Full wwPDB X-ray Structure Validation Report (i)

May 24, 2020 – 02:25 am BST

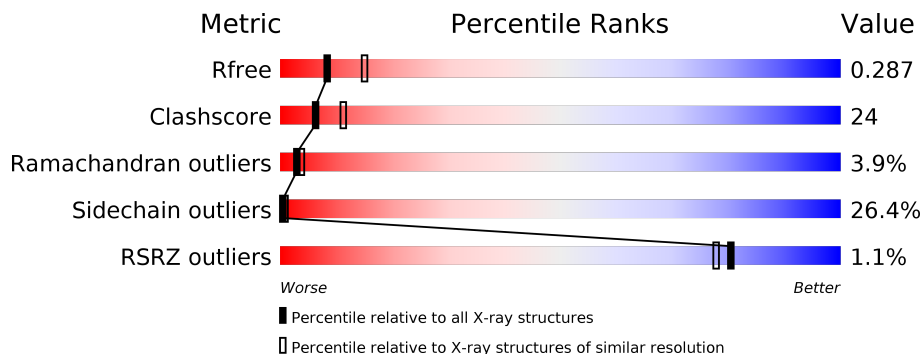|		
PDB ID	:	1P45
Title	:	Targeting tuberculosis and malaria through inhibition of enoyl reductase: compound activity and structural data
Authors	:	Kuo, M.R.; Morbidoni, H.R.; Alland, D.; Sneddon, S.F.; Gourlie, B.B.; Staveski, M.M.; Leonard, M.; Gregory, J.S.; Janjigian, A.D.; Yee, C.; Musser, J.M.; Kreiswirth, B.N.; Iwamoto, H.; Perozzo, R.; Jacobs Jr., W.R.; Sacchettini, J.C.; Fidock, D.A.; TB Structural Genomics Consortium (TBSGC)
Deposited on	:	2003-04-21
Resolution	:	2.60 Å(reported)

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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 2.60 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	Percentile Ranks	Value
Rfree		0.287
Clashscore		24
Ramachandran outliers		3.9%
Sidechain outliers		26.4%
RSRZ outliers		1.1%

Worse .... *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 on 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 <=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	269	48% 37% 14%
1	B	269	43% 36% 17%

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	TCL	B	500	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4171 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 [NADH].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			1994	1263	348	373	10			
1	B	268	Total	C	N	O	S	0	0	0
			1993	1263	348	372	10			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).
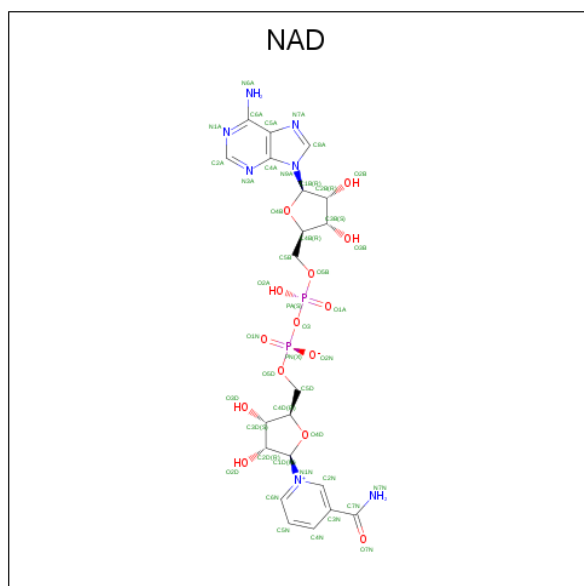
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is TRICLOSAN (three-letter code: TCL) (formula: $C_{12}H_7Cl_3O_2$).
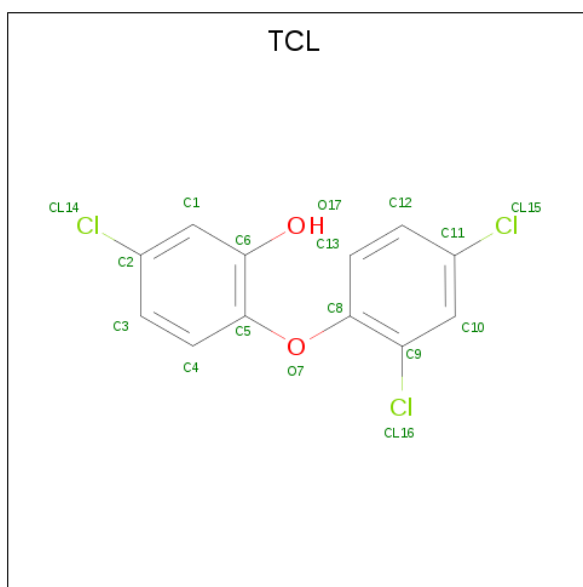
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	O	0	0
			17	12	3	2		
3	A	1	Total	C	Cl	O	0	0
			17	12	3	2		
3	B	1	Total	C	Cl	O	0	0
			17	12	3	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	20	Total	O	0	0
			20	20		
4	B	25	Total	O	0	0
			25	25		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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: Enoyl-[acyl-carrier-protein] reductase [NADH]
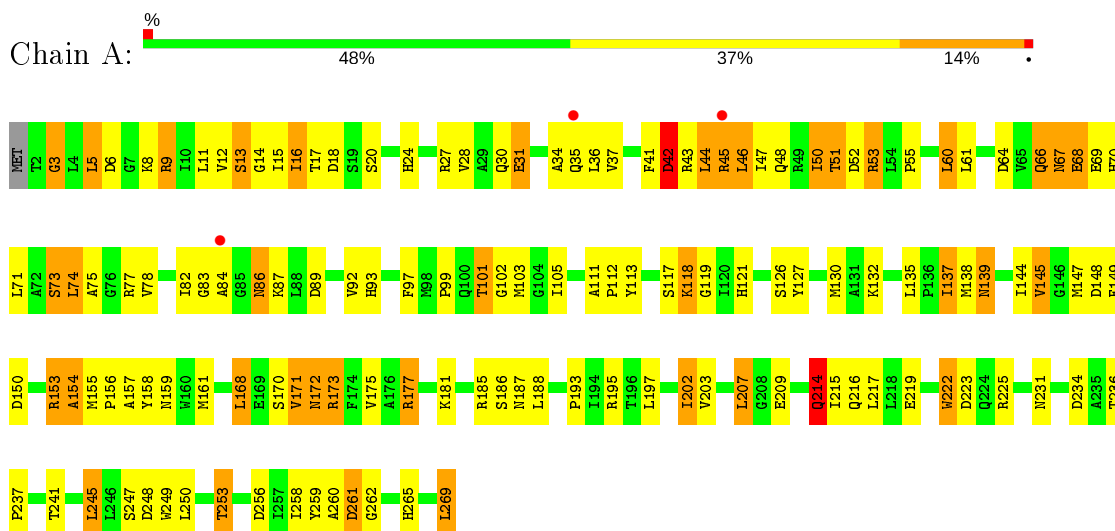
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]
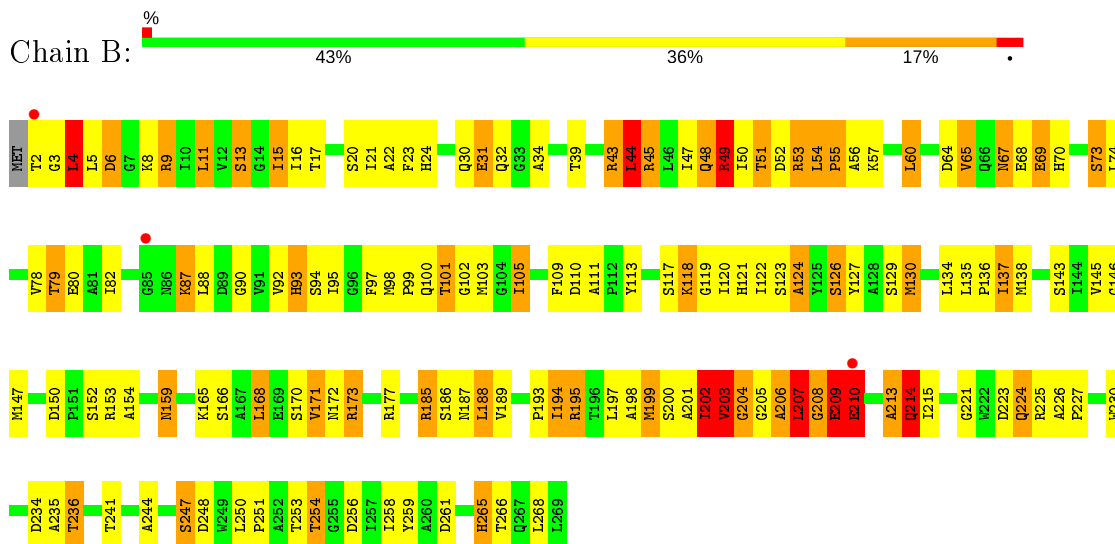
4   Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	94.82Å 104.12Å 189.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 29.18 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.8 (30.00-2.60) 94.9 (29.18-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.09 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.1, CNS	Depositor
R, R_{free}	0.225 , 0.290 0.228 , 0.287	Depositor DCC
R_{free} test set	1401 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	47.0	Xtriage
Anisotropy	0.734	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 36.7	EDS
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4171	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

Full wwPDB X-ray Structure Validation Report

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: TCL, NAD

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	1.29	9/2032 (0.4%)	1.54	29/2758 (1.1%)
1	B	1.41	10/2031 (0.5%)	1.46	22/2758 (0.8%)
All	All	1.35	19/4063 (0.5%)	1.50	51/5516 (0.9%)

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	3
1	B	0	10
All	All	0	13

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	214	GLN	CB-CG	12.02	1.85	1.52
1	B	214	GLN	CG-CD	7.05	1.67	1.51
1	A	181	LYS	CD-CE	6.35	1.67	1.51
1	B	261	ASP	CG-OD2	5.88	1.38	1.25
1	A	181	LYS	CB-CG	5.76	1.68	1.52
1	B	79	THR	CA-CB	5.76	1.68	1.53
1	B	153	ARG	CG-CD	5.65	1.66	1.51
1	A	259	TYR	CE2-CZ	-5.53	1.31	1.38
1	B	224	GLN	CG-CD	5.43	1.63	1.51
1	B	64	ASP	CB-CG	5.38	1.63	1.51
1	A	186	SER	CB-OG	5.35	1.49	1.42
1	A	171	VAL	CB-CG1	5.35	1.64	1.52
1	B	49	ARG	CB-CG	5.34	1.67	1.52
1	A	214	GLN	CG-CD	5.24	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	118	LYS	CB-CG	5.22	1.66	1.52
1	A	118	LYS	CD-CE	5.19	1.64	1.51
1	A	130	MET	CG-SD	5.08	1.94	1.81
1	A	147	MET	SD-CE	-5.07	1.49	1.77
1	B	31	GLU	CD-OE1	5.03	1.31	1.25

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	ARG	NE-CZ-NH2	-18.06	111.27	120.30
1	A	173	ARG	NE-CZ-NH1	14.47	127.53	120.30
1	A	18	ASP	CB-CG-OD2	11.36	128.53	118.30
1	A	261	ASP	CB-CG-OD1	10.93	128.14	118.30
1	A	148	ASP	CB-CG-OD1	10.09	127.38	118.30
1	A	150	ASP	CB-CG-OD1	9.65	126.98	118.30
1	A	6	ASP	CB-CG-OD2	9.48	126.83	118.30
1	A	64	ASP	CB-CG-OD1	8.95	126.36	118.30
1	A	223	ASP	CB-CG-OD1	8.83	126.24	118.30
1	B	130	MET	CG-SD-CE	-8.82	86.09	100.20
1	B	153	ARG	NE-CZ-NH2	-8.47	116.06	120.30
1	A	153	ARG	NE-CZ-NH1	-7.96	116.32	120.30
1	A	177	ARG	CB-CA-C	7.79	125.99	110.40
1	B	250	LEU	CA-CB-CG	7.54	132.64	115.30
1	B	173	ARG	CG-CD-NE	-7.17	96.74	111.80
1	B	173	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	A	18	ASP	CB-CG-OD1	-7.02	111.98	118.30
1	B	11	LEU	CA-CB-CG	7.01	131.42	115.30
1	B	225	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	A	168	LEU	CB-CG-CD2	6.56	122.16	111.00
1	B	214	GLN	CA-CB-CG	6.55	127.82	113.40
1	A	52	ASP	CB-CG-OD2	6.37	124.04	118.30
1	A	269	LEU	CA-CB-CG	6.22	129.62	115.30
1	B	153	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	B	248	ASP	CB-CG-OD2	6.07	123.77	118.30
1	A	43	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	A	177	ARG	CA-CB-CG	6.02	126.64	113.40
1	B	11	LEU	CB-CG-CD1	5.78	120.82	111.00
1	B	224	GLN	CA-CB-CG	5.67	125.88	113.40
1	A	261	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	B	110	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	43	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	150	ASP	CB-CG-OD1	5.48	123.23	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	185	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	262	GLY	CA-C-O	-5.40	110.88	120.60
1	A	139	ASN	N-CA-CB	-5.33	101.00	110.60
1	B	171	VAL	CB-CA-C	-5.32	101.30	111.40
1	B	223	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	256	ASP	CB-CG-OD2	5.25	123.02	118.30
1	B	87	LYS	CA-CB-CG	5.21	124.86	113.40
1	A	150	ASP	CB-CG-OD2	-5.21	113.62	118.30
1	A	154	ALA	CB-CA-C	5.18	117.87	110.10
1	B	153	ARG	CG-CD-NE	-5.17	100.94	111.80
1	A	234	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	225	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	A	193	PRO	N-CD-CG	-5.10	95.55	103.20
1	A	42	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	173	ARG	CD-NE-CZ	5.09	130.72	123.60
1	B	49	ARG	CG-CD-NE	5.07	122.44	111.80
1	A	64	ASP	CB-CG-OD2	-5.06	113.74	118.30
1	B	202	ILE	N-CA-C	5.06	124.65	111.00

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	138	MET	Peptide
1	A	3	GLY	Peptide
1	A	41	PHE	Peptide
1	B	123	SER	Peptide
1	B	197	LEU	Peptide
1	B	2	THR	Peptide
1	B	200	SER	Peptide
1	B	203	VAL	Peptide
1	B	207	LEU	Peptide
1	B	208	GLY	Peptide
1	B	209	GLU	Peptide
1	B	268	LEU	Peptide
1	B	44	LEU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1994	0	2008	79	0
1	B	1993	0	2008	121	0
2	A	44	0	25	1	0
2	B	44	0	26	3	0
3	A	34	0	12	2	0
3	B	17	0	6	6	0
4	A	20	0	0	1	0
4	B	25	0	0	3	0
All	All	4171	0	4085	197	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 24.

All (197) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:GLN:CG	1:B:214:GLN:CB	1.85	1.53
1:B:120:ILE:O	1:B:124:ALA:HB3	1.65	0.95
1:A:202:ILE:HD11	1:A:215:ILE:HG21	1.50	0.92
1:A:245:LEU:HD13	1:A:250:LEU:HD12	1.56	0.88
1:A:215:ILE:O	1:A:219:GLU:HB2	1.74	0.87
1:A:195:ARG:HH21	1:A:203:VAL:HG11	1.44	0.82
1:B:202:ILE:H	1:B:202:ILE:HD12	1.48	0.77
1:B:3:GLY:O	1:B:6:ASP:N	2.17	0.77
1:A:47:ILE:O	1:A:51:THR:HG22	1.84	0.76
1:A:172:ASN:ND2	4:A:451:HOH:O	2.19	0.75
1:B:103:MET:CE	3:B:500:TCL:H121	2.17	0.75
1:B:93:HIS:HD2	1:B:127:TYR:HA	1.53	0.73
1:B:209:GLU:OE1	1:B:209:GLU:HA	1.88	0.72
1:A:69:GLU:O	1:A:73:SER:HB3	1.88	0.72
1:B:254:THR:HG21	4:B:501:HOH:O	1.88	0.72
1:A:24:HIS:O	1:A:28:VAL:HG23	1.90	0.72
1:B:137:ILE:CG1	1:B:137:ILE:O	2.37	0.71
1:B:199:MET:O	1:B:202:ILE:HB	1.90	0.71
1:B:205:GLY:C	1:B:207:LEU:H	1.94	0.70
1:B:93:HIS:CE1	1:B:95:ILE:HB	2.27	0.69
1:A:45:ARG:NH1	1:A:45:ARG:HB2	2.07	0.69
1:B:259:TYR:CD2	1:B:265:HIS:CD2	2.81	0.69
1:A:46:LEU:O	1:A:50:ILE:HG12	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ILE:HB	1:A:207:LEU:HD22	1.75	0.67
1:B:201:ALA:O	1:B:204:GLY:HA3	1.95	0.67
1:B:103:MET:HE3	3:B:500:TCL:H121	1.76	0.67
1:B:203:VAL:H	1:B:204:GLY:HA3	1.62	0.65
1:B:202:ILE:H	1:B:202:ILE:CD1	2.11	0.64
1:A:214:GLN:HE21	1:A:214:GLN:HA	1.62	0.64
1:B:49:ARG:O	1:B:52:ASP:HB2	1.98	0.63
1:B:189:VAL:HA	1:B:258:ILE:O	1.98	0.62
1:B:67:ASN:HD22	1:B:70:HIS:H	1.48	0.62
1:A:47:ILE:O	1:A:51:THR:CG2	2.48	0.61
1:A:46:LEU:HD23	1:A:50:ILE:HD11	1.82	0.61
1:B:118:LYS:NZ	4:B:523:HOH:O	2.10	0.61
1:B:48:GLN:HG2	1:B:60:LEU:HD23	1.82	0.60
1:B:213:ALA:C	1:B:215:ILE:H	2.05	0.60
1:B:137:ILE:HG13	1:B:137:ILE:O	2.01	0.59
1:A:93:HIS:NE2	1:A:126:SER:OG	2.36	0.59
1:B:93:HIS:CD2	1:B:127:TYR:HA	2.38	0.59
1:B:93:HIS:O	1:B:146:GLY:HA2	2.03	0.59
1:B:30:GLN:C	1:B:32:GLN:N	2.54	0.59
1:A:83:GLY:O	1:A:86:ASN:HB2	2.03	0.58
1:B:103:MET:HE1	3:B:500:TCL:H121	1.85	0.58
1:B:168:LEU:HD22	1:B:188:LEU:HD21	1.84	0.58
1:B:185:ARG:HA	1:B:254:THR:HG23	1.85	0.58
1:B:93:HIS:HD2	1:B:127:TYR:CA	2.15	0.58
1:B:147:MET:O	1:B:165:LYS:NZ	2.36	0.58
1:A:67:ASN:OD1	1:A:70:HIS:CD2	2.58	0.57
1:B:205:GLY:C	1:B:207:LEU:N	2.58	0.57
1:A:195:ARG:HE	1:A:203:VAL:HG21	1.68	0.57
1:B:47:ILE:HG22	1:B:51:THR:CG2	2.33	0.57
1:A:261:ASP:OD2	1:A:265:HIS:HB3	2.04	0.57
1:A:45:ARG:HB2	1:A:45:ARG:HH11	1.68	0.57
1:A:245:LEU:HD21	1:A:258:ILE:HG13	1.87	0.56
1:A:9:ARG:HD2	1:A:87:LYS:O	2.05	0.56
1:B:194:ILE:O	1:B:199:MET:HE3	2.06	0.56
1:B:30:GLN:O	1:B:32:GLN:N	2.39	0.56
1:B:206:ALA:O	1:B:208:GLY:N	2.39	0.56
1:B:21:ILE:HG13	2:B:350:NAD:O1N	2.05	0.56
1:B:13:SER:HB3	1:B:92:VAL:O	2.06	0.56
1:B:234:ASP:OD1	1:B:236:THR:HG23	2.06	0.56
1:A:53:ARG:HB3	1:A:53:ARG:CZ	2.36	0.55
1:A:13:SER:HB2	1:A:92:VAL:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:GLN:C	1:B:32:GLN:H	2.09	0.55
1:A:121:HIS:CD2	1:B:113:TYR:CG	2.94	0.55
1:B:213:ALA:O	1:B:215:ILE:N	2.39	0.55
1:A:67:ASN:HB3	1:A:70:HIS:HD2	1.72	0.55
1:B:198:ALA:C	1:B:202:ILE:HD13	2.27	0.55
1:A:185:ARG:HG2	1:A:253:THR:O	2.07	0.54
1:A:50:ILE:O	1:A:53:ARG:HG2	2.07	0.54
1:B:193:PRO:HD2	1:B:230:TRP:NE1	2.22	0.54
1:B:199:MET:HA	1:B:202:ILE:HG12	1.89	0.54
2:B:350:NAD:C7N	3:B:500:TCL:C3	2.86	0.54
1:A:5:LEU:HB3	1:A:34:ALA:HB2	1.89	0.54
1:B:202:ILE:N	1:B:202:ILE:CD1	2.72	0.53
1:A:67:ASN:C	1:A:67:ASN:HD22	2.11	0.53
1:B:203:VAL:N	1:B:204:GLY:HA3	2.22	0.53
1:B:241:THR:O	1:B:244:ALA:HB3	2.07	0.53
1:B:202:ILE:N	1:B:202:ILE:HD12	2.22	0.53
1:B:54:LEU:O	1:B:55:PRO:O	2.26	0.53
1:B:201:ALA:O	1:B:204:GLY:CA	2.56	0.53
1:A:171:VAL:O	1:A:175:VAL:HG23	2.09	0.53
1:B:20:SER:O	1:B:23:PHE:HB3	2.08	0.53
1:B:135:LEU:N	1:B:136:PRO:CD	2.71	0.52
1:B:199:MET:N	1:B:202:ILE:HD13	2.25	0.52
1:B:44:LEU:N	1:B:44:LEU:CD2	2.72	0.52
1:B:67:ASN:ND2	1:B:70:HIS:H	2.08	0.52
1:A:30:GLN:HE21	1:A:36:LEU:HD12	1.74	0.52
1:A:245:LEU:CD1	1:A:250:LEU:HD12	2.36	0.52
1:A:60:LEU:HD22	1:A:61:LEU:N	2.25	0.52
1:B:122:ILE:O	1:B:126:SER:OG	2.26	0.52
1:B:78:VAL:O	1:B:82:ILE:HG12	2.10	0.52
1:B:22:ALA:HB2	1:B:94:SER:HB3	1.93	0.51
1:A:16:ILE:HG23	1:A:17:THR:HG23	1.90	0.51
1:B:259:TYR:CE2	1:B:265:HIS:HD2	2.28	0.51
1:B:120:ILE:O	1:B:124:ALA:CB	2.50	0.51
1:A:127:TYR:OH	1:A:144:ILE:HG22	2.11	0.50
1:A:11:LEU:HA	1:A:37:VAL:O	2.11	0.50
1:A:102:GLY:O	1:A:159:ASN:HB2	2.12	0.49
1:B:98:MET:SD	1:B:119:GLY:HA3	2.52	0.49
1:B:259:TYR:CE2	1:B:265:HIS:CD2	3.01	0.49
1:A:245:LEU:HD13	1:A:250:LEU:CD1	2.36	0.49
1:B:194:ILE:O	1:B:199:MET:CE	2.61	0.49
1:A:215:ILE:HG12	3:A:450:TCL:O17	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:HIS:O	1:A:74:LEU:HB2	2.12	0.49
1:B:226:ALA:O	1:B:227:PRO:C	2.50	0.48
1:B:4:LEU:H	1:B:32:GLN:HE21	1.62	0.48
1:B:90:GLY:HA2	1:B:143:SER:O	2.13	0.48
1:B:65:VAL:CG1	1:B:126:SER:HB3	2.44	0.48
1:A:112:PRO:O	1:A:113:TYR:C	2.51	0.47
1:A:145:VAL:HA	1:A:187:ASN:O	2.15	0.47
1:A:53:ARG:HB3	1:A:53:ARG:NH1	2.30	0.47
1:A:73:SER:O	1:A:77:ARG:HG3	2.14	0.47
1:B:50:ILE:O	1:B:53:ARG:HB2	2.15	0.47
1:A:67:ASN:HD22	1:A:68:GLU:N	2.13	0.47
1:B:213:ALA:C	1:B:215:ILE:N	2.68	0.46
1:B:205:GLY:O	1:B:207:LEU:N	2.49	0.46
1:B:3:GLY:O	1:B:5:LEU:N	2.48	0.46
1:A:153:ARG:HH11	1:A:153:ARG:HD2	1.47	0.46
1:A:173:ARG:HB3	1:B:154:ALA:HB2	1.96	0.46
1:B:105:ILE:HD12	1:B:105:ILE:H	1.81	0.46
1:B:13:SER:OG	1:B:95:ILE:HG13	2.16	0.46
1:A:236:THR:N	1:A:237:PRO:CD	2.79	0.46
2:B:350:NAD:N7N	3:B:500:TCL:C4	2.79	0.46
1:B:210:GLU:O	1:B:213:ALA:HB3	2.16	0.46
1:B:204:GLY:HA2	1:B:205:GLY:HA2	1.70	0.45
1:A:8:LYS:HE3	1:A:248:ASP:OD1	2.16	0.45
1:B:44:LEU:N	1:B:44:LEU:HD22	2.31	0.45
1:B:32:GLN:O	1:B:32:GLN:HG3	2.16	0.45
1:B:73:SER:O	1:B:74:LEU:C	2.55	0.45
1:B:198:ALA:C	1:B:202:ILE:CD1	2.86	0.44
1:B:65:VAL:HG11	1:B:126:SER:HB3	1.99	0.44
1:A:42:ASP:C	1:A:42:ASP:OD1	2.56	0.44
1:B:134:LEU:O	1:B:138:MET:HB2	2.16	0.44
1:B:93:HIS:CD2	1:B:127:TYR:CA	2.98	0.44
1:A:78:VAL:O	1:A:82:ILE:HG13	2.18	0.43
1:B:244:ALA:O	1:B:247:SER:HB3	2.18	0.43
1:A:66:GLN:HA	1:A:121:HIS:CE1	2.53	0.43
1:B:103:MET:HE1	3:B:500:TCL:CL15	2.55	0.43
1:A:249:TRP:O	1:A:250:LEU:HD23	2.18	0.43
1:A:132:LYS:HD2	1:B:109:PHE:HB3	2.00	0.43
1:B:137:ILE:HG12	1:B:137:ILE:O	2.18	0.43
1:B:5:LEU:O	1:B:8:LYS:HB2	2.18	0.43
1:A:11:LEU:HD23	1:A:12:VAL:N	2.34	0.43
1:A:158:TYR:CZ	1:A:161:MET:HG3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:VAL:HG12	1:A:175:VAL:HG21	2.00	0.43
1:A:67:ASN:CB	1:A:70:HIS:HD2	2.31	0.43
1:A:121:HIS:CD2	1:B:113:TYR:CD2	3.06	0.43
1:B:199:MET:HA	1:B:202:ILE:CG1	2.48	0.43
1:A:195:ARG:NH2	1:A:203:VAL:HG11	2.24	0.43
1:B:235:ALA:O	1:B:236:THR:C	2.56	0.43
1:A:97:PHE:O	1:A:119:GLY:HA2	2.19	0.43
1:B:101:THR:HG23	1:B:111:ALA:HA	2.01	0.43
1:B:145:VAL:HA	1:B:187:ASN:O	2.19	0.43
1:A:44:LEU:CD1	1:A:60:LEU:HD11	2.49	0.42
1:B:171:VAL:O	1:B:172:ASN:C	2.55	0.42
1:A:102:GLY:C	1:A:103:MET:HG3	2.40	0.42
1:B:47:ILE:O	1:B:51:THR:HG23	2.19	0.42
1:B:186:SER:H	1:B:254:THR:CG2	2.33	0.42
1:A:241:THR:HG21	1:A:260:ALA:HB2	2.02	0.42
1:B:102:GLY:O	1:B:159:ASN:HB2	2.20	0.42
1:B:5:LEU:HB3	1:B:34:ALA:HB2	2.02	0.42
1:A:75:ALA:CB	1:A:137:ILE:HD13	2.50	0.42
1:B:24:HIS:CD2	1:B:235:ALA:HB3	2.55	0.42
1:B:43:ARG:HD2	1:B:43:ARG:N	2.35	0.42
1:B:97:PHE:CE2	1:B:99:PRO:HD3	2.55	0.41
1:A:101:THR:HG23	1:A:111:ALA:HA	2.02	0.41
1:B:15:ILE:CD1	1:B:23:PHE:HA	2.51	0.41
1:B:265:HIS:ND1	1:B:266:THR:N	2.69	0.41
1:B:67:ASN:HD22	1:B:70:HIS:N	2.16	0.41
1:A:27:ARG:O	1:A:31:GLU:HG3	2.20	0.41
1:A:66:GLN:OE1	1:A:118:LYS:HE2	2.20	0.41
1:A:154:ALA:HB1	1:B:177:ARG:HD2	2.01	0.41
1:A:48:GLN:HA	1:A:51:THR:HG23	2.03	0.41
1:B:186:SER:H	1:B:254:THR:HG22	1.85	0.41
1:B:3:GLY:HA2	1:B:32:GLN:HG3	2.02	0.41
1:A:44:LEU:CD1	1:A:60:LEU:CD1	2.99	0.41
1:B:166:SER:HB3	4:B:502:HOH:O	2.21	0.41
1:B:195:ARG:HA	1:B:199:MET:CE	2.51	0.41
1:B:201:ALA:O	1:B:204:GLY:C	2.58	0.41
1:B:60:LEU:O	1:B:60:LEU:HG	2.19	0.41
1:B:78:VAL:HG11	1:B:88:LEU:HD11	2.03	0.41
1:B:47:ILE:O	1:B:50:ILE:N	2.53	0.41
1:A:101:THR:HG21	1:A:112:PRO:HD2	2.03	0.41
1:A:149:PHE:CZ	1:A:222:TRP:CH2	3.09	0.41
1:B:93:HIS:HE1	1:B:95:ILE:HB	1.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:GLY:O	2:A:300:NAD:O3B	2.37	0.40
1:B:23:PHE:CE2	1:B:54:LEU:HD13	2.57	0.40
1:B:67:ASN:ND2	1:B:69:GLU:CB	2.84	0.40
1:A:215:ILE:HG23	3:A:450:TCL:H11	2.03	0.40
1:B:9:ARG:O	1:B:88:LEU:HD23	2.21	0.40
1:A:155:MET:HG3	1:A:156:PRO:O	2.22	0.40
1:B:185:ARG:HA	1:B:254:THR:CG2	2.50	0.40
1:A:156:PRO:O	1:A:157:ALA:HB3	2.20	0.40
1:A:24:HIS:ND1	1:A:27:ARG:NH2	2.65	0.40
1:B:195:ARG:HA	1:B:199:MET:HE3	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	266/269 (99%)	242 (91%)	20 (8%)	4 (2%)	10	21
1	B	266/269 (99%)	223 (84%)	26 (10%)	17 (6%)	1	1
All	All	532/538 (99%)	465 (87%)	46 (9%)	21 (4%)	3	4

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	GLY
1	A	42	ASP
1	A	84	ALA
1	B	4	LEU
1	B	45	ARG
1	B	55	PRO
1	B	56	ALA
1	B	202	ILE

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Mol	Chain	Res	Type
1	B	206	ALA
1	B	207	LEU
1	B	31	GLU
1	B	213	ALA
1	B	214	GLN
1	A	55	PRO
1	B	204	GLY
1	B	210	GLU
1	B	124	ALA
1	B	16	ILE
1	B	159	ASN
1	B	199	MET
1	B	221	GLY

5.3.2   Protein sidechains (i)

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	203/205 (99%)	152 (75%)	51 (25%)	0	1
1	B	203/205 (99%)	147 (72%)	56 (28%)	0	1
All	All	406/410 (99%)	299 (74%)	107 (26%)	0	1

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	9	ARG
1	A	13	SER
1	A	15	ILE
1	A	16	ILE
1	A	20	SER
1	A	31	GLU
1	A	35	GLN
1	A	42	ASP
1	A	44	LEU

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Mol	Chain	Res	Type
1	A	45	ARG
1	A	46	LEU
1	A	50	ILE
1	A	51	THR
1	A	53	ARG
1	A	60	LEU
1	A	66	GLN
1	A	67	ASN
1	A	68	GLU
1	A	71	LEU
1	A	73	SER
1	A	74	LEU
1	A	86	ASN
1	A	89	ASP
1	A	99	PRO
1	A	101	THR
1	A	105	ILE
1	A	117	SER
1	A	135	LEU
1	A	137	ILE
1	A	139	ASN
1	A	145	VAL
1	A	168	LEU
1	A	170	SER
1	A	172	ASN
1	A	177	ARG
1	A	188	LEU
1	A	197	LEU
1	A	202	ILE
1	A	207	LEU
1	A	209	GLU
1	A	214	GLN
1	A	216	GLN
1	A	217	LEU
1	A	222	TRP
1	A	231	ASN
1	A	245	LEU
1	A	247	SER
1	A	253	THR
1	A	256	ASP
1	A	269	LEU
1	B	4	LEU

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Mol	Chain	Res	Type
1	B	6	ASP
1	B	9	ARG
1	B	11	LEU
1	B	13	SER
1	B	15	ILE
1	B	17	THR
1	B	39	THR
1	B	43	ARG
1	B	44	LEU
1	B	45	ARG
1	B	48	GLN
1	B	49	ARG
1	B	51	THR
1	B	53	ARG
1	B	54	LEU
1	B	57	LYS
1	B	60	LEU
1	B	65	VAL
1	B	67	ASN
1	B	68	GLU
1	B	69	GLU
1	B	73	SER
1	B	79	THR
1	B	80	GLU
1	B	87	LYS
1	B	93	HIS
1	B	100	GLN
1	B	101	THR
1	B	105	ILE
1	B	117	SER
1	B	121	HIS
1	B	126	SER
1	B	129	SER
1	B	130	MET
1	B	137	ILE
1	B	152	SER
1	B	168	LEU
1	B	170	SER
1	B	173	ARG
1	B	188	LEU
1	B	194	ILE
1	B	195	ARG

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Mol	Chain	Res	Type
1	B	202	ILE
1	B	203	VAL
1	B	207	LEU
1	B	209	GLU
1	B	210	GLU
1	B	214	GLN
1	B	224	GLN
1	B	236	THR
1	B	247	SER
1	B	251	PRO
1	B	253	THR
1	B	254	THR
1	B	265	HIS

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

Mol	Chain	Res	Type
1	A	30	GLN
1	A	67	ASN
1	A	70	HIS
1	A	139	ASN
1	A	214	GLN
1	A	265	HIS
1	B	32	GLN
1	B	48	GLN
1	B	66	GLN
1	B	67	ASN
1	B	86	ASN
1	B	93	HIS
1	B	100	GLN
1	B	159	ASN
1	B	187	ASN
1	B	216	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

5 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	350	1	42,48,48	1.87	5 (11%)	50,73,73	2.13	13 (26%)
3	TCL	A	400	-	18,18,18	1.59	6 (33%)	25,25,25	1.67	6 (24%)
3	TCL	A	450	-	18,18,18	1.73	6 (33%)	25,25,25	1.79	5 (20%)
2	NAD	A	300	1	42,48,48	1.77	6 (14%)	50,73,73	2.03	16 (32%)
3	TCL	B	500	-	18,18,18	1.89	5 (27%)	25,25,25	1.57	4 (16%)

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	350	1	-	12/26/62/62	0/5/5/5
3	TCL	A	400	-	-	0/4/4/4	0/2/2/2
3	TCL	A	450	-	-	0/4/4/4	0/2/2/2
2	NAD	A	300	1	-	9/26/62/62	0/5/5/5
3	TCL	B	500	-	-	0/4/4/4	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	350	NAD	O7N-C7N	8.16	1.39	1.24
2	A	300	NAD	O7N-C7N	7.73	1.38	1.24
2	B	350	NAD	C2A-N3A	5.26	1.40	1.32
3	B	500	TCL	C10-C11	4.25	1.45	1.38
3	B	500	TCL	C8-C9	3.76	1.46	1.39
2	B	350	NAD	C2A-N1A	3.70	1.40	1.33
3	A	450	TCL	C11-CL15	-3.19	1.67	1.74
2	A	300	NAD	C2A-N3A	3.10	1.37	1.32
2	A	300	NAD	C7N-N7N	-3.08	1.27	1.33
2	A	300	NAD	O2B-C2B	-3.07	1.35	1.43
3	A	450	TCL	C8-C9	2.74	1.44	1.39
3	A	400	TCL	C13-C12	2.72	1.43	1.38
3	A	450	TCL	C13-C12	2.71	1.43	1.38
3	B	500	TCL	C3-C2	2.68	1.43	1.38
3	A	450	TCL	C3-C2	2.65	1.43	1.38
3	A	400	TCL	C10-C11	2.54	1.42	1.38
3	A	400	TCL	C8-C9	2.52	1.44	1.39
3	A	450	TCL	C12-C11	2.50	1.42	1.38
3	B	500	TCL	C12-C11	2.46	1.42	1.38
3	A	400	TCL	O7-C8	2.43	1.44	1.39
2	B	350	NAD	O4B-C4B	-2.36	1.39	1.45
3	B	500	TCL	O7-C8	2.28	1.44	1.39
3	A	400	TCL	C12-C11	2.25	1.42	1.38
3	A	400	TCL	C6-C5	2.14	1.44	1.40
2	A	300	NAD	O4D-C4D	-2.14	1.40	1.45
3	A	450	TCL	O17-C6	-2.13	1.32	1.36
2	B	350	NAD	C6A-C5A	-2.07	1.35	1.43
2	A	300	NAD	PN-O2N	-2.00	1.45	1.55

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	350	NAD	O7N-C7N-C3N	-6.38	112.00	119.63
2	A	300	NAD	N3A-C2A-N1A	-5.47	120.13	128.68
2	B	350	NAD	C3N-C7N-N7N	5.35	124.17	117.75
2	A	300	NAD	O7N-C7N-N7N	-4.93	115.58	122.58
3	A	450	TCL	C10-C11-CL15	-4.84	113.10	119.15
2	B	350	NAD	C3B-C2B-C1B	-4.79	93.77	100.98
2	A	300	NAD	C1B-N9A-C4A	-4.62	118.52	126.64
2	B	350	NAD	N3A-C2A-N1A	-4.24	122.05	128.68
3	B	500	TCL	C10-C11-CL15	4.21	124.41	119.15
2	B	350	NAD	C1B-N9A-C4A	-4.17	119.31	126.64
3	A	400	TCL	C10-C9-C8	4.14	126.56	121.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	500	TCL	C13-C12-C11	3.75	123.20	119.24
2	B	350	NAD	C3N-C2N-N1N	-3.62	116.88	120.43
2	A	300	NAD	C3D-C2D-C1D	-3.61	95.54	100.98
2	A	300	NAD	PN-O3-PA	-3.58	120.55	132.83
2	A	300	NAD	O7N-C7N-C3N	3.51	123.83	119.63
3	A	400	TCL	C10-C11-CL15	3.27	123.24	119.15
3	A	450	TCL	O7-C8-C9	-3.25	111.89	119.58
2	B	350	NAD	O4B-C1B-C2B	3.17	111.56	106.93
2	A	300	NAD	O4B-C1B-C2B	-2.89	102.70	106.93
3	A	400	TCL	C13-C12-C11	2.70	122.09	119.24
3	A	450	TCL	C12-C11-C10	2.68	125.09	121.53
2	B	350	NAD	C2B-C3B-C4B	2.62	107.73	102.64
3	B	500	TCL	C12-C11-C10	-2.58	118.10	121.53
2	A	300	NAD	C2B-C3B-C4B	-2.48	97.82	102.64
2	A	300	NAD	O3D-C3D-C2D	-2.43	103.95	111.82
2	B	350	NAD	O2B-C2B-C1B	2.39	119.66	110.85
2	A	300	NAD	C3N-C7N-N7N	2.35	120.57	117.75
2	B	350	NAD	C2N-C3N-C4N	2.29	120.85	118.26
3	A	450	TCL	O17-C6-C5	-2.28	114.76	120.09
3	A	400	TCL	C8-C9-CL16	-2.27	116.75	119.43
3	A	400	TCL	O7-C8-C13	2.23	126.69	120.73
2	A	300	NAD	O5D-C5D-C4D	2.21	116.60	108.99
3	B	500	TCL	C8-O7-C5	2.21	123.29	118.04
2	A	300	NAD	O4B-C4B-C3B	2.16	109.38	105.11
2	A	300	NAD	C2N-C3N-C4N	2.14	120.69	118.26
2	A	300	NAD	C4A-C5A-N7A	-2.13	107.18	109.40
2	B	350	NAD	O2N-PN-O1N	2.12	122.73	112.24
3	A	400	TCL	C1-C6-C5	-2.10	117.66	119.81
2	B	350	NAD	N6A-C6A-N1A	2.09	122.92	118.57
2	A	300	NAD	O2D-C2D-C1D	2.08	118.53	110.85
2	A	300	NAD	C2A-N1A-C6A	2.07	122.30	118.75
2	B	350	NAD	C4A-C5A-N7A	2.05	111.53	109.40
3	A	450	TCL	C13-C8-C9	2.04	122.05	118.84

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	350	NAD	C5B-O5B-PA-O1A
2	B	350	NAD	C5D-O5D-PN-O3
2	B	350	NAD	C5D-O5D-PN-O1N
2	B	350	NAD	C5D-O5D-PN-O2N

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Mol	Chain	Res	Type	Atoms
2	B	350	NAD	O4D-C1D-N1N-C2N
2	B	350	NAD	O4D-C1D-N1N-C6N
2	B	350	NAD	C2D-C1D-N1N-C2N
2	B	350	NAD	C2D-C1D-N1N-C6N
2	A	300	NAD	C5B-O5B-PA-O1A
2	A	300	NAD	PN-O3-PA-O5B
2	A	300	NAD	C5D-O5D-PN-O3
2	A	300	NAD	C5D-O5D-PN-O1N
2	A	300	NAD	C5D-O5D-PN-O2N
2	A	300	NAD	O4D-C1D-N1N-C2N
2	B	350	NAD	O4B-C4B-C5B-O5B
2	B	350	NAD	PN-O3-PA-O5B
2	A	300	NAD	C5B-O5B-PA-O3
2	A	300	NAD	C5B-O5B-PA-O2A
2	B	350	NAD	C5B-O5B-PA-O3
2	A	300	NAD	O4B-C4B-C5B-O5B
2	B	350	NAD	C5B-O5B-PA-O2A

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	350	NAD	3	0
3	A	450	TCL	2	0
2	A	300	NAD	1	0
3	B	500	TCL	6	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 then 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.

Ligand NAD B 350

Bond lengths

Bond angles

Torsions

Rings

Ligand TCL A 400

Bond lengths

Bond angles

Torsions

Rings

Ligand TCL A 450

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD A 300

Bond lengths

Bond angles

Torsions

Rings

Ligand TCL B 500

Bond lengths

Bond angles

Torsions

Rings
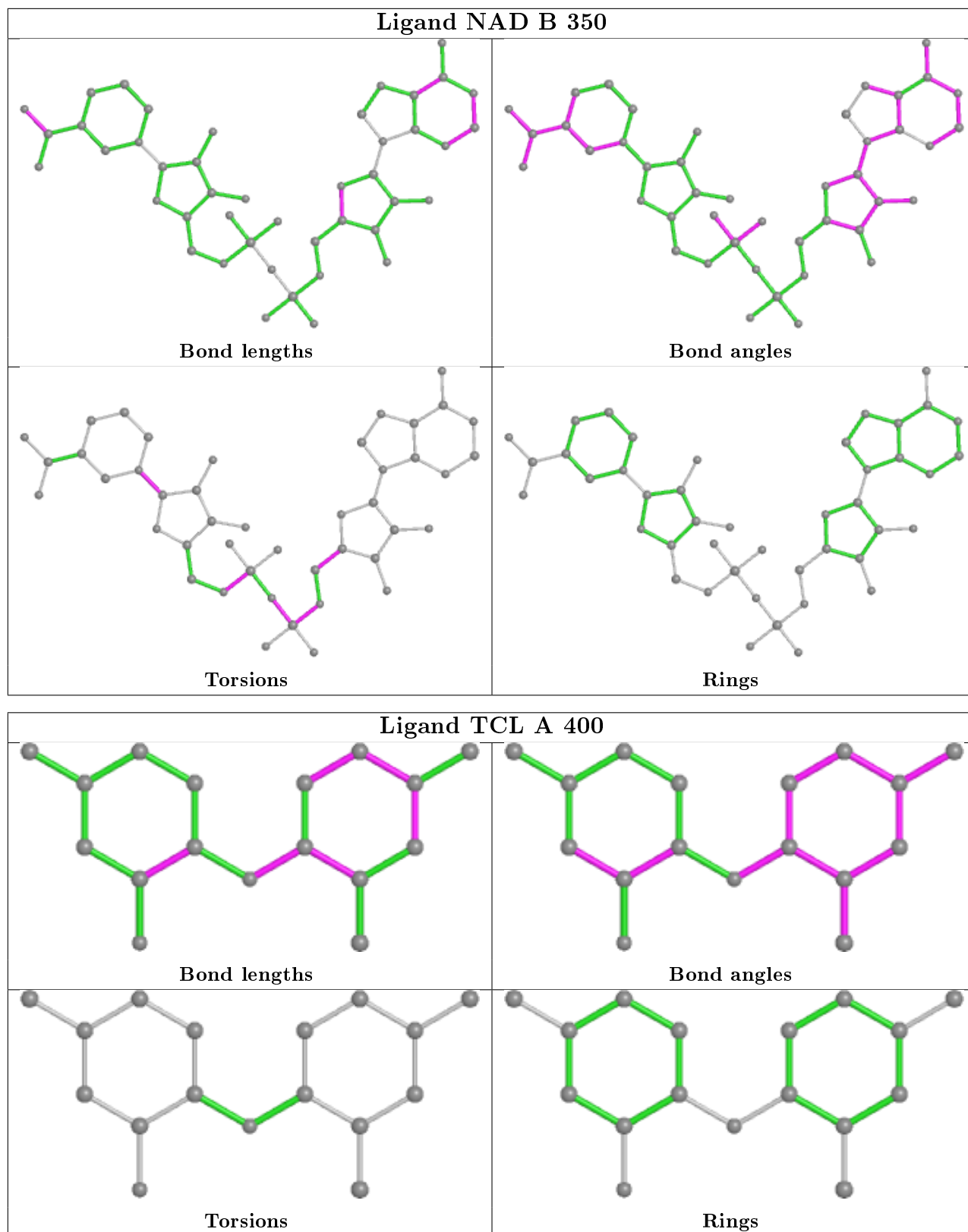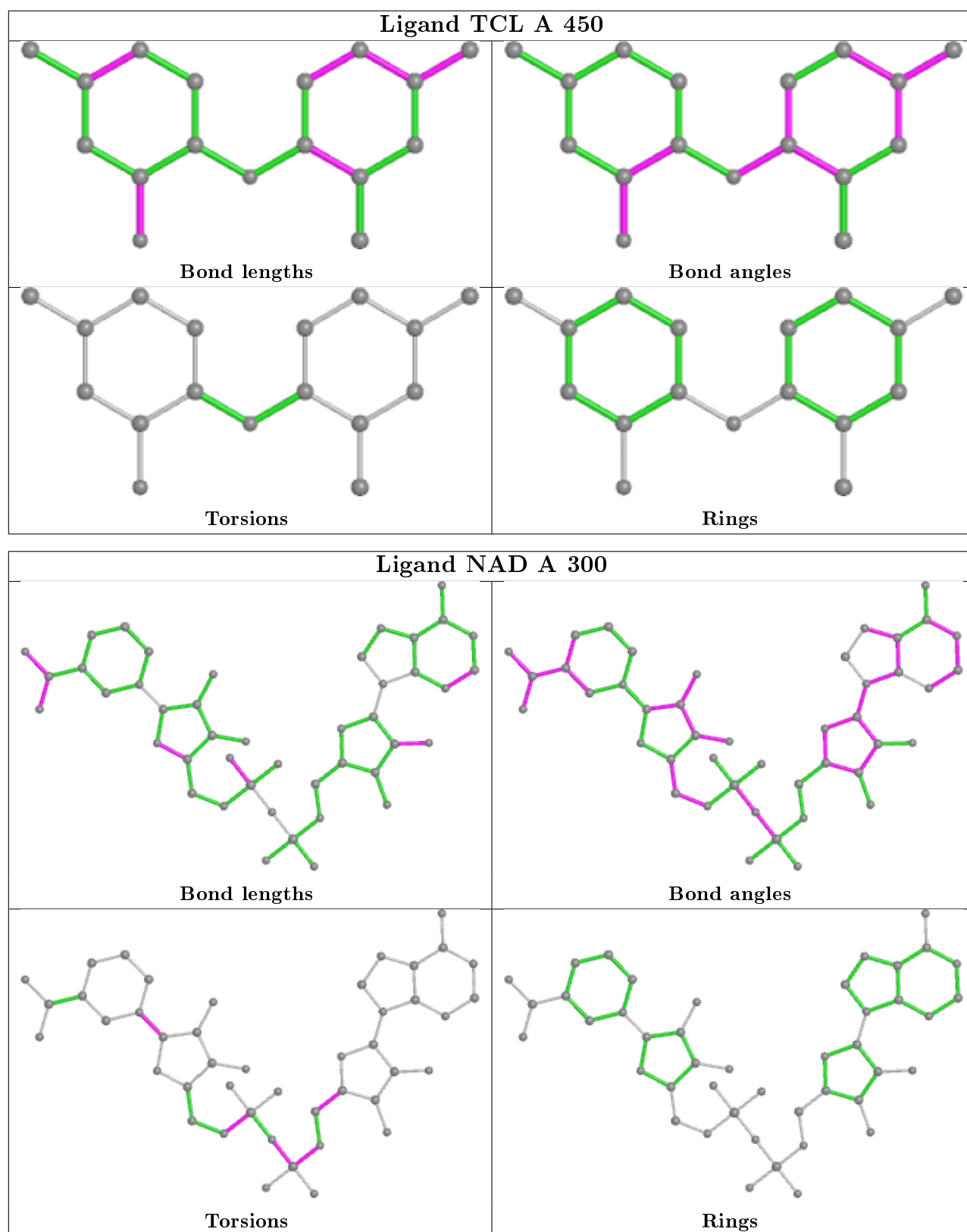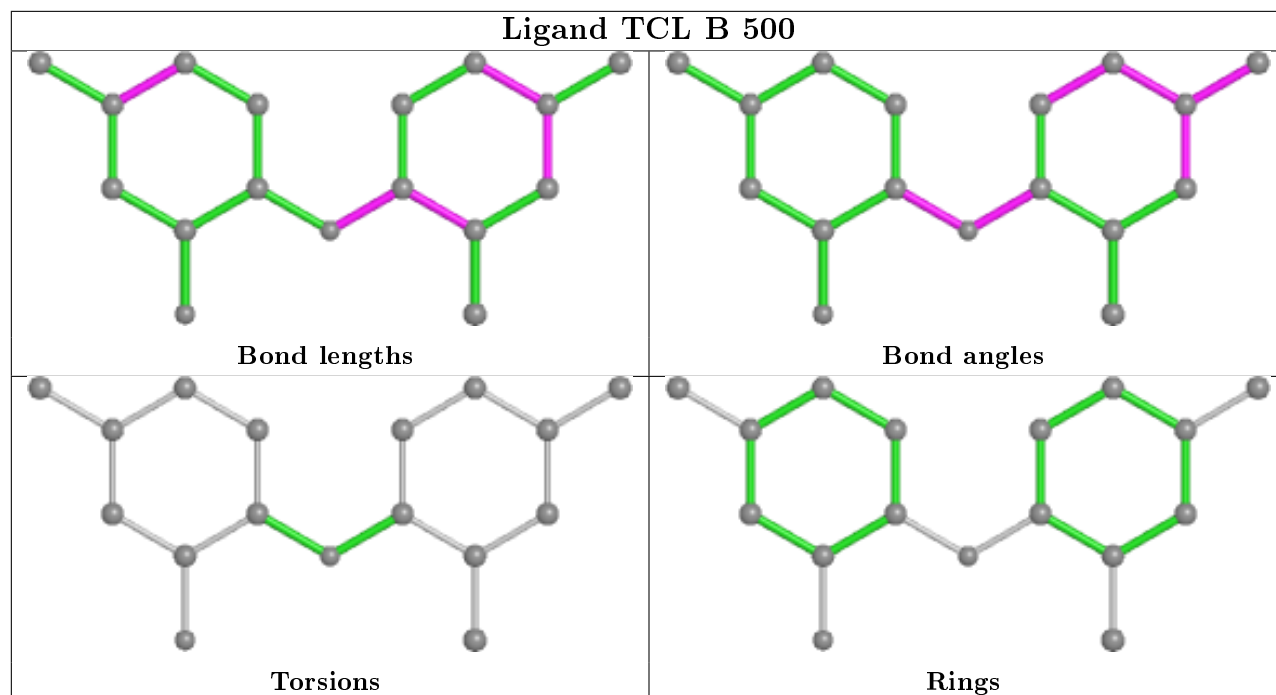
5.7 Other polymers (i)

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(Å²)	Q<0.9
1	A	268/269 (99%)	-0.37	3 (1%)	80	78	32, 51, 72, 87	0
1	B	268/269 (99%)	-0.27	3 (1%)	80	78	29, 50, 82, 102	0
All	All	536/538 (99%)	-0.32	6 (1%)	80	78	29, 51, 77, 102	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	THR	3.8
1	B	210	GLU	3.6
1	B	85	GLY	2.7
1	A	84	ALA	2.6
1	A	45	ARG	2.3
1	A	35	GLN	2.1

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 carbohydrates 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
3	TCL	A	450	17/17	0.92	0.17	62,66,73,75	0
3	TCL	A	400	17/17	0.93	0.14	49,54,58,64	0
3	TCL	B	500	17/17	0.94	0.13	45,49,57,69	0
2	NAD	B	350	44/44	0.95	0.15	35,48,61,61	0
2	NAD	A	300	44/44	0.97	0.14	35,46,53,57	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.
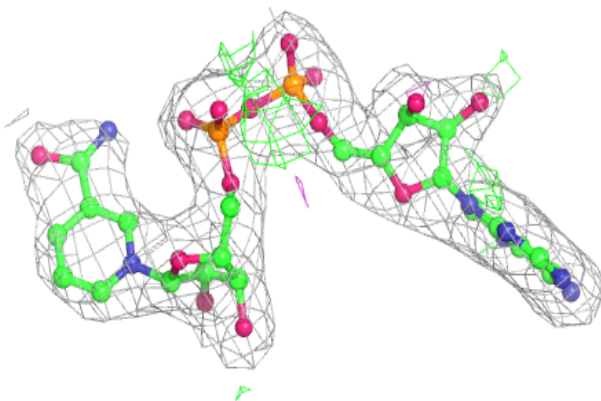

Electron density around TCL A 450:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
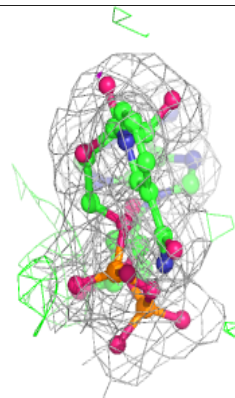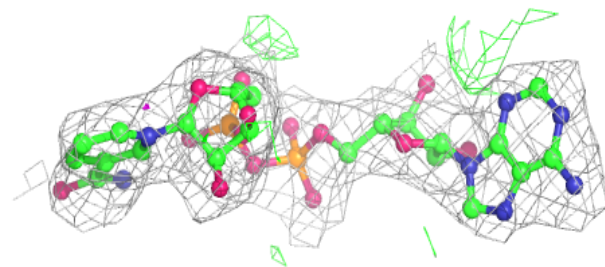mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
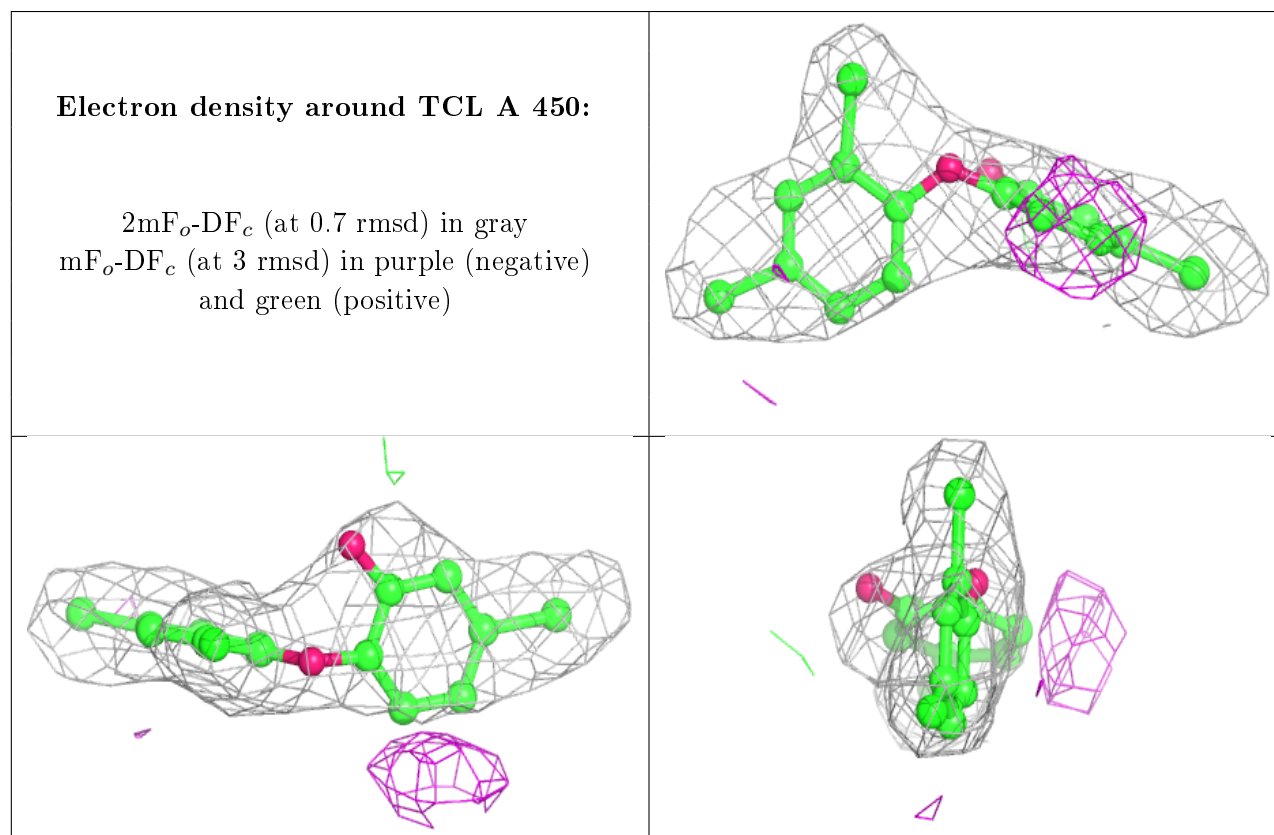
Electron density around TCL A 400:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
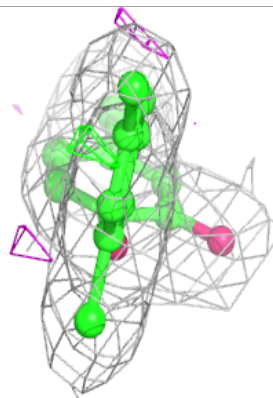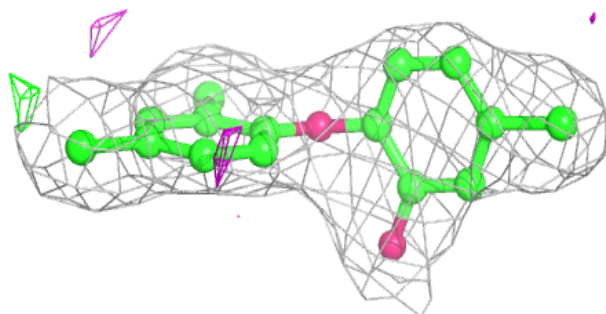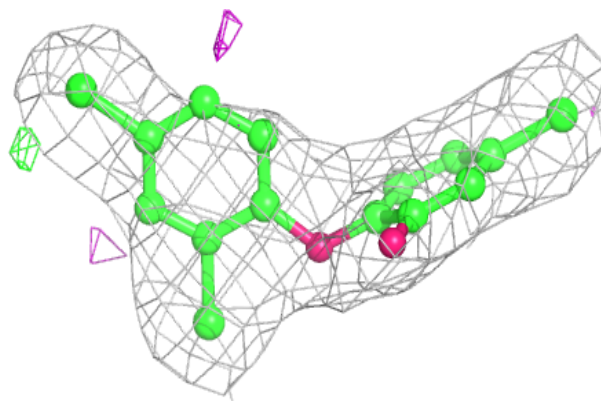
Electron density around TCL B 500:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
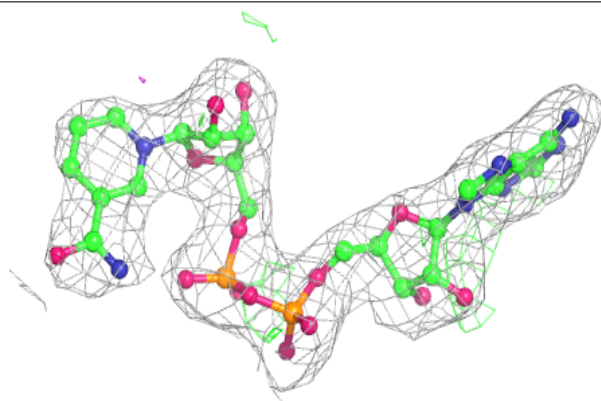$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
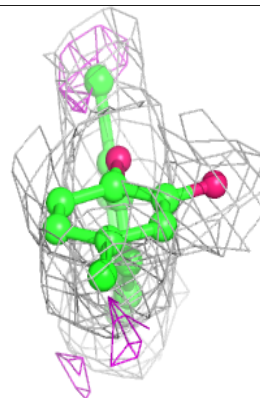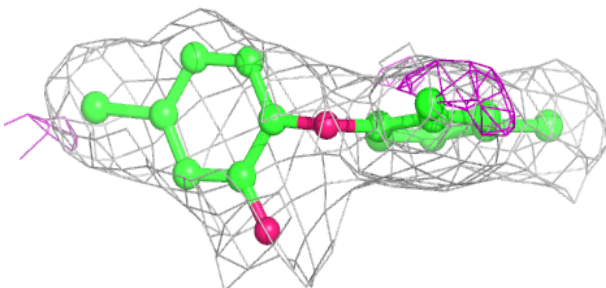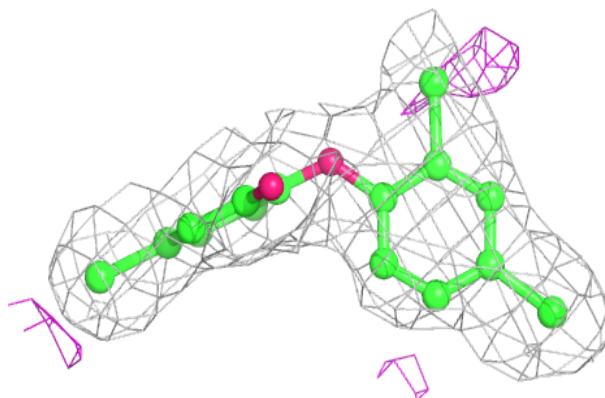
Electron density around NAD B 350:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
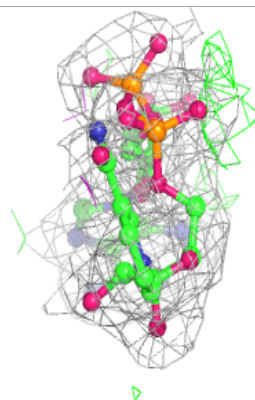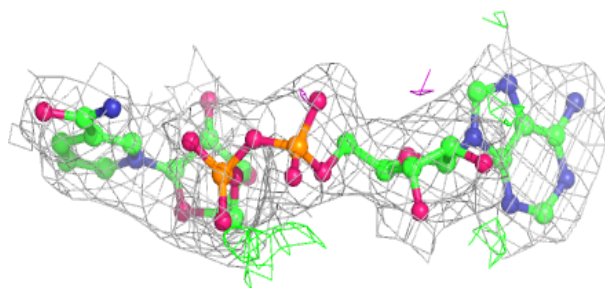
Electron density around NAD A 300:

$2mF_o$-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.