



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:20 am BST

PDB ID : 2OP0
Title : Crystal structure of plasmodium falciparum enoyl ACP reductase with triclosan reductase
Authors : Tsai, H.
Deposited on : 2007-01-26
Resolution : 2.80 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

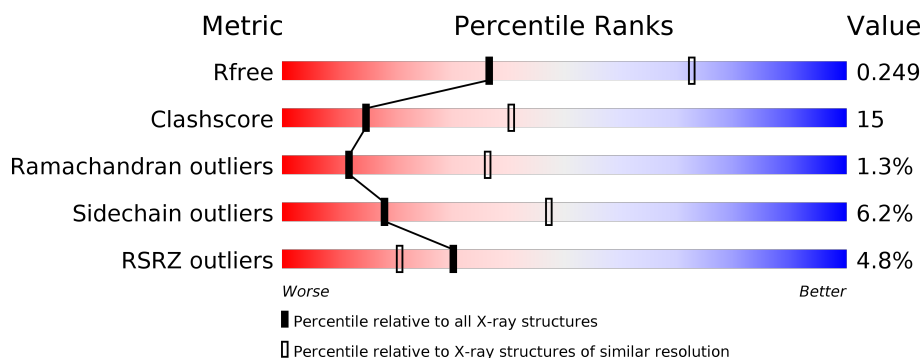
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	338	<div> <div>4%</div> <div> <div></div> <div>56%</div> <div>23%</div> <div>••</div> <div>18%</div> </div> </div>
1	B	338	<div> <div>4%</div> <div> <div></div> <div>61%</div> <div>20%</div> <div>•</div> <div>17%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4597 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 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	0	0
			2192	1400	366	415	11			
1	B	282	Total	C	N	O	S	0	0	0
			2224	1420	374	419	11			

There are 16 discrepancies between the modelled and reference sequences:

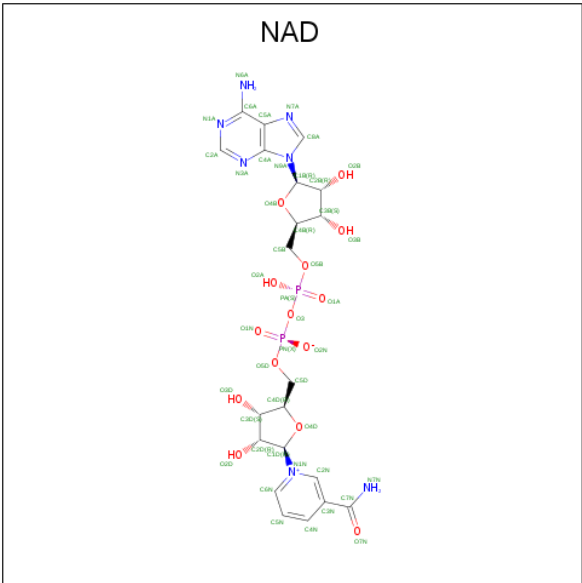
Chain	Residue	Modelled	Actual	Comment	Reference
A	88	MET	-	CLONING ARTIFACT	UNP Q9BH77
A	89	VAL	-	CLONING ARTIFACT	UNP Q9BH77
A	90	HIS	-	EXPRESSION TAG	UNP Q9BH77
A	91	HIS	-	EXPRESSION TAG	UNP Q9BH77
A	92	HIS	-	EXPRESSION TAG	UNP Q9BH77
A	93	HIS	-	EXPRESSION TAG	UNP Q9BH77
A	94	HIS	-	EXPRESSION TAG	UNP Q9BH77
A	95	HIS	-	EXPRESSION TAG	UNP Q9BH77
B	88	MET	-	CLONING ARTIFACT	UNP Q9BH77
B	89	VAL	-	CLONING ARTIFACT	UNP Q9BH77
B	90	HIS	-	EXPRESSION TAG	UNP Q9BH77
B	91	HIS	-	EXPRESSION TAG	UNP Q9BH77
B	92	HIS	-	EXPRESSION TAG	UNP Q9BH77
B	93	HIS	-	EXPRESSION TAG	UNP Q9BH77
B	94	HIS	-	EXPRESSION TAG	UNP Q9BH77
B	95	HIS	-	EXPRESSION TAG	UNP Q9BH77

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



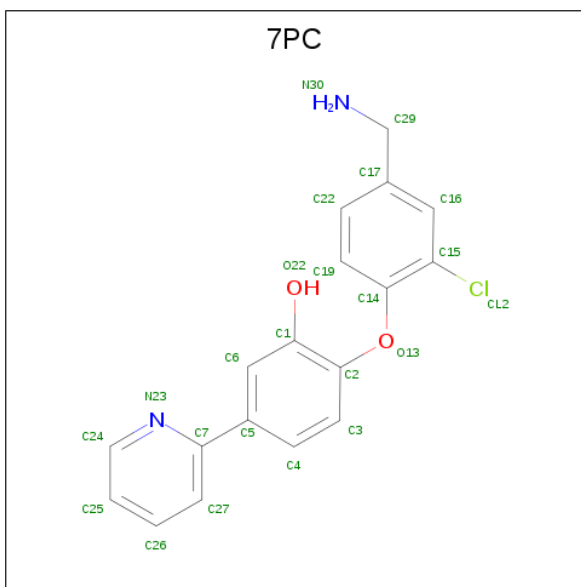
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

- Molecule 4 is 2-[4-(AMINOMETHYL)-2-CHLOROPHENOXY]-5-PYRIDIN-2-YLPHENOL (three-letter code: 7PC) (formula: C₁₈H₁₅ClN₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	Cl	N	O	
			23	18	1	2	2	
							0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	51	Total	O		
			51	51	0	0
5	B	58	Total	O		
			58	58	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	132.31Å 132.31Å 82.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.66 – 2.80 29.93 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.9 (93.66-2.80) 98.0 (29.93-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.04 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.187 , 0.274 0.183 , 0.249	Depositor DCC
R_{free} test set	931 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	40.3	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4597	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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: SO4, NAD, 7PC

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	0.39	0/2232	0.53	0/3009
1	B	0.38	0/2264	0.56	0/3053
All	All	0.39	0/4496	0.54	0/6062

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2192	0	2201	74	0
1	B	2224	0	2241	67	0
2	A	5	0	0	0	0
3	B	44	0	26	1	0
4	B	23	0	10	6	0
5	A	51	0	0	2	0
5	B	58	0	0	5	1
All	All	4597	0	4478	136	1

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 (136) 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:153:ILE:HB	1:B:157:LYS:HB2	1.55	0.89
1:B:254:ASN:HD22	1:B:254:ASN:H	1.22	0.85
1:B:201:LEU:HD21	1:B:205:LYS:HE2	1.62	0.82
1:A:174:ALA:O	1:A:177:ILE:HG22	1.81	0.81
1:A:179:GLU:HA	1:A:180:GLU:C	2.02	0.78
1:A:316:LYS:HA	1:A:316:LYS:HE3	1.66	0.77
1:B:367:THR:HG22	1:B:370:ASP:HB2	1.68	0.76
1:A:105:ILE:HD11	1:A:113:TRP:HE3	1.52	0.75
1:B:372:ALA:HB1	4:B:500:7PC:H25	1.73	0.71
1:A:369:ILE:O	1:A:373:ILE:HG13	1.91	0.70
1:B:219:ALA:HB2	1:B:281:MET:CE	2.23	0.69
1:A:301:ARG:HH21	1:B:379:TYR:HA	1.59	0.68
1:B:201:LEU:O	1:B:202:ILE:HB	1.95	0.66
1:A:301:ARG:NH2	1:B:379:TYR:HA	2.11	0.65
1:A:301:ARG:CD	1:B:383:ARG:HD2	2.26	0.64
1:B:319:ALA:CB	4:B:500:7PC:CL2	2.84	0.63
1:B:319:ALA:HB1	4:B:500:7PC:C15	2.30	0.62
1:A:166:PRO:HB2	1:A:193:TYR:HB3	1.83	0.61
1:A:315:LEU:O	1:A:316:LYS:HB2	2.02	0.59
1:B:254:ASN:HD22	1:B:254:ASN:N	1.91	0.59
1:B:368:PHE:O	1:B:369:ILE:HB	2.02	0.59
1:A:314:PRO:HB2	1:A:373:ILE:HG12	1.85	0.58
1:A:315:LEU:HD21	1:A:388:SER:HB3	1.85	0.58
1:B:219:ALA:HB2	1:B:281:MET:HE1	1.85	0.58
1:A:180:GLU:O	1:A:182:LYS:N	2.38	0.56
1:A:301:ARG:HH11	1:A:301:ARG:HG3	1.70	0.56
1:A:125:LYS:HD2	1:A:160:ASN:HD22	1.70	0.56
1:A:201:LEU:HD22	1:A:205:LYS:HE3	1.88	0.56
1:B:166:PRO:HD2	5:B:539:HOH:O	2.05	0.56
1:B:121:LYS:HG2	1:B:153:ILE:HG21	1.88	0.55
1:A:125:LYS:HD2	1:A:160:ASN:ND2	2.21	0.55
1:A:120:SER:HB3	1:A:153:ILE:HD12	1.89	0.55
1:B:132:PRO:HG2	1:B:187:TYR:CE2	2.41	0.55
1:B:319:ALA:HB1	4:B:500:7PC:C16	2.37	0.54
1:A:422:LEU:HD12	1:A:422:LEU:O	2.07	0.54
1:A:149:ASN:O	1:A:152:ILE:HG12	2.08	0.54
1:A:301:ARG:NH1	1:A:301:ARG:HG3	2.23	0.52
1:A:214:HIS:O	1:A:264:SER:HA	2.09	0.52
1:A:373:ILE:O	1:A:377:GLU:HG3	2.09	0.52
1:A:383:ARG:HE	1:B:301:ARG:HH21	1.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:PHE:O	1:B:151:MET:HG3	2.09	0.52
1:B:319:ALA:HB1	4:B:500:7PC:CL2	2.47	0.51
1:B:369:ILE:HG23	1:B:370:ASP:N	2.25	0.51
1:A:128:PHE:HZ	1:A:159:MET:HE1	1.74	0.51
1:A:131:TRP:CG	1:A:133:PRO:HD2	2.44	0.51
1:B:372:ALA:CB	4:B:500:7PC:H25	2.40	0.51
1:A:378:LYS:HD3	1:A:379:TYR:CE2	2.45	0.51
1:B:144:ASN:HB3	1:B:146:LYS:HE3	1.92	0.50
1:B:201:LEU:HD23	1:B:202:ILE:H	1.77	0.50
1:A:116:ALA:HB1	1:A:159:MET:HE1	1.94	0.50
1:B:125:LYS:HB3	1:B:162:LEU:HD12	1.93	0.50
1:A:151:MET:HE3	1:A:161:ILE:HD12	1.92	0.50
1:B:113:TRP:HE1	1:B:117:LYS:HZ3	1.59	0.50
1:B:368:PHE:O	1:B:369:ILE:CB	2.59	0.50
1:B:127:ILE:HG23	1:B:163:ASP:HB3	1.95	0.49
1:B:244:SER:O	1:B:248:LEU:HB2	2.13	0.49
1:A:301:ARG:HH21	1:B:379:TYR:CA	2.26	0.49
1:B:219:ALA:CB	1:B:281:MET:CE	2.91	0.48
1:B:212:LEU:HB3	1:B:262:ILE:HG12	1.94	0.48
1:B:184:ASN:ND2	1:B:186:ARG:H	2.12	0.48
1:A:277:TYR:CE2	1:A:281:MET:HB3	2.49	0.47
1:B:202:ILE:N	5:B:556:HOH:O	2.47	0.47
1:B:277:TYR:CZ	1:B:281:MET:HG3	2.50	0.46
1:A:109:ASN:HB3	1:A:317:SER:HA	1.96	0.46
1:A:131:TRP:CE2	1:A:133:PRO:HG2	2.50	0.46
1:B:119:LEU:HB3	1:B:124:VAL:HG22	1.96	0.46
1:A:147:PHE:O	1:A:151:MET:HB2	2.14	0.46
1:B:221:GLU:HB3	1:B:224:LYS:HD2	1.96	0.46
1:B:369:ILE:HA	1:B:372:ALA:HB3	1.97	0.46
1:B:204:GLN:HB2	5:B:556:HOH:O	2.16	0.46
1:B:416:GLY:O	1:B:419:ILE:HG12	2.15	0.46
1:B:201:LEU:CD2	1:B:205:LYS:HE2	2.40	0.45
1:B:369:ILE:CG2	1:B:370:ASP:N	2.79	0.45
1:A:166:PRO:HD2	5:A:468:HOH:O	2.17	0.45
1:B:119:LEU:O	1:B:124:VAL:HG13	2.17	0.45
1:B:108:THR:HG22	1:B:113:TRP:CD2	2.51	0.45
1:B:320:ALA:HB1	1:B:369:ILE:HG12	1.98	0.45
1:A:157:LYS:HA	5:A:469:HOH:O	2.16	0.45
1:A:138:PHE:HE2	1:A:164:MET:CE	2.30	0.45
1:A:203:HIS:HB2	1:A:255:ILE:HG21	1.98	0.45
1:B:122:ARG:HH22	1:B:211:MET:CE	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:ILE:HD11	1:B:113:TRP:HE3	1.81	0.45
1:B:288:LEU:HA	5:B:525:HOH:O	2.16	0.45
1:A:281:MET:O	1:A:285:LYS:HG2	2.17	0.44
1:B:182:LYS:HE2	1:B:182:LYS:HB2	1.66	0.44
1:A:378:LYS:HD3	1:A:379:TYR:CZ	2.52	0.44
1:B:122:ARG:HH22	1:B:211:MET:HE2	1.83	0.44
1:B:122:ARG:CG	1:B:122:ARG:O	2.65	0.44
1:A:111:TYR:O	1:A:115:ILE:HG13	2.17	0.44
1:B:108:THR:HG22	1:B:113:TRP:CE2	2.52	0.44
3:B:450:NAD:O2N	3:B:450:NAD:H2N	2.18	0.44
1:A:138:PHE:CE2	1:A:164:MET:CE	3.00	0.44
1:A:128:PHE:CZ	1:A:159:MET:HE1	2.51	0.44
1:A:210:ASN:HA	1:A:260:SER:OG	2.17	0.44
1:A:138:PHE:CE2	1:A:164:MET:HE2	2.52	0.44
1:B:103:ALA:HB1	1:B:167:PHE:CE2	2.53	0.44
1:A:212:LEU:HD21	1:A:248:LEU:HG	1.99	0.43
1:A:398:LEU:HD11	1:A:411:ILE:HG13	1.99	0.43
1:B:252:PHE:O	1:B:256:MET:HG3	2.18	0.43
1:A:109:ASN:CB	1:A:317:SER:HA	2.48	0.43
1:A:259:GLN:HG2	1:A:304:ASN:ND2	2.33	0.43
1:A:306:ARG:HD3	1:A:404:ARG:O	2.17	0.43
1:B:201:LEU:HA	5:B:556:HOH:O	2.17	0.43
1:A:132:PRO:N	1:A:133:PRO:CD	2.82	0.43
1:A:143:LYS:C	1:A:145:GLY:H	2.22	0.43
1:A:131:TRP:CD2	1:A:133:PRO:HD2	2.54	0.43
1:B:138:PHE:CE2	1:B:164:MET:CE	3.02	0.43
1:A:122:ARG:HH22	1:A:211:MET:HE2	1.84	0.42
1:A:265:LEU:HD22	1:A:265:LEU:N	2.34	0.42
1:A:162:LEU:HA	1:A:162:LEU:HD23	1.84	0.42
1:B:113:TRP:HE1	1:B:117:LYS:NZ	2.18	0.42
1:B:255:ILE:O	1:B:255:ILE:HG13	2.18	0.42
1:B:144:ASN:HB2	1:B:146:LYS:HG2	2.01	0.42
1:A:215:SER:HA	1:A:265:LEU:HD23	2.02	0.42
1:A:252:PHE:CD1	1:A:255:ILE:HD11	2.54	0.42
1:A:383:ARG:HD2	1:A:383:ARG:HA	1.53	0.42
1:A:377:GLU:O	1:A:383:ARG:NH1	2.52	0.42
1:A:153:ILE:HD11	1:A:157:LYS:HD3	2.01	0.41
1:A:177:ILE:CD1	1:A:181:THR:HB	2.50	0.41
1:B:121:LYS:HG2	1:B:153:ILE:CG2	2.49	0.41
1:A:171:PHE:CZ	1:A:181:THR:HG21	2.55	0.41
1:A:109:ASN:O	1:A:317:SER:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:ASP:O	1:B:374:GLU:HB2	2.20	0.41
1:A:140:LYS:HB2	1:A:140:LYS:HE3	1.80	0.41
1:A:123:ASN:OD1	1:A:157:LYS:HE2	2.21	0.41
1:A:177:ILE:HD11	1:A:181:THR:HB	2.01	0.41
1:A:234:TYR:O	1:A:237:ALA:HB3	2.20	0.41
1:A:111:TYR:OH	1:A:313:GLY:O	2.38	0.41
1:A:120:SER:HB3	1:A:153:ILE:CD1	2.50	0.41
1:A:222:VAL:HG22	1:A:222:VAL:O	2.19	0.41
1:A:301:ARG:NE	1:B:383:ARG:HD2	2.36	0.40
1:B:261:SER:OG	1:B:399:LEU:HD23	2.20	0.40
1:A:222:VAL:HG13	1:A:223:GLN:HG2	2.03	0.40
1:B:131:TRP:HA	1:B:132:PRO:HD3	1.91	0.40
1:B:382:LEU:HB2	1:B:415:ASN:HB3	2.03	0.40
1:A:156:ASP:CG	1:A:156:ASP:O	2.60	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:543:HOH:O	5:B:545:HOH:O[8_665]	2.03	0.17

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	271/338 (80%)	251 (93%)	16 (6%)	4 (2%)	10	33
1	B	276/338 (82%)	256 (93%)	17 (6%)	3 (1%)	14	41
All	All	547/676 (81%)	507 (93%)	33 (6%)	7 (1%)	12	36

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	181	THR
1	A	316	LYS
1	A	423	PRO
1	B	369	ILE
1	B	404	ARG
1	A	144	ASN
1	B	423	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	241/297 (81%)	226 (94%)	15 (6%)	18	47
1	B	243/297 (82%)	228 (94%)	15 (6%)	18	47
All	All	484/594 (82%)	454 (94%)	30 (6%)	18	47

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	150	ASP
1	A	151	MET
1	A	153	ILE
1	A	162	LEU
1	A	175	ASN
1	A	180	GLU
1	A	181	THR
1	A	183	ASN
1	A	316	LYS
1	A	317	SER
1	A	369	ILE
1	A	383	ARG
1	A	384	GLN
1	A	417	LEU
1	A	422	LEU
1	B	108	THR
1	B	124	VAL

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Mol	Chain	Res	Type
1	B	126	ILE
1	B	137	ILE
1	B	162	LEU
1	B	189	MET
1	B	201	LEU
1	B	226	LEU
1	B	238	LEU
1	B	254	ASN
1	B	261	SER
1	B	290	SER
1	B	323	ILE
1	B	382	LEU
1	B	417	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	ASN
1	A	183	ASN
1	A	200	ASN
1	A	228	ASN
1	A	302	ASN
1	A	304	ASN
1	B	184	ASN
1	B	254	ASN
1	B	302	ASN

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

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAD	B	450	-	42,48,48	1.33	6 (14%)	50,73,73	1.35	9 (18%)
2	SO4	A	426	-	4,4,4	0.42	0	6,6,6	0.26	0
4	7PC	B	500	-	25,25,25	1.51	2 (8%)	34,34,34	2.29	2 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	B	450	-	-	10/26/62/62	0/5/5/5
4	7PC	B	500	-	-	6/10/10/10	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	500	7PC	C29-C17	-6.30	1.29	1.51
3	B	450	NAD	O7N-C7N	4.73	1.33	1.24
3	B	450	NAD	C7N-N7N	-3.15	1.27	1.33
4	B	500	7PC	C15-CL2	2.94	1.80	1.73
3	B	450	NAD	C2A-N1A	-2.93	1.28	1.33
3	B	450	NAD	C2A-N3A	-2.68	1.27	1.32
3	B	450	NAD	C8A-N7A	2.16	1.38	1.34
3	B	450	NAD	O4D-C1D	2.02	1.43	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	500	7PC	C17-C29-N30	12.07	178.76	115.47
3	B	450	NAD	C4A-C5A-N7A	-3.77	105.47	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	450	NAD	C3N-C7N-N7N	3.61	122.08	117.75
3	B	450	NAD	C2A-N1A-C6A	2.63	123.26	118.75
3	B	450	NAD	C3B-C2B-C1B	2.57	104.84	100.98
3	B	450	NAD	PN-O3-PA	-2.40	124.61	132.83
4	B	500	7PC	C24-N23-C7	2.37	120.56	117.23
3	B	450	NAD	N6A-C6A-N1A	2.25	123.25	118.57
3	B	450	NAD	C5A-C6A-N1A	-2.25	115.25	120.35
3	B	450	NAD	N3A-C2A-N1A	-2.24	125.18	128.68
3	B	450	NAD	O7N-C7N-N7N	-2.18	119.48	122.58

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	450	NAD	C5B-O5B-PA-O1A
3	B	450	NAD	PN-O3-PA-O5B
3	B	450	NAD	C5D-O5D-PN-O1N
3	B	450	NAD	C5D-O5D-PN-O2N
3	B	450	NAD	O4B-C4B-C5B-O5B
3	B	450	NAD	C3B-C4B-C5B-O5B
4	B	500	7PC	C6-C5-C7-C27
4	B	500	7PC	C6-C5-C7-N23
4	B	500	7PC	C4-C5-C7-N23
4	B	500	7PC	C4-C5-C7-C27
4	B	500	7PC	C15-C14-O13-C2
3	B	450	NAD	C5B-O5B-PA-O3
3	B	450	NAD	C4B-C5B-O5B-PA
3	B	450	NAD	C5B-O5B-PA-O2A
4	B	500	7PC	C1-C2-O13-C14
3	B	450	NAD	C5D-O5D-PN-O3

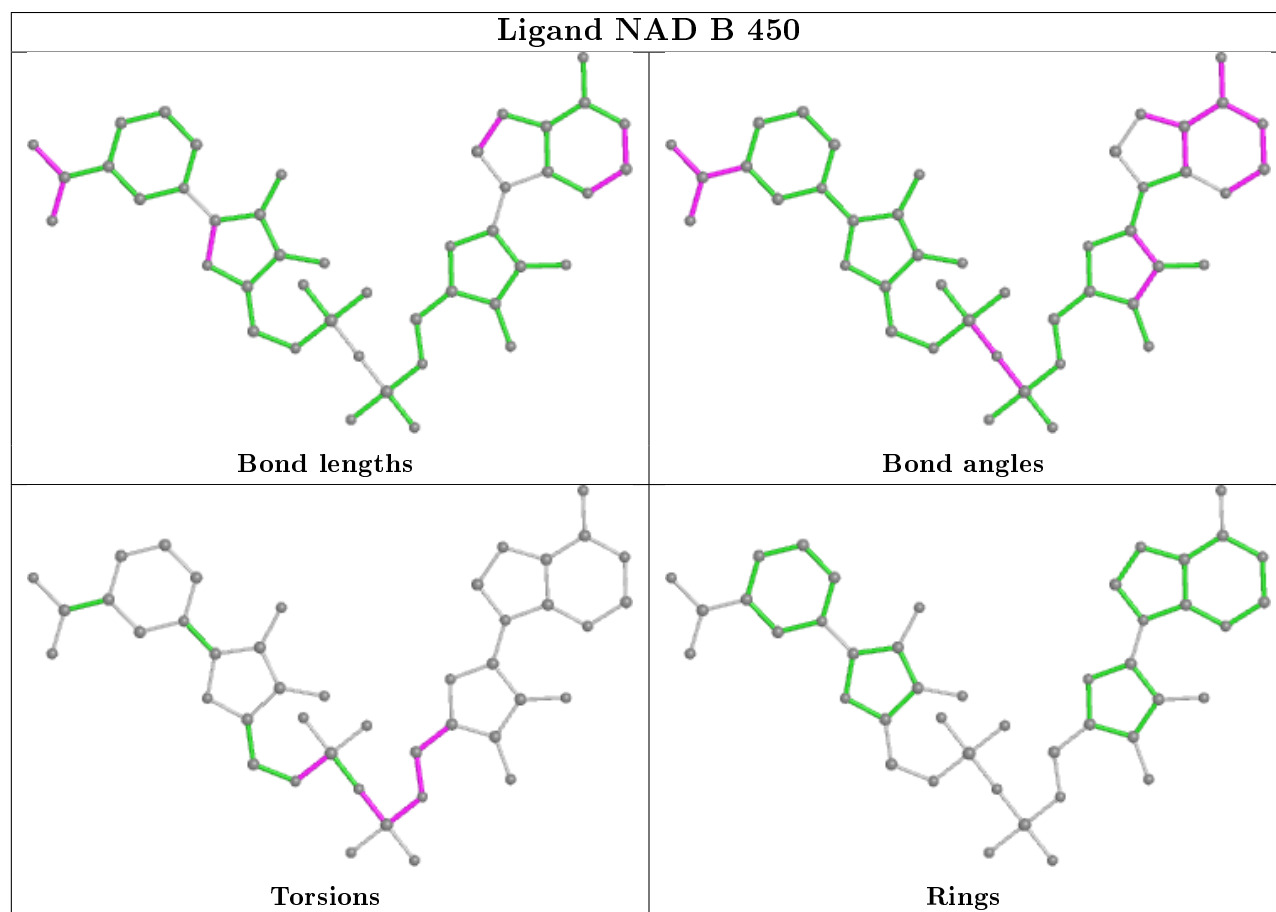
There are no ring outliers.

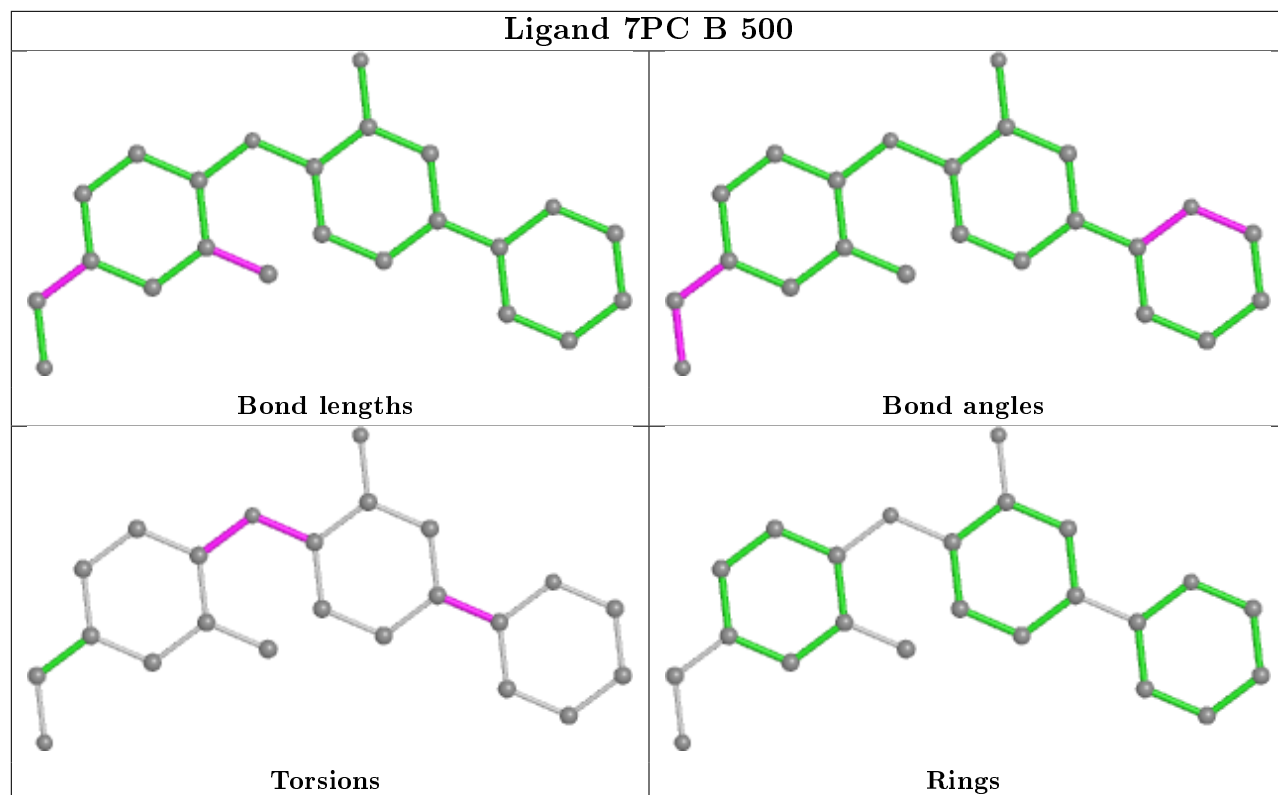
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	450	NAD	1	0
4	B	500	7PC	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	277/338 (81%)	-0.30	15 (5%) 25 17	0, 6, 47, 82	0
1	B	282/338 (83%)	-0.27	12 (4%) 35 25	0, 8, 48, 97	0
All	All	559/676 (82%)	-0.29	27 (4%) 30 21	0, 7, 48, 97	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	367	THR	4.9
1	B	144	ASN	4.7
1	A	181	THR	4.5
1	A	317	SER	4.3
1	A	183	ASN	4.2
1	A	182	LYS	3.8
1	B	149	ASN	3.6
1	B	150	ASP	3.2
1	B	146	LYS	3.1
1	B	145	GLY	3.1
1	B	143	LYS	3.0
1	A	222	VAL	2.9
1	A	180	GLU	2.9
1	A	224	LYS	2.9
1	A	178	ASP	2.8
1	B	371	TYR	2.8
1	B	157	LYS	2.8
1	A	188	ASN	2.7
1	A	179	GLU	2.6
1	B	158	LYS	2.6
1	B	141	ASN	2.5
1	B	152	ILE	2.3
1	A	316	LYS	2.3
1	A	108	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	156	ASP	2.1
1	A	221	GLU	2.1
1	A	123	ASN	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 carbohydrates in this entry.

6.4 Ligands [i](#)

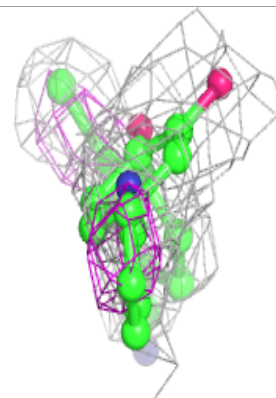
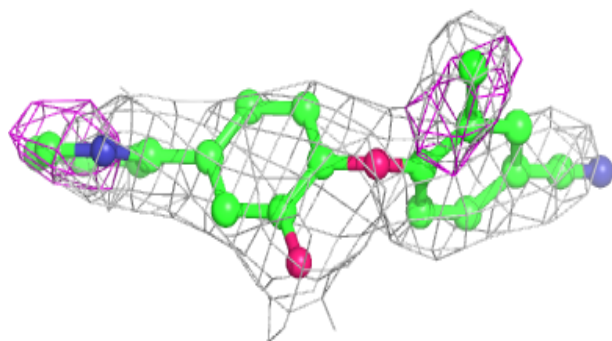
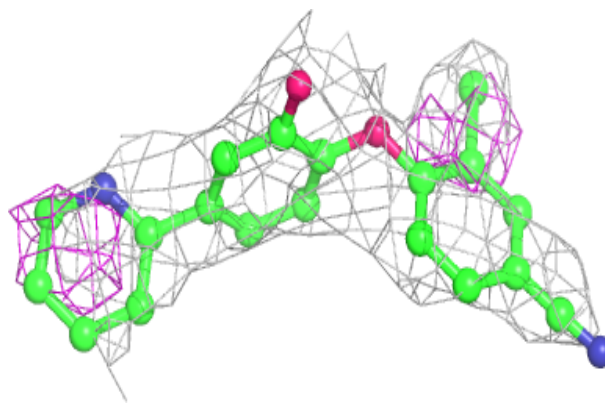
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	A	426	5/5	0.84	0.28	21,30,59,87	0
4	7PC	B	500	23/23	0.91	0.27	8,29,41,42	0
3	NAD	B	450	44/44	0.96	0.12	3,13,26,29	0

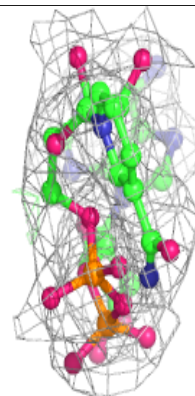
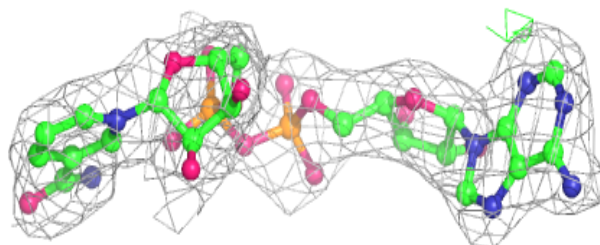
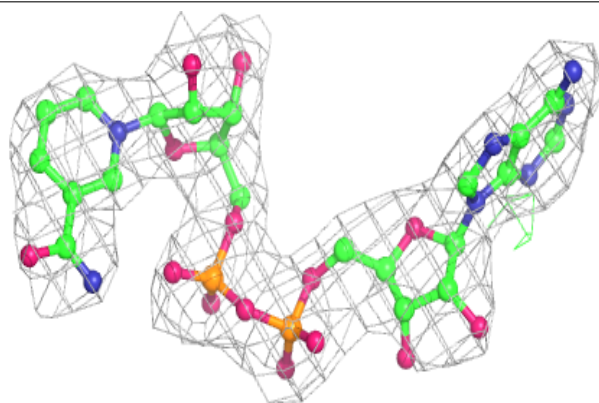
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 7PC 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 B 450:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.