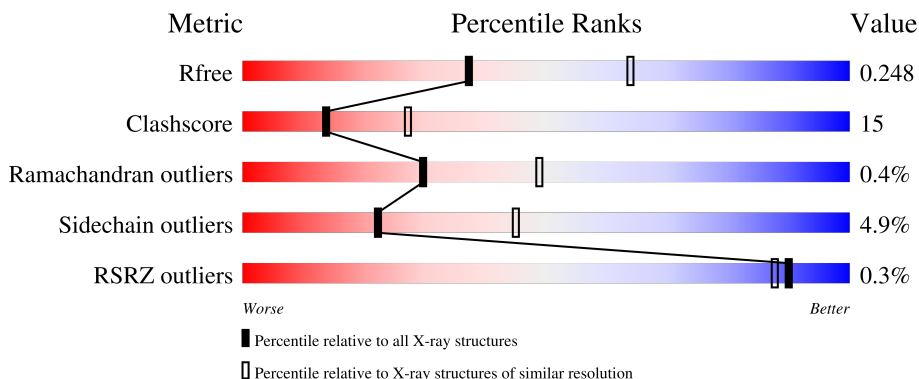
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	323	 67% 20% 12%
1	B	323	 59% 27% 11%
1	C	323	 58% 26% 13%
1	D	323	 62% 25% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9407 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 Enoyl-acyl carrier protein reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	0	0
			2208	1406	367	426	9			
1	B	289	Total	C	N	O	S	0	0	0
			2250	1430	374	437	9			
1	C	282	Total	C	N	O	S	0	0	0
			2191	1396	363	423	9			
1	D	289	Total	C	N	O	S	0	0	0
			2250	1430	374	437	9			

There are 4 discrepancies between the modelled and reference sequences:

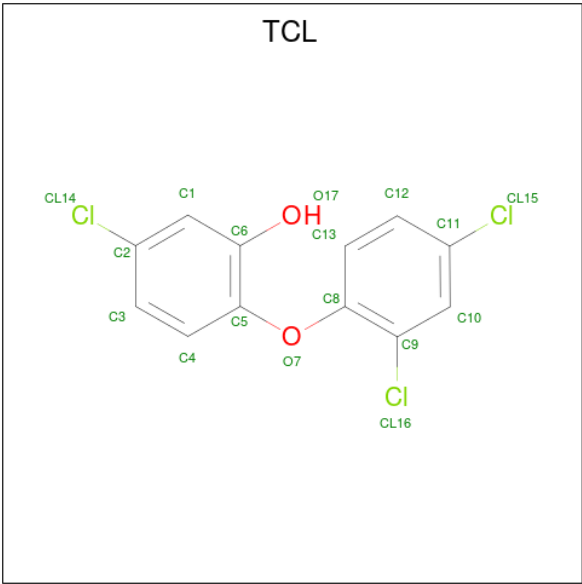
Chain	Residue	Modelled	Actual	Comment	Reference
A	74	MET	-	expression tag	UNP Q6TEI5
B	74	MET	-	expression tag	UNP Q6TEI5
C	74	MET	-	expression tag	UNP Q6TEI5
D	74	MET	-	expression tag	UNP Q6TEI5

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

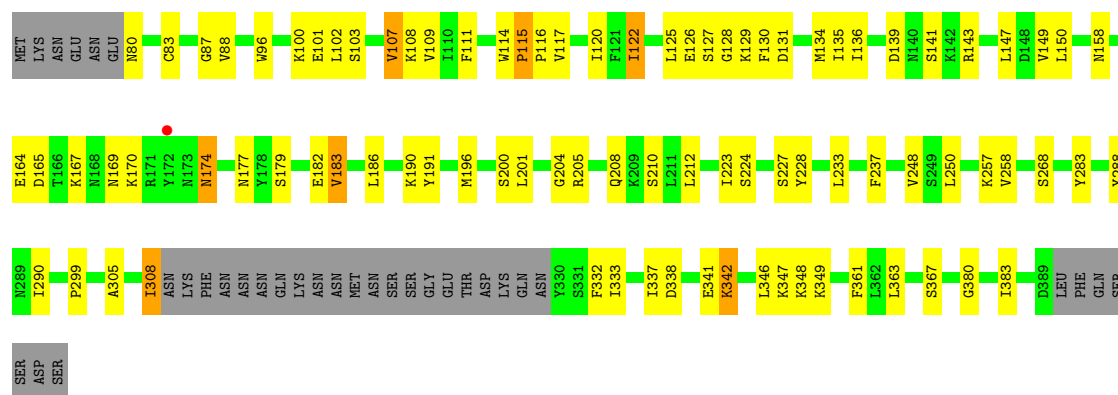
- Molecule 3 is TRICLOSAN (CCD ID: TCL) (formula: C₁₂H₇Cl₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	O	0	0
			17	12	3	2		
3	B	1	Total	C	Cl	O	0	0
			17	12	3	2		
3	C	1	Total	C	Cl	O	0	0
			17	12	3	2		
3	D	1	Total	C	Cl	O	0	0
			17	12	3	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	79	Total	O	0	0
			79	79		
4	B	54	Total	O	0	0
			54	54		
4	C	66	Total	O	0	0
			66	66		
4	D	65	Total	O	0	0
			65	65		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.34Å 121.20Å 87.83Å 90.00° 108.97° 90.00°	Depositor
Resolution (Å)	36.33 – 2.49 36.33 – 2.49	Depositor EDS
% Data completeness (in resolution range)	92.2 (36.33-2.49) 92.6 (36.33-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.48Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.183 , 0.254 (Not available) , 0.248	Depositor DCC
R_{free} test set	2075 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å ²)	60.7	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9407	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.50	0/2246	0.83	1/3026 (0.0%)
1	B	0.43	0/2290	0.81	1/3088 (0.0%)
1	C	0.48	0/2229	0.79	0/3004
1	D	0.46	0/2290	0.81	3/3088 (0.1%)
All	All	0.47	0/9055	0.81	5/12206 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	141	SER	N-CA-C	-6.59	104.71	112.89
1	A	118	TYR	N-CA-C	5.63	117.09	111.07
1	D	115	PRO	N-CA-C	5.45	117.35	110.70
1	B	143	ARG	N-CA-C	5.30	117.36	110.53
1	D	109	VAL	N-CA-C	5.27	115.55	108.17

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2208	0	2210	53	0
1	B	2250	0	2241	76	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2191	0	2191	86	0
1	D	2250	0	2241	65	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	1	0
2	D	44	0	26	1	0
3	A	17	0	6	1	0
3	B	17	0	6	2	0
3	C	17	0	7	0	0
3	D	17	0	6	1	0
4	A	79	0	0	9	0
4	B	54	0	0	3	0
4	C	66	0	0	8	0
4	D	65	0	0	9	0
All	All	9407	0	9012	264	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 15.

All (264) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:ARG:NH1	1:C:364:SER:HB3	1.71	1.04
1:D:88:VAL:HG11	1:D:111:PHE:CD1	2.07	0.90
1:C:105:ARG:HH12	1:C:364:SER:HB3	1.39	0.85
1:B:80:ASN:HD22	1:B:108:LYS:HE2	1.42	0.85
1:B:80:ASN:ND2	1:B:108:LYS:HE2	1.92	0.84
1:C:341:GLU:OE2	1:C:349:LYS:HG3	1.80	0.81
1:A:288:TYR:HB2	1:A:290:ILE:HG13	1.61	0.80
1:D:122:ILE:O	1:D:126:GLU:HG2	1.82	0.79
1:D:135:ILE:HG23	1:D:139:ASP:HA	1.66	0.78
1:A:303:ARG:HD3	4:A:58:HOH:O	1.83	0.78
1:C:88:VAL:HG21	1:C:111:PHE:CD1	2.18	0.77
1:C:196:MET:HG2	1:C:363:LEU:HB3	1.64	0.77
1:A:208:GLN:HG3	4:A:439:HOH:O	1.85	0.76
1:A:199:HIS:HD2	1:A:233:LEU:HD12	1.50	0.76
1:B:382:ASN:HD21	1:C:373:GLN:HE22	1.31	0.75
1:D:108:LYS:HE2	1:D:147:LEU:HD22	1.67	0.75
1:A:257:LYS:HE2	1:B:385:PHE:HA	1.70	0.74
1:C:385:PHE:HA	1:D:257:LYS:HE2	1.69	0.73
1:B:91:SER:HA	1:B:96:TRP:CG	2.23	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:ILE:O	1:C:126:GLU:HG2	1.89	0.73
1:C:102:LEU:HB3	1:C:107:VAL:CG1	2.18	0.73
1:A:179:SER:O	1:A:183:VAL:HG13	1.89	0.72
1:C:119:ASN:HA	4:C:445:HOH:O	1.89	0.71
1:D:182:GLU:HG3	4:D:423:HOH:O	1.90	0.70
1:A:127:SER:OG	1:A:129:LYS:HE2	1.92	0.70
1:B:237:PHE:O	1:B:241:MET:HG3	1.92	0.69
1:B:139:ASP:HA	1:B:141:SER:HA	1.73	0.69
1:B:190:LYS:HD3	1:B:191:TYR:CE2	2.28	0.69
1:C:102:LEU:O	1:C:107:VAL:HG12	1.92	0.69
1:D:190:LYS:HD3	1:D:191:TYR:CZ	2.27	0.69
1:C:94:TYR:O	1:C:98:ILE:HG13	1.93	0.68
1:A:80:ASN:ND2	1:A:108:LYS:HG3	2.08	0.68
1:B:197:LEU:HB3	1:B:247:VAL:HG22	1.73	0.68
1:B:170:LYS:HG2	1:B:171:ARG:NH1	2.08	0.67
1:A:163:ASP:OD1	1:A:166:THR:HG23	1.95	0.67
1:D:299:PRO:HB2	1:D:337:ILE:HG13	1.77	0.67
1:C:122:ILE:HB	4:C:445:HOH:O	1.95	0.66
1:A:122:ILE:O	1:A:126:GLU:HG2	1.97	0.65
1:D:341:GLU:O	1:D:347:LYS:HD3	1.97	0.65
1:A:254:ALA:HB2	1:A:259:VAL:HG21	1.79	0.65
1:C:202:ALA:HB1	1:C:266:MET:CE	2.26	0.64
1:D:150:LEU:HD13	1:D:186:LEU:HD22	1.78	0.64
1:C:105:ARG:NH1	1:C:364:SER:CB	2.57	0.64
1:A:248:VAL:HG22	1:A:363:LEU:HD21	1.79	0.64
1:C:108:LYS:HB3	1:C:147:LEU:HG	1.80	0.64
1:C:307:ALA:O	1:C:308:ILE:HG12	1.98	0.64
1:C:102:LEU:HD22	1:C:107:VAL:HG11	1.80	0.63
1:B:299:PRO:HB2	1:B:337:ILE:HG13	1.80	0.63
1:C:190:LYS:HD2	1:C:191:TYR:CE2	2.34	0.63
1:D:164:GLU:HA	1:D:167:LYS:HD2	1.81	0.63
1:C:380:GLY:O	1:C:383:ILE:HG12	1.98	0.63
1:D:83:CYS:HB2	1:D:196:MET:HB2	1.81	0.63
1:B:202:ALA:HB3	3:B:500:TCL:CL16	2.36	0.63
1:C:226:SER:OG	1:C:266:MET:HE1	1.99	0.62
1:B:209:LYS:O	1:B:263:GLY:HA3	1.99	0.62
1:C:131:ASP:O	1:C:135:ILE:HG23	1.99	0.61
1:C:163:ASP:O	1:C:167:LYS:HG3	2.00	0.61
1:A:259:VAL:HG23	1:A:259:VAL:O	2.00	0.61
1:B:220:LEU:HD11	1:D:224:SER:HB2	1.81	0.61
1:D:174:ASN:OD1	1:D:174:ASN:N	2.32	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:LYS:HD2	1:A:147:LEU:HD13	1.81	0.61
1:B:89:GLY:O	1:B:90:ASP:HB3	2.00	0.60
1:D:338:ASP:O	1:D:342:LYS:HB2	2.02	0.60
1:A:205:ARG:HG3	4:A:414:HOH:O	2.01	0.60
1:C:202:ALA:HB1	1:C:266:MET:HE1	1.83	0.60
1:B:131:ASP:CG	1:B:143:ARG:HH12	2.09	0.60
1:A:196:MET:HG2	1:A:363:LEU:HB3	1.83	0.60
1:B:109:VAL:HG11	1:B:111:PHE:HE1	1.66	0.60
1:D:101:GLU:HB3	4:D:404:HOH:O	2.01	0.59
1:B:111:PHE:HB2	1:B:149:VAL:HG22	1.84	0.59
1:C:180:ILE:HD13	1:C:232:SER:HB3	1.84	0.59
1:B:91:SER:HA	1:B:96:TRP:CB	2.32	0.58
1:B:109:VAL:CG1	1:B:111:PHE:HE1	2.16	0.58
1:D:127:SER:OG	1:D:129:LYS:HG2	2.03	0.58
1:A:205:ARG:NH2	1:A:217:ASP:OD2	2.35	0.57
1:C:102:LEU:HB3	1:C:107:VAL:HG11	1.86	0.57
1:D:177:ASN:HA	1:D:182:GLU:OE1	2.05	0.57
1:D:196:MET:HG2	1:D:363:LEU:HB3	1.86	0.57
1:B:179:SER:HB2	1:B:182:GLU:OE1	2.04	0.56
1:A:238:CYS:HB2	4:A:55:HOH:O	2.05	0.56
1:C:301:LYS:HG3	1:C:301:LYS:O	2.05	0.56
1:D:88:VAL:HG11	1:D:111:PHE:CG	2.39	0.56
1:D:125:LEU:CD1	1:D:134:MET:HE1	2.35	0.56
1:A:130:PHE:O	1:A:134:MET:HG3	2.06	0.56
1:C:105:ARG:HH11	1:C:364:SER:HB3	1.68	0.56
1:C:115:PRO:HB2	1:C:116:PRO:HD3	1.87	0.56
1:B:186:LEU:C	1:B:186:LEU:HD23	2.31	0.56
1:C:265:GLY:O	1:C:268:SER:HB3	2.05	0.56
1:B:181:GLU:HB2	1:B:236:HIS:CE1	2.41	0.56
1:C:108:LYS:HE3	4:C:427:HOH:O	2.06	0.56
1:D:149:VAL:O	1:D:150:LEU:HD23	2.05	0.55
1:D:102:LEU:O	1:D:107:VAL:HG13	2.06	0.55
1:A:142:LYS:HA	4:A:446:HOH:O	2.06	0.54
1:D:342:LYS:O	1:D:347:LYS:HE3	2.08	0.54
1:A:80:ASN:HD21	1:A:108:LYS:HG3	1.71	0.54
1:A:211:LEU:HD22	1:C:231:ILE:HD13	1.89	0.53
1:D:179:SER:HB2	4:D:423:HOH:O	2.08	0.53
1:C:305:ALA:O	1:C:308:ILE:HG13	2.09	0.53
1:C:105:ARG:NH2	1:C:196:MET:SD	2.81	0.53
1:D:258:VAL:HA	4:D:429:HOH:O	2.09	0.53
1:A:288:TYR:CB	1:A:290:ILE:HG13	2.38	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:ASN:CG	4:A:429:HOH:O	2.52	0.52
1:C:237:PHE:O	1:C:241:MET:HG3	2.09	0.52
1:B:94:TYR:O	1:B:98:ILE:HG13	2.08	0.52
1:A:163:ASP:CG	1:A:166:THR:HG23	2.35	0.52
1:C:88:VAL:HG12	4:C:426:HOH:O	2.10	0.52
1:A:162:ILE:HG22	1:A:167:LYS:HG3	1.92	0.51
1:A:257:LYS:HE3	1:B:257:LYS:HZ3	1.75	0.51
1:C:193:LYS:HD3	4:C:421:HOH:O	2.09	0.51
1:D:204:GLY:N	3:D:500:TCL:CL15	2.80	0.51
1:B:190:LYS:HD3	1:B:191:TYR:CZ	2.45	0.51
1:C:132:LYS:O	1:C:135:ILE:HG12	2.11	0.51
1:B:205:ARG:HD3	4:B:430:HOH:O	2.10	0.51
1:C:125:LEU:HD13	1:C:130:PHE:HD2	1.74	0.51
1:D:257:LYS:HD2	4:D:435:HOH:O	2.10	0.51
1:B:205:ARG:CD	4:B:430:HOH:O	2.59	0.51
1:B:210:SER:HB2	1:D:283:TYR:CZ	2.46	0.50
1:C:98:ILE:HG12	1:C:356:GLY:HA2	1.94	0.50
1:B:104:LYS:HB3	1:B:136:ILE:HG21	1.94	0.50
1:B:156:PHE:CE1	1:B:162:ILE:HA	2.47	0.50
1:B:190:LYS:HG2	1:B:191:TYR:CD2	2.47	0.50
1:B:301:LYS:HE3	1:B:306:THR:OG1	2.12	0.50
1:C:348:LYS:HE3	4:C:430:HOH:O	2.12	0.50
1:D:158:ASN:HA	4:D:423:HOH:O	2.12	0.50
1:C:100:LYS:HD3	1:C:133:ASP:O	2.11	0.50
1:C:170:LYS:O	1:C:170:LYS:HG2	2.11	0.50
1:C:80:ASN:HB2	1:C:108:LYS:NZ	2.28	0.49
1:C:176:LYS:O	1:C:177:ASN:HB2	2.12	0.49
1:D:114:TRP:CD1	1:D:115:PRO:HD2	2.47	0.49
1:D:288:TYR:HB2	1:D:290:ILE:HG13	1.93	0.49
1:A:259:VAL:HG23	1:A:262:TYR:HB3	1.93	0.49
1:B:100:LYS:O	1:B:103:SER:HB2	2.11	0.49
1:D:80:ASN:HB3	1:D:108:LYS:NZ	2.27	0.49
1:D:305:ALA:HB1	1:D:333:ILE:HG12	1.94	0.49
1:D:130:PHE:O	1:D:134:MET:HG3	2.13	0.49
1:B:199:HIS:HD2	1:B:233:LEU:HD12	1.78	0.49
1:B:170:LYS:HG2	1:B:171:ARG:HH12	1.77	0.49
1:B:346:LEU:HD11	1:C:291:ARG:HG2	1.94	0.49
1:B:174:ASN:OD1	1:B:174:ASN:N	2.45	0.49
1:C:248:VAL:HA	1:C:293:ASN:O	2.13	0.49
1:C:147:LEU:HD13	1:C:191:TYR:CE1	2.48	0.48
1:B:115:PRO:HB2	1:B:116:PRO:HD3	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:LYS:HB3	1:C:123:LYS:HE2	1.65	0.48
1:B:87:GLY:HA3	1:B:200:SER:O	2.14	0.48
1:B:159:TYR:O	1:B:162:ILE:HG23	2.13	0.48
1:C:117:VAL:HA	1:C:120:ILE:HD12	1.95	0.48
1:C:80:ASN:HB2	1:C:108:LYS:HZ3	1.78	0.48
1:B:90:ASP:OD1	1:B:92:ASN:HB2	2.14	0.48
1:B:114:TRP:CE2	1:B:116:PRO:HG2	2.49	0.48
1:C:130:PHE:O	1:C:134:MET:HG3	2.14	0.48
1:D:341:GLU:OE2	1:D:349:LYS:HG3	2.13	0.48
1:A:257:LYS:CE	1:B:257:LYS:HZ3	2.27	0.47
1:D:341:GLU:HA	4:D:422:HOH:O	2.13	0.47
1:A:205:ARG:HH22	1:A:217:ASP:CG	2.23	0.47
1:C:135:ILE:HG22	1:C:143:ARG:HH11	1.79	0.47
1:B:205:ARG:HB2	4:B:430:HOH:O	2.14	0.47
1:A:131:ASP:HB3	1:A:143:ARG:HH12	1.80	0.47
1:C:118:TYR:CD2	1:C:175:LEU:HD22	2.50	0.47
1:C:186:LEU:C	1:C:186:LEU:HD23	2.40	0.47
1:C:123:LYS:O	1:C:126:GLU:HB2	2.15	0.47
1:C:170:LYS:HA	1:C:173:ASN:ND2	2.30	0.47
1:D:208:GLN:HE21	1:D:308:ILE:HA	1.80	0.47
1:B:109:VAL:CG1	1:B:111:PHE:CE1	2.96	0.46
1:D:170:LYS:HE2	1:D:170:LYS:HB3	1.73	0.46
1:A:382:ASN:OD1	4:A:429:HOH:O	2.20	0.46
1:D:201:LEU:C	1:D:201:LEU:HD12	2.39	0.46
1:A:203:ASN:O	1:A:222:ALA:HA	2.14	0.46
1:C:202:ALA:HB1	1:C:266:MET:HE2	1.96	0.46
1:B:152:LEU:HD23	1:B:178:TYR:O	2.15	0.46
1:C:342:LYS:HG2	1:C:343:TYR:CZ	2.50	0.46
1:D:179:SER:O	1:D:183:VAL:HG13	2.15	0.46
1:B:283:TYR:CZ	1:D:210:SER:HB2	2.51	0.46
1:B:368:SER:HB2	1:C:348:LYS:NZ	2.31	0.46
1:B:139:ASP:HB2	1:B:140:ASN:OD1	2.15	0.46
1:A:348:LYS:HG2	1:A:349:LYS:N	2.31	0.46
1:C:381:LEU:HD23	4:C:444:HOH:O	2.15	0.46
1:D:200:SER:O	2:D:550:NAD:H52N	2.16	0.46
1:A:206:GLU:HA	1:A:208:GLN:HE21	1.81	0.45
1:A:261:GLY:N	4:A:427:HOH:O	2.23	0.45
1:B:137:ASN:HA	1:B:138:ASN:C	2.40	0.45
1:D:115:PRO:HB2	1:D:116:PRO:HD3	1.97	0.45
1:C:307:ALA:C	1:C:308:ILE:HG12	2.41	0.45
1:C:81:GLU:HB3	1:C:196:MET:HE1	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:LEU:O	1:D:237:PHE:HB2	2.16	0.45
1:A:254:ALA:CB	1:A:259:VAL:CG2	2.94	0.45
1:B:162:ILE:HG13	1:B:166:THR:CG2	2.47	0.45
1:B:308:ILE:H	1:B:308:ILE:HG13	1.33	0.45
1:A:208:GLN:HG3	1:A:208:GLN:H	1.49	0.44
1:D:380:GLY:O	1:D:383:ILE:HG12	2.16	0.44
1:C:88:VAL:O	1:C:113:VAL:HG22	2.17	0.44
1:A:210:SER:HB2	1:C:283:TYR:CZ	2.52	0.44
1:A:260:PRO:HA	4:A:427:HOH:O	2.17	0.44
1:B:164:GLU:OE1	1:B:167:LYS:HD2	2.18	0.44
1:B:132:LYS:HG3	1:B:133:ASP:OD1	2.17	0.44
1:B:248:VAL:HA	1:B:293:ASN:O	2.18	0.44
1:B:83:CYS:HB2	1:B:196:MET:HB2	2.00	0.44
1:B:130:PHE:O	1:B:134:MET:HG3	2.18	0.43
1:D:87:GLY:HA3	1:D:201:LEU:HB3	2.00	0.43
1:A:202:ALA:HB3	3:A:400:TCL:CL16	2.55	0.43
1:B:331:SER:OG	1:B:334:ASP:CG	2.61	0.43
1:C:205:ARG:NH2	1:C:217:ASP:OD2	2.50	0.43
1:D:136:ILE:HD11	1:D:143:ARG:C	2.43	0.43
1:D:288:TYR:CB	1:D:290:ILE:HG13	2.48	0.43
1:C:81:GLU:HB3	1:C:196:MET:CE	2.48	0.43
1:C:103:SER:OG	1:C:144:MET:HG3	2.18	0.43
1:A:119:ASN:O	1:A:123:LYS:HG3	2.18	0.43
1:D:117:VAL:HA	1:D:120:ILE:HD12	2.01	0.43
1:D:204:GLY:HA2	4:D:426:HOH:O	2.19	0.43
1:B:142:LYS:O	1:B:142:LYS:HG3	2.19	0.43
1:D:128:GLY:HA2	1:D:131:ASP:OD1	2.18	0.43
1:A:85:ILE:HG12	1:A:198:VAL:HB	1.99	0.43
1:A:88:VAL:HG22	1:A:95:GLY:HA3	2.01	0.43
1:B:366:GLU:O	1:C:357:SER:OG	2.37	0.43
1:D:83:CYS:HB2	1:D:196:MET:CB	2.48	0.43
1:C:107:VAL:O	1:C:107:VAL:HG13	2.17	0.43
1:C:345:PRO:HD2	1:C:379:ASN:O	2.19	0.43
1:D:96:TRP:O	1:D:100:LYS:HG3	2.19	0.43
1:B:275:SER:HA	1:B:278:ARG:NH2	2.33	0.42
1:C:253:GLN:HG2	1:C:253:GLN:O	2.20	0.42
1:A:177:ASN:O	1:A:183:VAL:HG12	2.19	0.42
1:C:193:LYS:HA	1:C:240:PHE:O	2.20	0.42
1:C:308:ILE:HB	1:C:332:PHE:HB3	2.01	0.42
1:B:172:TYR:C	1:B:174:ASN:H	2.27	0.42
1:C:102:LEU:C	1:C:107:VAL:HG12	2.44	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:450:NAD:O2N	2:C:450:NAD:N7N	2.48	0.42
1:C:257:LYS:CE	4:D:408:HOH:O	2.67	0.42
1:D:149:VAL:C	1:D:150:LEU:HD23	2.44	0.42
1:D:223:ILE:O	1:D:227:SER:HB2	2.20	0.42
1:B:196:MET:HG2	1:B:363:LEU:HB3	2.02	0.42
1:A:362:LEU:HD23	1:A:362:LEU:HA	1.88	0.42
1:B:382:ASN:ND2	1:C:373:GLN:HE22	2.07	0.42
1:A:257:LYS:NZ	1:B:257:LYS:NZ	2.67	0.42
1:B:86:ALA:O	1:B:112:GLY:O	2.37	0.42
1:B:216:ARG:HB2	1:D:228:TYR:CE2	2.55	0.42
1:C:239:LYS:HG2	4:C:67:HOH:O	2.20	0.42
1:A:200:SER:CB	1:A:250:LEU:HD23	2.50	0.41
1:B:88:VAL:O	1:B:113:VAL:HG22	2.20	0.41
1:B:171:ARG:HA	1:B:171:ARG:HD3	1.96	0.41
1:D:248:VAL:HG23	1:D:363:LEU:HD21	2.02	0.41
1:C:114:TRP:CG	1:C:116:PRO:HD2	2.55	0.41
1:D:361:PHE:CZ	1:D:367:SER:HB3	2.55	0.41
1:A:207:VAL:HA	1:A:263:GLY:C	2.45	0.41
1:C:205:ARG:HD3	1:C:221:ASP:OD2	2.20	0.41
1:D:169:ASN:OD1	1:D:170:LYS:N	2.52	0.41
1:D:248:VAL:HG23	1:D:363:LEU:CD2	2.50	0.41
1:A:101:GLU:HG3	1:A:357:SER:N	2.36	0.41
1:B:180:ILE:O	1:B:183:VAL:HG22	2.20	0.41
1:C:206:GLU:C	1:C:208:GLN:N	2.77	0.41
1:D:117:VAL:HG12	1:D:120:ILE:HD12	2.02	0.41
1:B:114:TRP:CG	1:B:116:PRO:HD2	2.56	0.41
1:B:253:GLN:OE1	1:B:257:LYS:HE3	2.21	0.41
1:C:170:LYS:HE3	1:C:171:ARG:HD2	2.03	0.41
1:C:233:LEU:HD23	1:C:233:LEU:HA	1.84	0.41
1:A:211:LEU:HD12	1:C:279:VAL:HB	2.03	0.41
1:A:303:ARG:HG3	1:A:304:ALA:N	2.36	0.40
1:B:301:LYS:O	1:B:301:LYS:HG3	2.21	0.40
1:C:114:TRP:CD1	1:C:116:PRO:HD2	2.56	0.40
1:D:100:LYS:O	1:D:103:SER:HB2	2.20	0.40
1:B:305:ALA:HB2	3:B:500:TCL:H41	2.03	0.40
1:A:332:PHE:CD1	1:A:332:PHE:C	2.99	0.40
1:B:139:ASP:HA	1:B:140:ASN:HA	1.64	0.40
1:C:115:PRO:C	1:C:117:VAL:H	2.28	0.40
1:D:103:SER:HB3	1:D:136:ILE:HD13	2.03	0.40
1:D:200:SER:HA	1:D:250:LEU:HD23	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	278/323 (86%)	266 (96%)	11 (4%)	1 (0%)	30	49
1	B	285/323 (88%)	270 (95%)	13 (5%)	2 (1%)	18	34
1	C	276/323 (85%)	258 (94%)	17 (6%)	1 (0%)	30	49
1	D	285/323 (88%)	266 (93%)	19 (7%)	0	100	100
All	All	1124/1292 (87%)	1060 (94%)	60 (5%)	4 (0%)	30	49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	90	ASP
1	A	90	ASP
1	C	173	ASN
1	B	86	ALA

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	242/280 (86%)	232 (96%)	10 (4%)	27	53
1	B	247/280 (88%)	236 (96%)	11 (4%)	24	49
1	C	240/280 (86%)	226 (94%)	14 (6%)	18	38
1	D	247/280 (88%)	234 (95%)	13 (5%)	20	42
All	All	976/1120 (87%)	928 (95%)	48 (5%)	22	45

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	ILE
1	A	166	THR
1	A	183	VAL
1	A	201	LEU
1	A	208	GLN
1	A	211	LEU
1	A	212	LEU
1	A	273	LEU
1	A	309	ASN
1	A	383	ILE
1	B	88	VAL
1	B	129	LYS
1	B	152	LEU
1	B	162	ILE
1	B	174	ASN
1	B	179	SER
1	B	227	SER
1	B	248	VAL
1	B	268	SER
1	B	308	ILE
1	B	337	ILE
1	C	88	VAL
1	C	119	ASN
1	C	122	ILE
1	C	147	LEU
1	C	148	ASP
1	C	175	LEU
1	C	183	VAL
1	C	205	ARG
1	C	208	GLN
1	C	217	ASP
1	C	223	ILE
1	C	248	VAL
1	C	306	THR
1	C	308	ILE
1	D	107	VAL
1	D	122	ILE
1	D	165	ASP
1	D	174	ASN
1	D	183	VAL
1	D	205	ARG
1	D	212	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	268	SER
1	D	308	ILE
1	D	332	PHE
1	D	342	LYS
1	D	346	LEU
1	D	348	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	208	GLN
1	A	242	ASN
1	A	373	GLN
1	B	177	ASN
1	B	236	HIS
1	B	253	GLN
1	B	373	GLN
1	B	382	ASN
1	C	119	ASN
1	C	174	ASN
1	C	242	ASN
1	C	253	GLN
1	C	373	GLN
1	C	382	ASN
1	D	208	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	B	550	-	46,48,48	0.92	4 (8%)	64,73,73	1.62	10 (15%)
2	NAD	C	450	-	46,48,48	0.93	3 (6%)	64,73,73	1.57	10 (15%)
3	TCL	A	400	-	18,18,18	1.07	1 (5%)	25,25,25	0.87	0
3	TCL	C	400	-	18,18,18	1.04	1 (5%)	25,25,25	0.82	0
2	NAD	A	450	-	46,48,48	0.89	3 (6%)	64,73,73	1.70	14 (21%)
3	TCL	D	500	-	18,18,18	1.11	2 (11%)	25,25,25	0.83	1 (4%)
2	NAD	D	550	-	46,48,48	0.92	4 (8%)	64,73,73	1.58	10 (15%)
3	TCL	B	500	-	18,18,18	1.18	2 (11%)	25,25,25	1.05	2 (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
2	NAD	B	550	-	-	9/30/62/62	0/5/5/5
2	NAD	C	450	-	-	7/30/62/62	0/5/5/5
3	TCL	A	400	-	-	0/4/4/4	0/2/2/2
3	TCL	C	400	-	-	0/4/4/4	0/2/2/2
2	NAD	A	450	-	-	5/30/62/62	0/5/5/5
3	TCL	D	500	-	-	0/4/4/4	0/2/2/2
2	NAD	D	550	-	-	8/30/62/62	0/5/5/5
3	TCL	B	500	-	-	0/4/4/4	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	500	TCL	C9-CL16	3.36	1.81	1.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	500	TCL	C9-CL16	3.03	1.80	1.73
2	B	550	NAD	O4D-C1D	2.89	1.44	1.40
2	D	550	NAD	PN-O3	2.44	1.62	1.59
2	C	450	NAD	O4D-C1D	2.40	1.44	1.40
2	B	550	NAD	PA-O3	2.39	1.62	1.59
2	D	550	NAD	C8A-N7A	2.39	1.36	1.31
3	A	400	TCL	C9-CL16	2.38	1.79	1.73
3	C	400	TCL	C9-CL16	2.38	1.79	1.73
2	A	450	NAD	O4D-C1D	2.33	1.43	1.40
2	B	550	NAD	C8A-N7A	2.29	1.36	1.31
2	C	450	NAD	C4A-N9A	-2.27	1.33	1.37
3	D	500	TCL	C11-CL15	2.27	1.79	1.74
2	A	450	NAD	PA-O3	2.23	1.61	1.59
3	B	500	TCL	C11-CL15	2.17	1.79	1.74
2	C	450	NAD	C5A-N7A	-2.06	1.35	1.39
2	A	450	NAD	C5A-N7A	-2.06	1.35	1.39
2	D	550	NAD	PA-O3	2.05	1.61	1.59
2	D	550	NAD	O4D-C1D	2.05	1.43	1.40
2	B	550	NAD	C5A-N7A	-2.01	1.35	1.39

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	550	NAD	C5A-C4A-N3A	-5.56	119.07	126.72
2	A	450	NAD	N3A-C2A-N1A	-5.39	120.42	128.58
2	A	450	NAD	C5A-C4A-N3A	-5.37	119.32	126.72
2	D	550	NAD	N3A-C2A-N1A	-4.94	121.10	128.58
2	B	550	NAD	N3A-C2A-N1A	-4.84	121.25	128.58
2	D	550	NAD	C5A-C4A-N3A	-4.78	120.14	126.72
2	C	450	NAD	N3A-C2A-N1A	-4.76	121.37	128.58
2	C	450	NAD	N9A-C8A-N7A	-4.33	107.79	113.94
2	C	450	NAD	C5A-C4A-N3A	-3.98	121.23	126.72
2	C	450	NAD	C4A-N9A-C8A	3.93	109.86	105.74
2	A	450	NAD	C2A-N3A-C4A	3.88	121.30	111.83
2	D	550	NAD	N9A-C8A-N7A	-3.73	108.64	113.94
2	B	550	NAD	C2A-N3A-C4A	3.57	120.55	111.83
2	B	550	NAD	N9A-C8A-N7A	-3.53	108.93	113.94
2	A	450	NAD	N9A-C8A-N7A	-3.49	108.98	113.94
2	B	550	NAD	N3A-C4A-N9A	3.42	132.98	127.17
2	D	550	NAD	C2A-N3A-C4A	3.36	120.05	111.83
2	A	450	NAD	N3A-C4A-N9A	3.25	132.69	127.17
2	D	550	NAD	N3A-C4A-N9A	3.08	132.41	127.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	550	NAD	C4A-C5A-N7A	-3.04	107.11	110.58
2	A	450	NAD	C4A-C5A-N7A	-3.02	107.13	110.58
2	D	550	NAD	C4A-N9A-C8A	2.99	108.88	105.74
2	D	550	NAD	O4B-C1B-N9A	2.92	113.70	108.09
2	B	550	NAD	O4B-C1B-N9A	2.90	113.66	108.09
2	C	450	NAD	C2A-N3A-C4A	2.89	118.89	111.83
2	C	450	NAD	C5A-N7A-C8A	2.88	107.97	103.45
2	D	550	NAD	C4A-C5A-N7A	-2.85	107.33	110.58
2	A	450	NAD	O4B-C1B-N9A	2.84	113.54	108.09
2	B	550	NAD	C5A-N7A-C8A	2.81	107.87	103.45
2	A	450	NAD	C5A-N7A-C8A	2.77	107.80	103.45
2	C	450	NAD	N3A-C4A-N9A	2.77	131.88	127.17
2	C	450	NAD	C4A-C5A-N7A	-2.71	107.49	110.58
2	D	550	NAD	C5A-N7A-C8A	2.70	107.69	103.45
3	D	500	TCL	O7-C5-C6	2.54	120.89	116.59
3	B	500	TCL	C8-C9-CL16	2.50	122.31	119.44
3	B	500	TCL	O7-C5-C6	2.33	120.54	116.59
2	B	550	NAD	C4A-N9A-C8A	2.28	108.14	105.74
2	A	450	NAD	C5N-C4N-C3N	-2.25	118.16	120.36
2	A	450	NAD	C4A-N9A-C8A	2.24	108.09	105.74
2	A	450	NAD	C3N-C7N-N7N	2.13	120.36	117.74
2	C	450	NAD	C5B-C4B-C3B	-2.11	107.62	115.21
2	D	550	NAD	O2N-PN-O1N	2.08	122.13	112.44
2	B	550	NAD	C5B-C4B-C3B	-2.07	107.76	115.21
2	A	450	NAD	C5B-C4B-C3B	-2.05	107.82	115.21
2	C	450	NAD	C4A-N9A-C1B	-2.03	121.89	126.63
2	A	450	NAD	O7N-C7N-C3N	-2.02	117.13	119.60
2	A	450	NAD	C5A-C4A-N9A	2.00	107.99	105.81

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	450	NAD	C5D-O5D-PN-O3
2	A	450	NAD	C5D-O5D-PN-O1N
2	A	450	NAD	C5D-O5D-PN-O2N
2	A	450	NAD	O4D-C1D-N1N-C2N
2	B	550	NAD	C5D-O5D-PN-O3
2	B	550	NAD	C5D-O5D-PN-O1N
2	B	550	NAD	C5D-O5D-PN-O2N
2	B	550	NAD	O4D-C1D-N1N-C2N
2	B	550	NAD	O4D-C1D-N1N-C6N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	450	NAD	C5D-O5D-PN-O3
2	C	450	NAD	C5D-O5D-PN-O1N
2	C	450	NAD	C5D-O5D-PN-O2N
2	C	450	NAD	O4D-C1D-N1N-C2N
2	D	550	NAD	C5D-O5D-PN-O3
2	D	550	NAD	C5D-O5D-PN-O1N
2	D	550	NAD	O4D-C1D-N1N-C2N
2	C	450	NAD	O4B-C4B-C5B-O5B
2	C	450	NAD	C3B-C4B-C5B-O5B
2	D	550	NAD	O4B-C4B-C5B-O5B
2	D	550	NAD	C3B-C4B-C5B-O5B
2	D	550	NAD	C5D-O5D-PN-O2N
2	B	550	NAD	C2D-C1D-N1N-C6N
2	A	450	NAD	O4D-C1D-N1N-C6N
2	C	450	NAD	O4D-C1D-N1N-C6N
2	D	550	NAD	O4D-C1D-N1N-C6N
2	B	550	NAD	C2B-C1B-N9A-C8A
2	B	550	NAD	PA-O3-PN-O1N
2	B	550	NAD	PA-O3-PN-O2N
2	D	550	NAD	PA-O3-PN-O2N

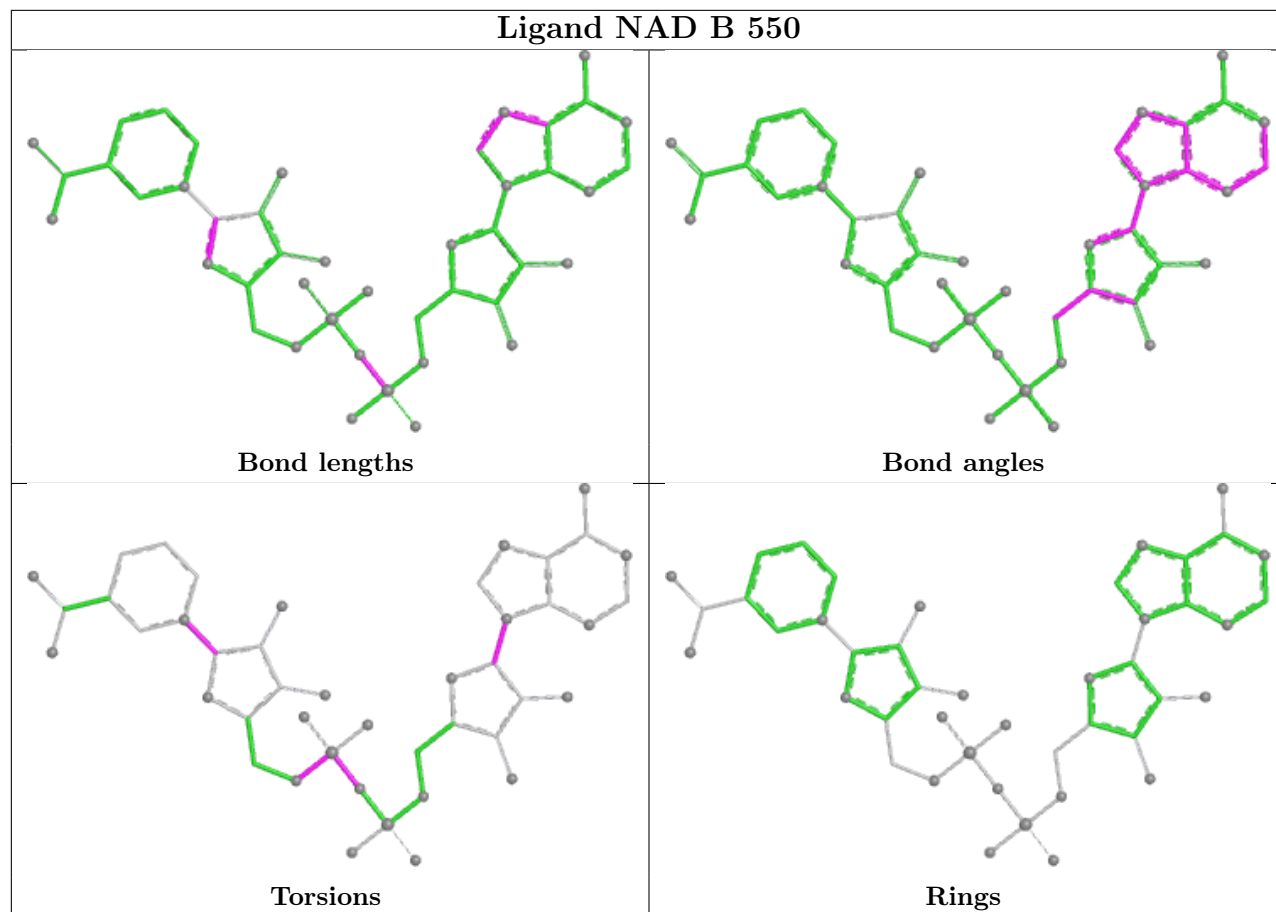
There are no ring outliers.

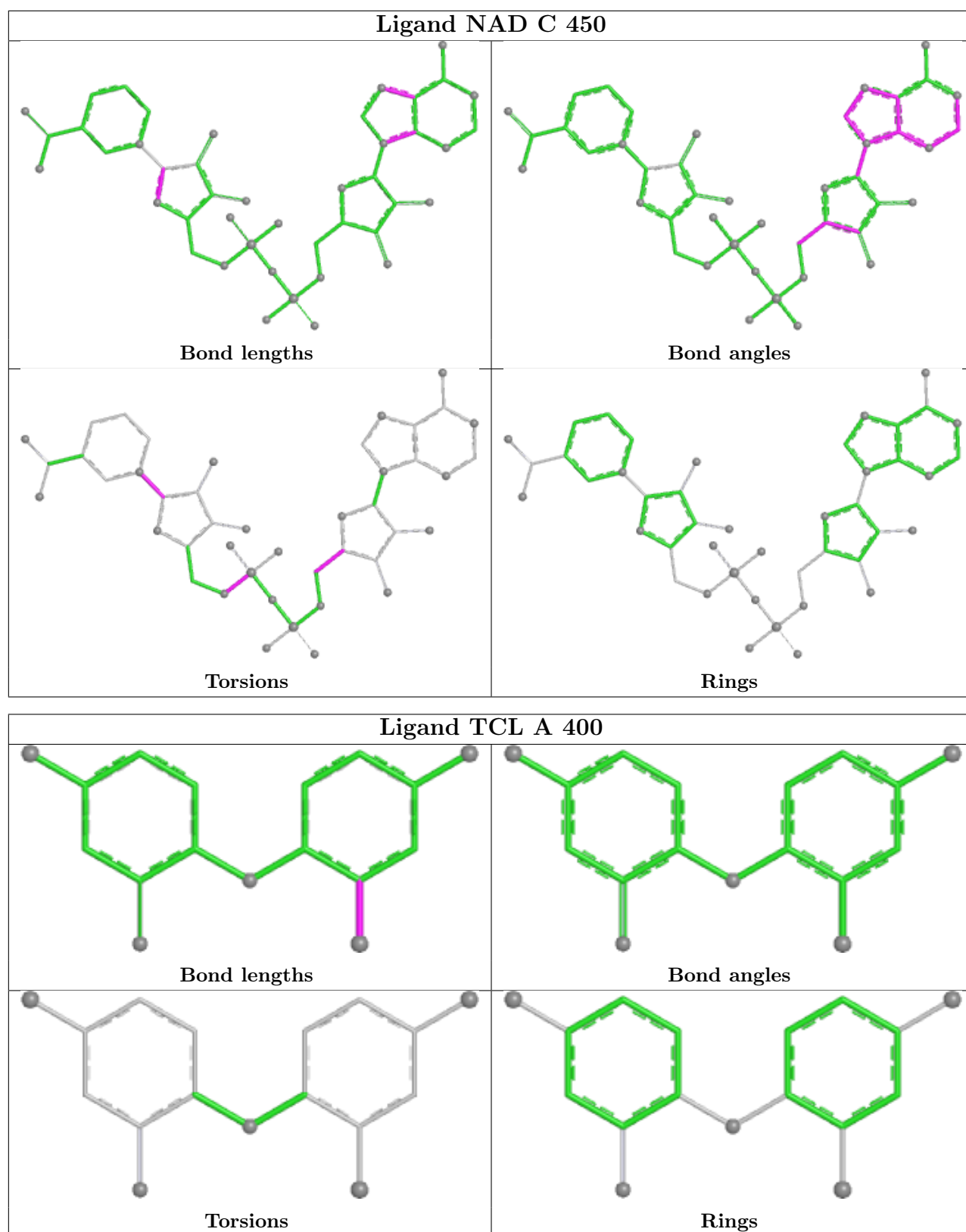
5 monomers are involved in 6 short contacts:

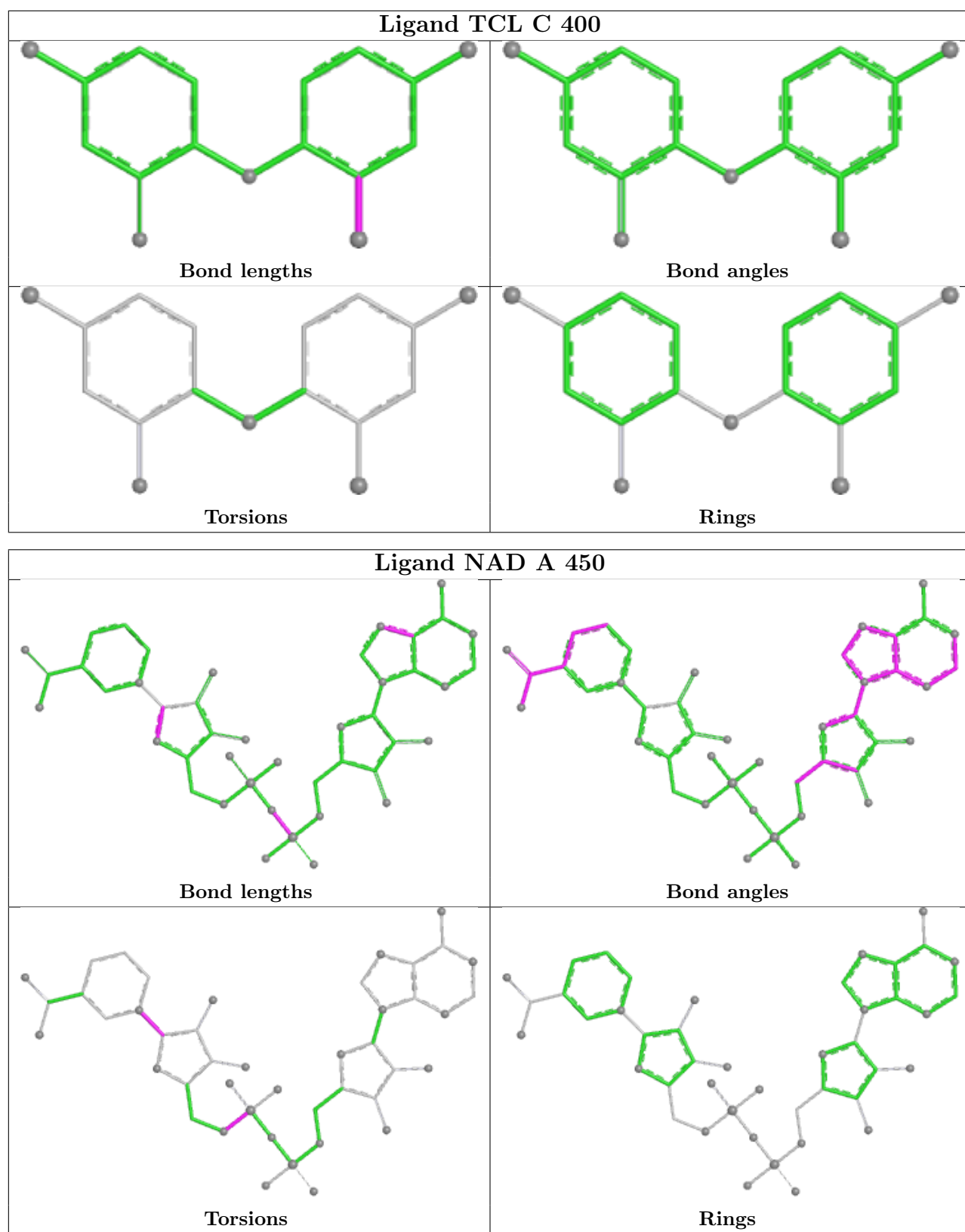
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	450	NAD	1	0
3	A	400	TCL	1	0
3	D	500	TCL	1	0
2	D	550	NAD	1	0
3	B	500	TCL	2	0

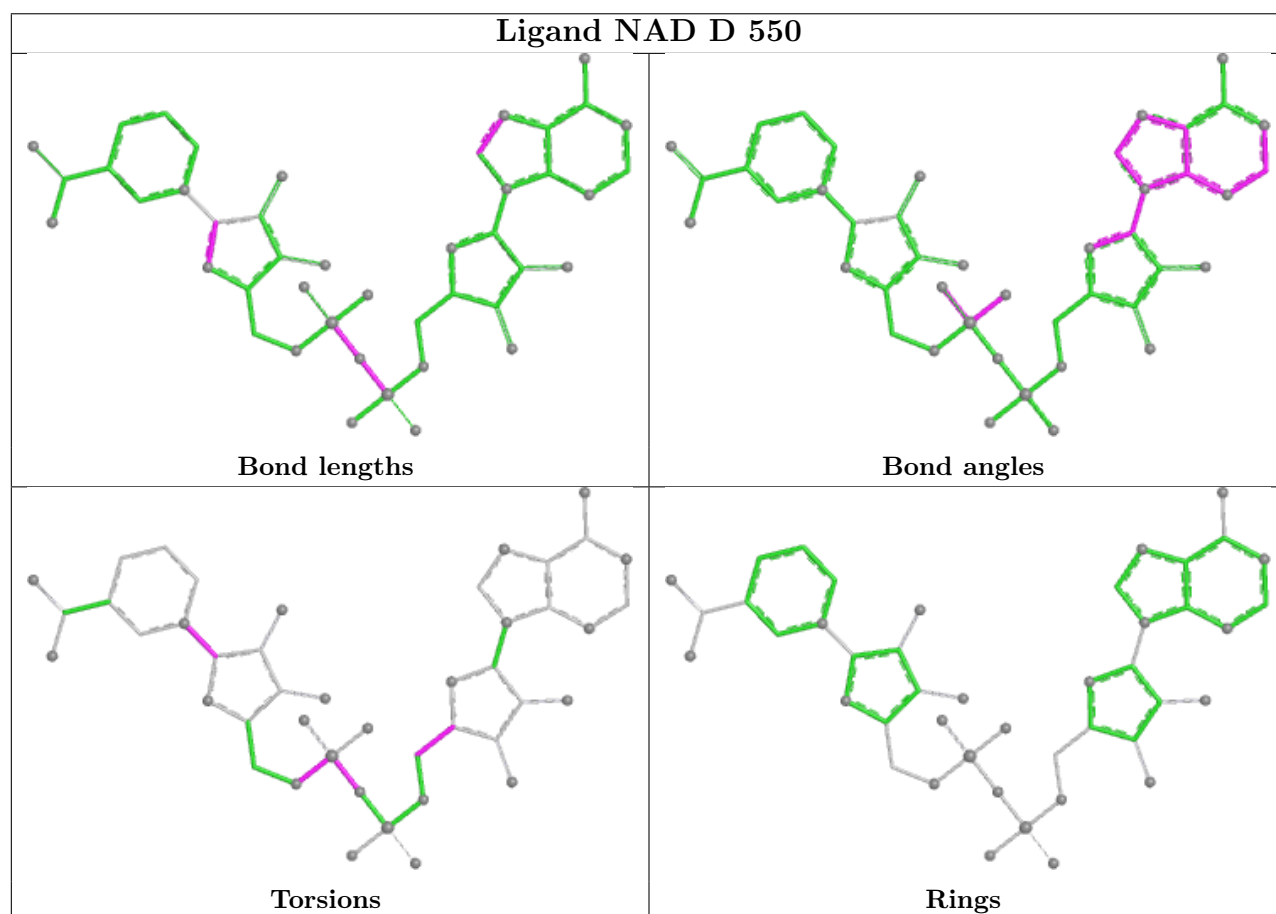
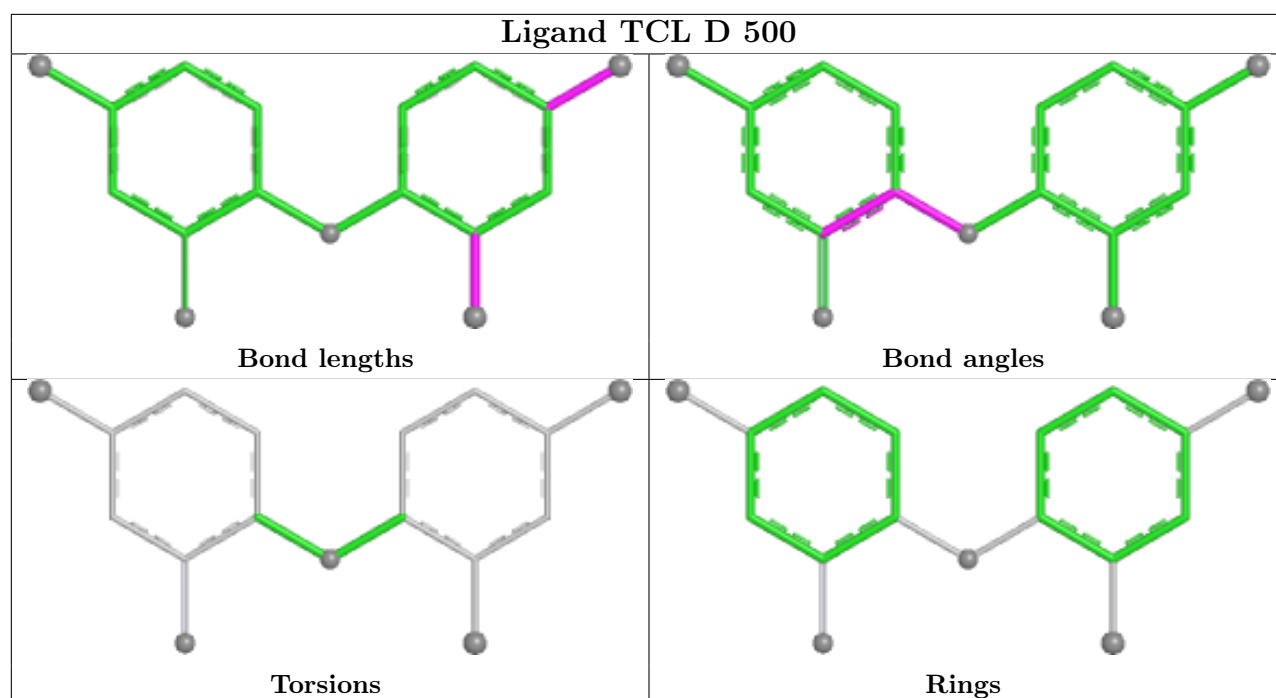
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

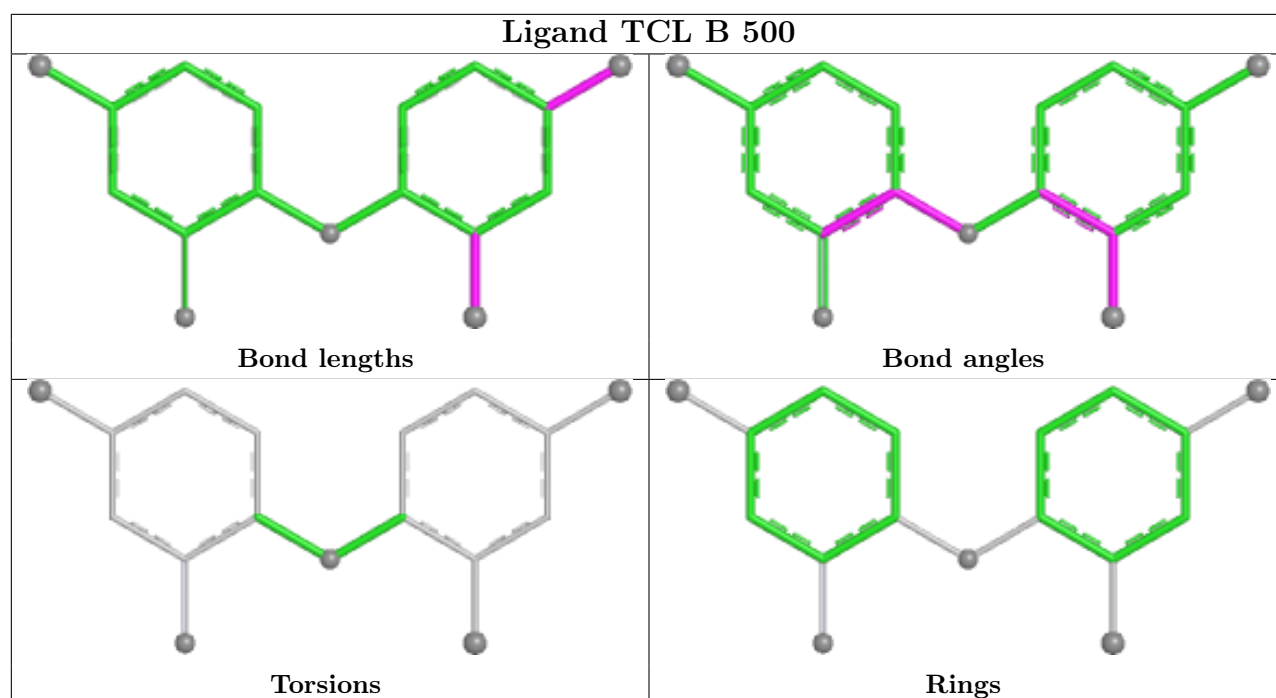
equivalents in the CSD to analyse the geometry.











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	284/323 (87%)	-0.40	0 100 100	43, 58, 78, 93	0
1	B	289/323 (89%)	-0.23	1 (0%) 90 87	47, 68, 110, 140	0
1	C	282/323 (87%)	-0.21	2 (0%) 84 81	46, 66, 90, 109	0
1	D	289/323 (89%)	-0.22	1 (0%) 90 87	46, 67, 109, 138	0
All	All	1144/1292 (88%)	-0.26	4 (0%) 90 87	43, 64, 98, 140	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	172	TYR	2.4
1	B	282	TYR	2.3
1	C	308	ILE	2.2
1	C	136	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

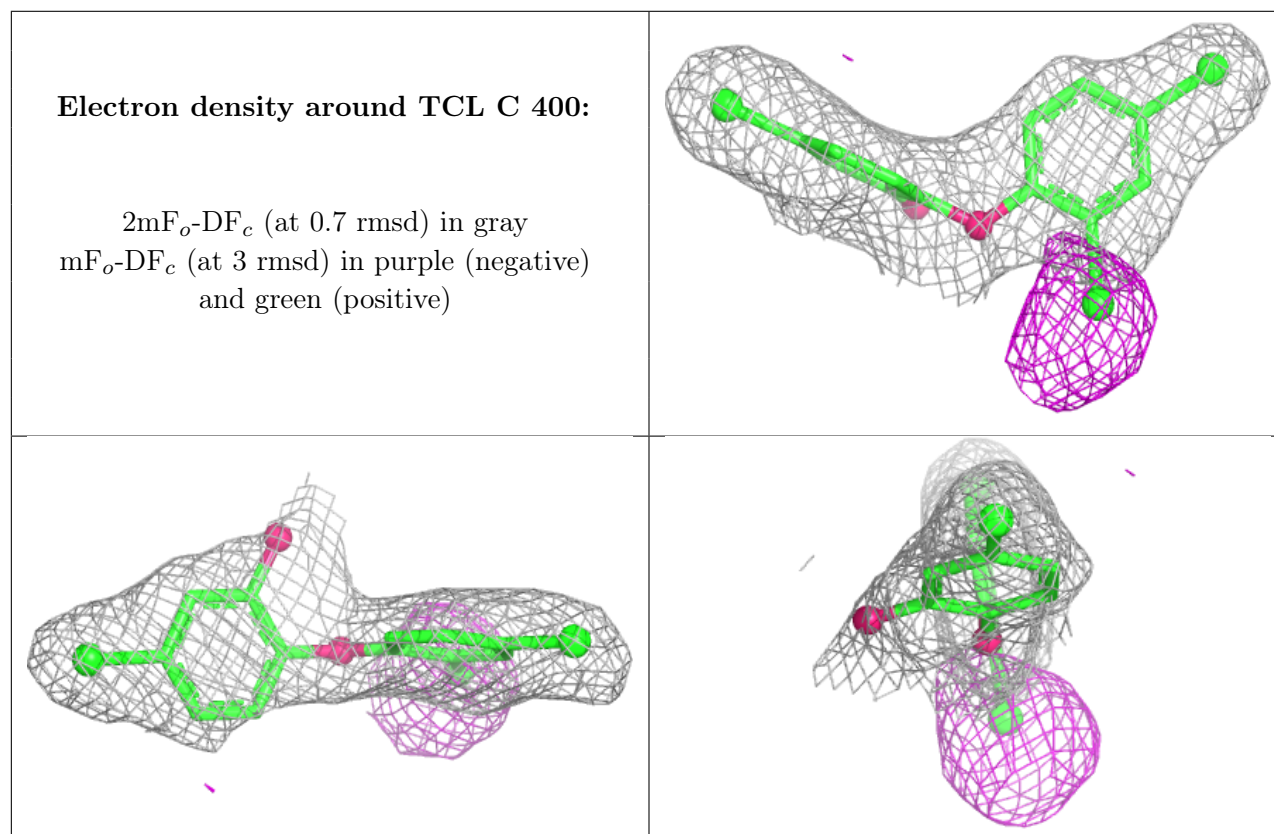
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

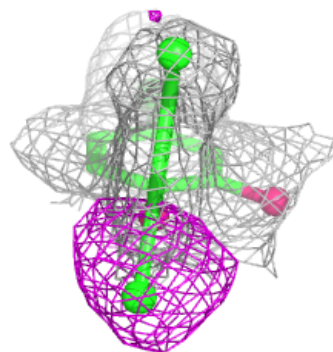
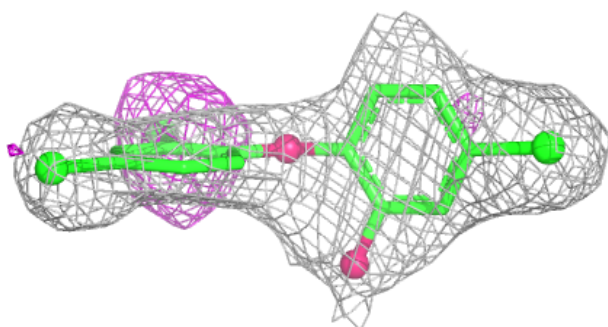
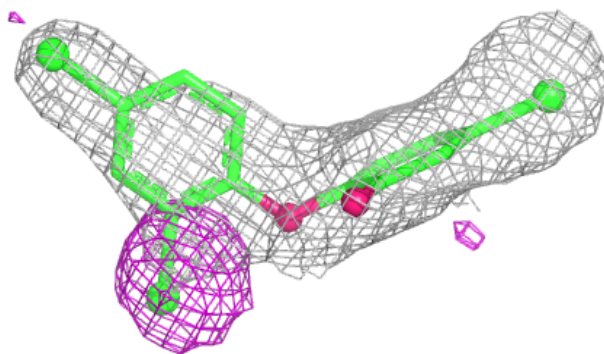
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	TCL	C	400	17/17	0.87	0.10	57,65,80,90	0
3	TCL	B	500	17/17	0.92	0.08	57,67,84,90	0
2	NAD	D	550	44/44	0.92	0.09	53,71,85,88	0
3	TCL	D	500	17/17	0.92	0.10	57,68,79,86	0
3	TCL	A	400	17/17	0.93	0.09	49,58,74,86	0
2	NAD	C	450	44/44	0.94	0.08	59,69,77,82	0
2	NAD	B	550	44/44	0.94	0.07	56,72,79,82	0
2	NAD	A	450	44/44	0.96	0.07	44,56,64,68	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.

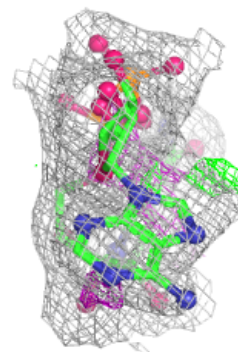
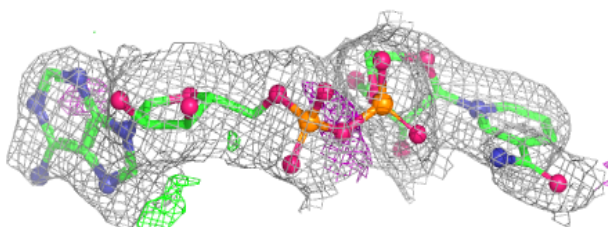
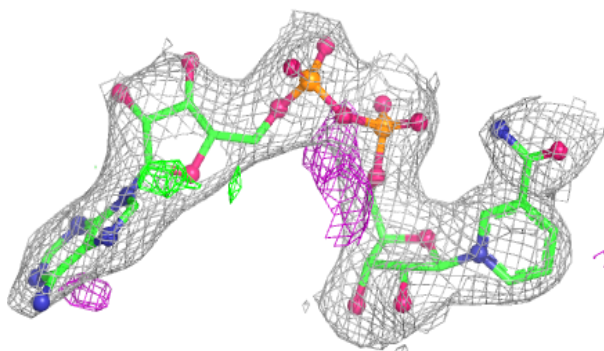


Electron density around TCL B 500:

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

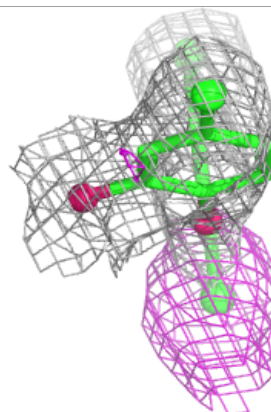
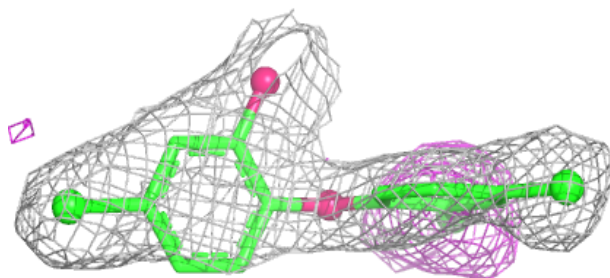
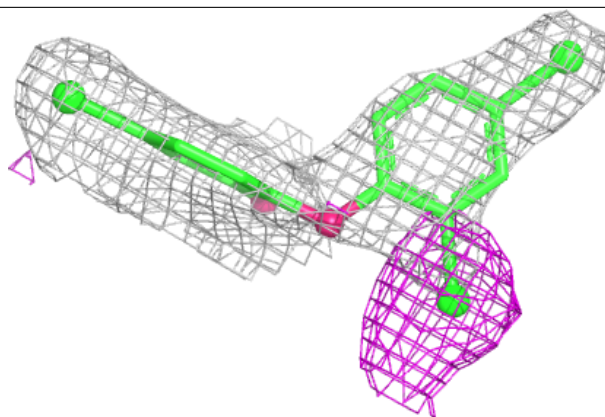
**Electron density around NAD D 550:**

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

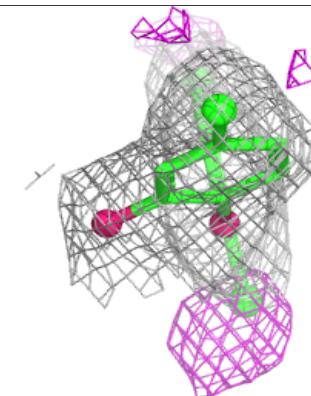
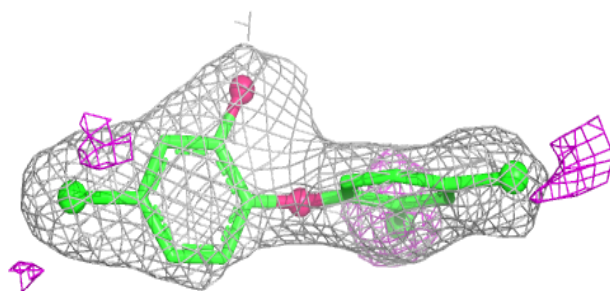
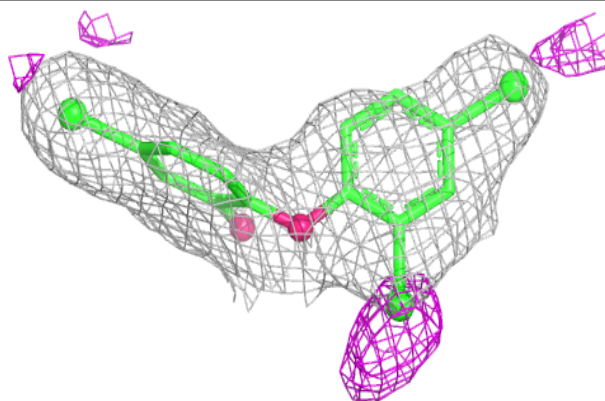


Electron density around TCL D 500:

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

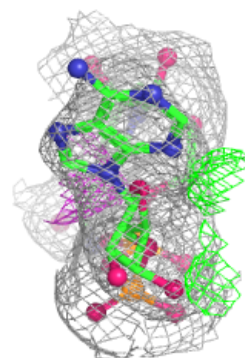
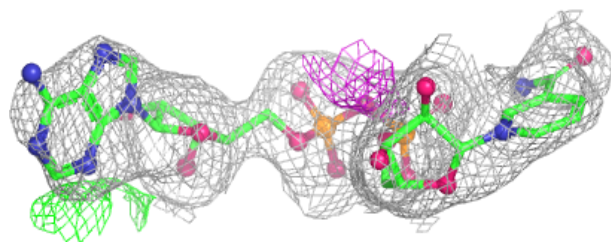
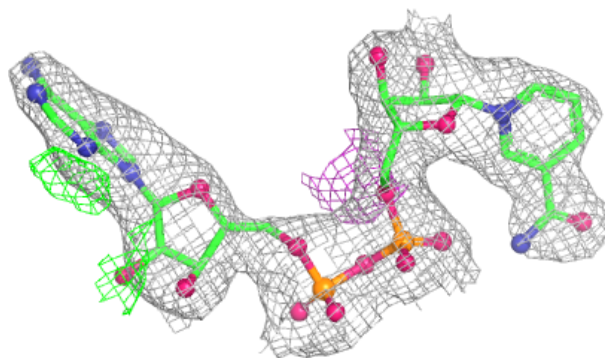
**Electron density around TCL A 400:**

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

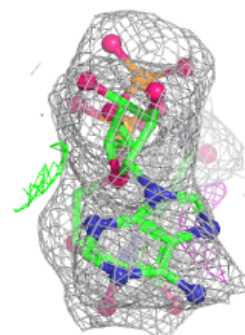
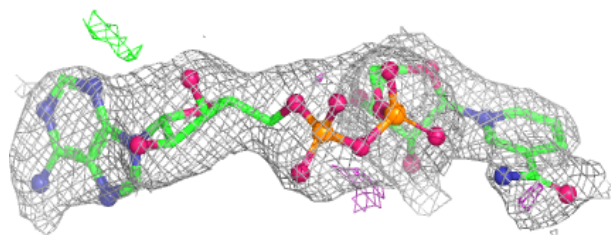
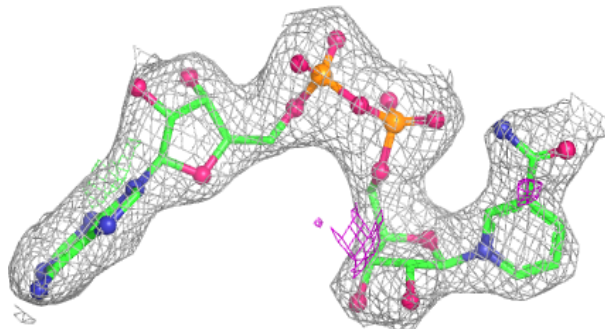


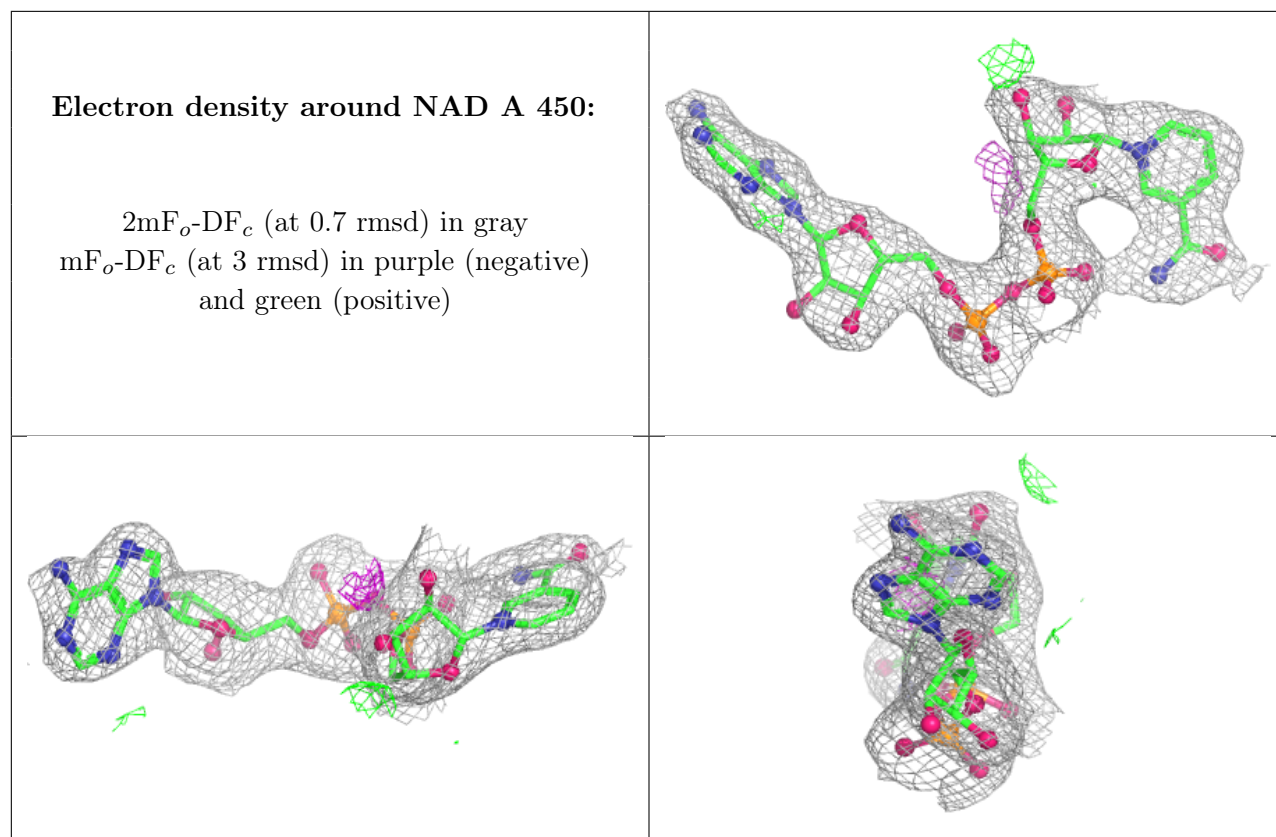
Electron density around NAD C 450:

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

**Electron density around NAD 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.