



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:01 PM UTC

PDB ID : 3FNF / pdb_00003fnf
Title : Crystal structure of InhA bound to triclosan derivative
Authors : Wang, F.
Deposited on : 2008-12-24
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

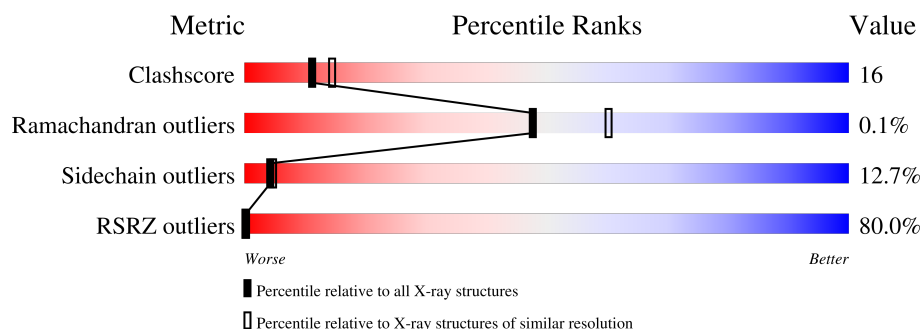
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	269	77% 70% 23% 5%
1	B	269	75% 64% 24% 5% 7%
1	C	269	78% 70% 22% • • •
1	D	269	77% 66% 26% • •

2 Entry composition [i](#)

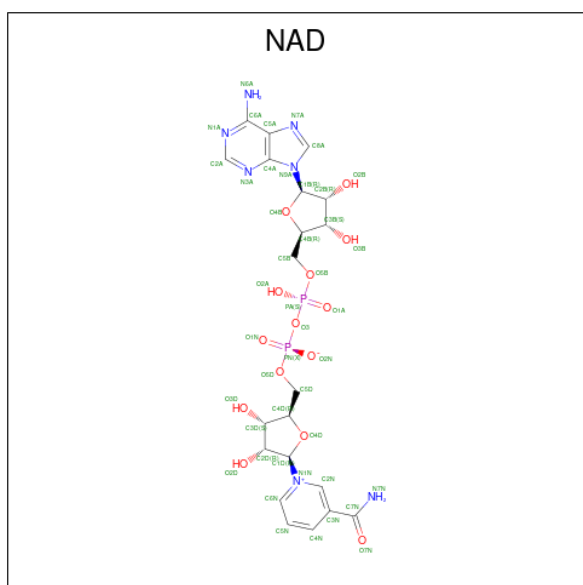
There are 4 unique types of molecules in this entry. The entry contains 8260 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	249	Total	C	N	O	S	0	0	0
			1866	1183	327	346	10			
1	C	261	Total	C	N	O	S	0	0	0
			1953	1238	341	364	10			
1	D	257	Total	C	N	O	S	0	0	0
			1926	1221	337	358	10			

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



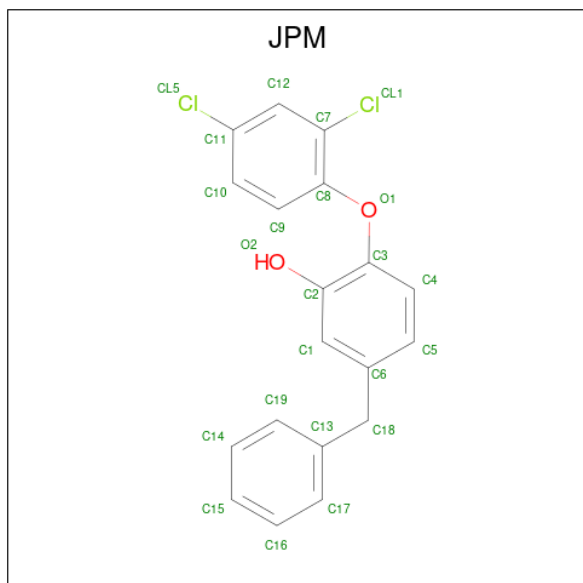
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0
			44	21	7	14	2	0
2	B	1	Total	C	N	O	P	0
			44	21	7	14	2	0

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

- Molecule 3 is 5-benzyl-2-(2,4-dichlorophenoxy)phenol (CCD ID: JPM) (formula: C₁₉H₁₄Cl₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	O		
			23	19	2	2	0	0
3	B	1	Total	C	Cl	O		
			23	19	2	2	0	0
3	C	1	Total	C	Cl	O		
			23	19	2	2	0	0
3	D	1	Total	C	Cl	O		
			23	19	2	2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	68	Total	O		
			68	68	0	0
4	B	64	Total	O		
			64	64	0	0
4	C	63	Total	O		
			63	63	0	0

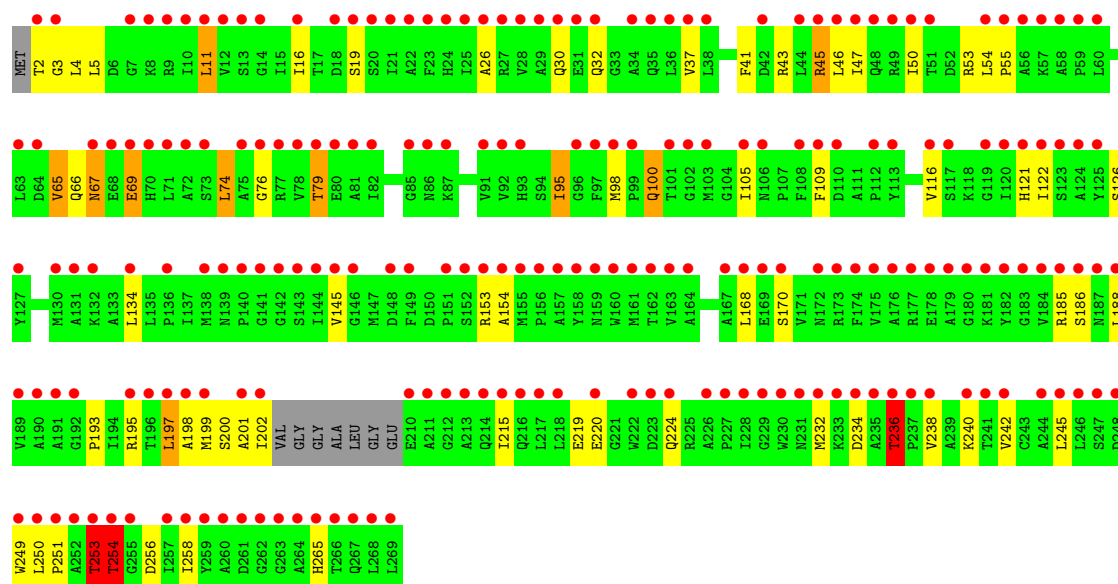
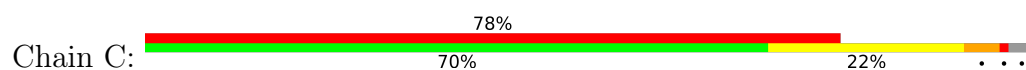
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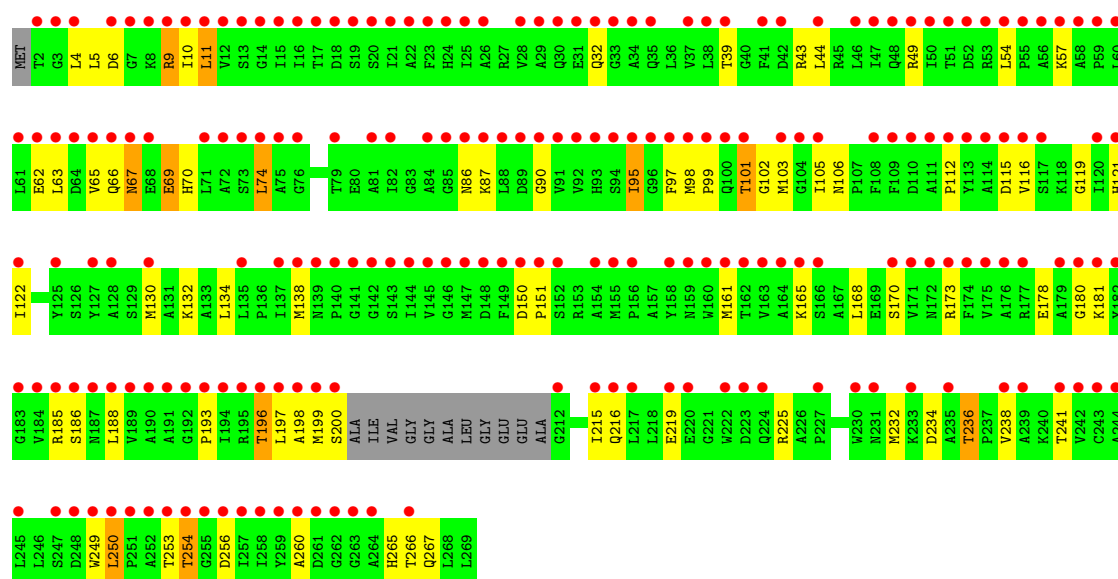
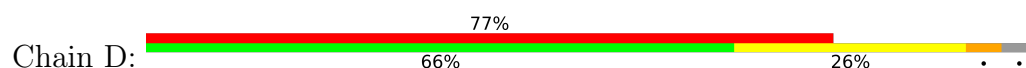
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	58	Total	O	0	0
			58	58		



• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	125.65Å 92.38Å 102.41Å 90.00° 106.51° 90.00°	Depositor
Resolution (Å)	19.85 – 2.30 19.85 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.8 (19.85-2.30) 8.6 (19.85-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.200 , 0.260 0.581 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 996.5	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.36	EDS
Total number of atoms	8260	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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: NAD, JPM

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	0.88	3/2032 (0.1%)	1.08	4/2758 (0.1%)
1	B	0.87	0/1903	1.07	3/2582 (0.1%)
1	C	0.82	2/1990 (0.1%)	1.04	1/2700 (0.0%)
1	D	0.78	0/1963	1.02	1/2663 (0.0%)
All	All	0.84	5/7888 (0.1%)	1.05	9/10703 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	238	VAL	CA-CB	5.71	1.62	1.54
1	A	253	THR	CA-CB	5.71	1.62	1.53
1	C	236	THR	CA-CB	5.68	1.61	1.53
1	C	253	THR	CA-CB	5.29	1.61	1.53
1	A	236	THR	CA-CB	5.17	1.61	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	198	ALA	N-CA-C	9.59	124.97	113.28
1	A	200	SER	N-CA-C	7.52	120.20	111.02
1	D	103	MET	N-CA-C	5.74	117.25	108.12
1	A	254	THR	CB-CA-C	-5.51	98.61	110.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	ALA	CA-C-N	-5.41	114.67	120.03
1	A	111	ALA	C-N-CA	-5.41	114.67	120.03
1	B	198	ALA	CA-C-N	5.09	130.87	121.70
1	B	198	ALA	C-N-CA	5.09	130.87	121.70
1	C	254	THR	CB-CA-C	-5.09	99.32	110.67

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	211	ALA	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1994	0	2008	74	0
1	B	1866	0	1877	68	0
1	C	1953	0	1967	67	0
1	D	1926	0	1940	71	0
2	A	44	0	26	2	0
2	B	44	0	26	2	0
2	C	44	0	26	1	0
2	D	44	0	26	3	0
3	A	23	0	13	0	0
3	B	23	0	13	2	0
3	C	23	0	13	1	0
3	D	23	0	13	3	0
4	A	68	0	0	6	0
4	B	64	0	0	5	0
4	C	63	0	0	9	0
4	D	58	0	0	4	0
All	All	8260	0	7948	260	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 16.

All (260) 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:16:ILE:HG23	1:B:197:LEU:CD2	1.73	1.18
1:B:197:LEU:H	1:B:197:LEU:HD12	1.15	1.09
1:B:106:ASN:HB2	4:B:304:HOH:O	1.50	1.08
1:A:211:ALA:HA	1:A:214:GLN:HB2	1.36	1.05
1:C:186:SER:H	1:C:254:THR:HG22	1.25	0.97
1:B:197:LEU:H	1:B:197:LEU:CD1	1.75	0.96
1:B:98:MET:HE1	1:B:116:VAL:HA	1.48	0.94
1:B:16:ILE:CG2	1:B:197:LEU:CD2	2.47	0.93
1:D:186:SER:H	1:D:254:THR:HG22	1.32	0.92
1:C:100:GLN:HG3	4:C:327:HOH:O	1.69	0.91
1:D:106:ASN:HB2	4:D:279:HOH:O	1.69	0.91
1:C:4:LEU:H	1:C:32:GLN:HE21	1.17	0.90
1:C:98:MET:HE1	1:C:116:VAL:HA	1.51	0.90
1:A:254:THR:HG21	4:A:273:HOH:O	1.72	0.88
1:C:195:ARG:HE	1:C:232:MET:HE2	1.39	0.88
1:D:98:MET:HE1	1:D:116:VAL:HA	1.55	0.86
1:B:16:ILE:HG23	1:B:197:LEU:HD21	1.57	0.86
1:B:256:ASP:OD2	1:C:265:HIS:HE1	1.58	0.86
1:C:215:ILE:HG23	1:C:232:MET:HE1	1.58	0.85
1:B:196:THR:HG23	1:B:198:ALA:H	1.44	0.83
1:B:221:GLY:HA2	4:B:284:HOH:O	1.77	0.83
1:B:101:THR:HG21	1:B:112:PRO:HD2	1.60	0.82
1:D:95:ILE:HD11	1:D:122:ILE:HG23	1.60	0.82
1:C:220:GLU:O	1:C:224:GLN:HG3	1.80	0.81
1:A:195:ARG:HG3	1:A:195:ARG:HH11	1.47	0.80
1:D:95:ILE:CD1	1:D:122:ILE:HG23	2.11	0.79
1:B:197:LEU:HD12	1:B:197:LEU:N	1.96	0.79
1:C:65:VAL:HG11	1:C:126:SER:HB3	1.65	0.79
1:A:186:SER:H	1:A:254:THR:CG2	1.96	0.79
1:C:65:VAL:CG1	1:C:126:SER:HB3	2.13	0.79
1:B:16:ILE:HG23	1:B:197:LEU:HD23	1.64	0.77
1:D:74:LEU:HD13	1:D:134:LEU:HD21	1.67	0.77
1:D:196:THR:HG22	1:D:199:MET:H	1.49	0.77
1:C:245:LEU:HD11	1:C:258:ILE:HD13	1.68	0.76
1:A:153:ARG:HD2	4:A:331:HOH:O	1.84	0.76
1:C:4:LEU:H	1:C:32:GLN:NE2	1.84	0.75
1:A:4:LEU:H	1:A:32:GLN:HE21	1.33	0.75
1:B:4:LEU:H	1:B:32:GLN:HE21	1.34	0.75
1:D:74:LEU:CD1	1:D:134:LEU:HD21	2.18	0.74
1:A:105:ILE:HD11	1:A:210:GLU:O	1.87	0.74
1:A:153:ARG:NH2	1:C:153:ARG:NH2	2.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:THR:HG21	4:B:272:HOH:O	1.88	0.72
1:A:186:SER:H	1:A:254:THR:HG22	1.55	0.72
1:B:253:THR:HG23	4:C:272:HOH:O	1.88	0.72
1:A:256:ASP:OD2	1:D:265:HIS:HE1	1.73	0.72
1:A:196:THR:HG23	1:A:198:ALA:H	1.55	0.71
1:C:45:ARG:H	1:C:45:ARG:HE	1.36	0.71
1:B:75:ALA:O	1:B:79:THR:HG23	1.90	0.71
1:B:16:ILE:CG2	1:B:197:LEU:HD22	2.20	0.71
1:A:68:GLU:HB2	4:A:314:HOH:O	1.92	0.70
1:C:65:VAL:HG11	1:C:126:SER:CB	2.21	0.70
1:D:44:LEU:HD21	1:D:62:GLU:HB2	1.73	0.70
1:A:259:TYR:O	1:D:253:THR:HG22	1.92	0.70
1:B:256:ASP:OD2	1:C:265:HIS:CE1	2.45	0.70
1:D:185:ARG:HA	1:D:254:THR:CG2	2.22	0.69
1:D:196:THR:HG23	1:D:198:ALA:H	1.56	0.69
1:B:101:THR:HG23	1:B:111:ALA:HA	1.72	0.69
1:A:101:THR:HG23	1:A:111:ALA:HA	1.76	0.68
1:A:2:THR:O	1:A:6:ASP:OD2	2.11	0.68
1:B:196:THR:HG21	2:B:310:NAD:O1N	1.93	0.67
4:A:271:HOH:O	1:D:253:THR:HG23	1.94	0.67
1:B:153:ARG:HD2	1:D:265:HIS:O	1.93	0.67
1:A:67:ASN:C	1:A:67:ASN:HD22	2.03	0.66
1:B:253:THR:CG2	4:C:272:HOH:O	2.44	0.66
1:C:234:ASP:OD1	1:C:236:THR:HG23	1.96	0.65
1:A:35:GLN:HB3	4:A:294:HOH:O	1.96	0.65
1:A:196:THR:HG21	2:A:300:NAD:O1N	1.97	0.65
1:C:186:SER:N	1:C:254:THR:HG22	2.08	0.64
1:C:185:ARG:HD3	4:C:289:HOH:O	1.98	0.64
1:C:254:THR:HG21	4:C:299:HOH:O	1.98	0.64
1:A:153:ARG:CD	4:A:331:HOH:O	2.46	0.63
1:D:215:ILE:HG22	1:D:219:GLU:OE1	1.99	0.63
1:C:199:MET:O	1:C:201:ALA:HA	1.98	0.63
1:B:186:SER:H	1:B:254:THR:HG23	1.62	0.63
1:D:241:THR:HG21	1:D:260:ALA:HB2	1.82	0.62
1:B:153:ARG:HD2	1:D:266:THR:HA	1.80	0.62
1:A:227:PRO:O	1:D:180:GLY:HA3	2.00	0.62
1:B:265:HIS:HE1	1:C:256:ASP:OD2	1.83	0.61
1:D:67:ASN:HD21	1:D:69:GLU:HB3	1.65	0.61
1:D:196:THR:HG21	2:D:330:NAD:O1N	2.01	0.61
1:A:100:GLN:CD	1:A:100:GLN:H	2.09	0.61
1:A:101:THR:HG21	1:A:115:ASP:OD2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ARG:HA	1:A:254:THR:HG23	1.84	0.60
1:B:200:SER:O	1:B:200:SER:OG	2.16	0.60
1:C:185:ARG:HA	1:C:254:THR:CG2	2.31	0.60
1:C:79:THR:HG23	4:C:296:HOH:O	2.02	0.59
1:D:4:LEU:H	1:D:32:GLN:HE21	1.49	0.59
1:C:43:ARG:O	1:C:47:ILE:HG13	2.02	0.59
1:C:202:ILE:HG22	1:C:202:ILE:O	2.03	0.58
1:B:220:GLU:HA	4:B:298:HOH:O	2.03	0.58
1:D:161:MET:HE3	1:D:165:LYS:HE2	1.85	0.58
1:B:67:ASN:HD21	1:B:69:GLU:HG2	1.68	0.58
1:C:65:VAL:CG1	1:C:126:SER:CB	2.81	0.57
1:B:185:ARG:NH2	4:B:334:HOH:O	2.37	0.57
1:D:4:LEU:HB3	1:D:32:GLN:HG3	1.86	0.57
1:A:49:ARG:O	1:A:53:ARG:NE	2.38	0.57
1:D:9:ARG:HH21	1:D:86:ASN:CG	2.13	0.57
1:A:173:ARG:HB3	1:B:154:ALA:HB2	1.85	0.57
1:C:67:ASN:C	1:C:67:ASN:HD22	2.12	0.57
1:B:222:TRP:HE1	1:B:261:ASP:HB2	1.69	0.57
1:C:16:ILE:HD11	1:C:43:ARG:HD2	1.86	0.56
1:D:4:LEU:H	1:D:32:GLN:HG3	1.71	0.56
1:D:70:HIS:O	1:D:74:LEU:HB2	2.05	0.56
1:B:258:ILE:HD12	1:B:258:ILE:N	2.22	0.55
1:C:95:ILE:CD1	1:C:122:ILE:HG23	2.36	0.55
1:A:186:SER:H	1:A:254:THR:HG23	1.71	0.55
1:B:153:ARG:CD	1:D:266:THR:HA	2.37	0.55
1:D:101:THR:HG21	1:D:115:ASP:OD2	2.07	0.55
1:D:134:LEU:O	1:D:138:MET:HG3	2.06	0.55
1:A:265:HIS:HE1	1:D:256:ASP:OD2	1.90	0.54
1:D:234:ASP:OD1	1:D:236:THR:HG23	2.07	0.54
1:A:16:ILE:HG23	1:A:17:THR:HG23	1.89	0.54
1:A:256:ASP:OD2	1:D:265:HIS:CE1	2.58	0.54
1:C:65:VAL:HG13	1:C:126:SER:HB3	1.87	0.54
1:B:186:SER:H	1:B:254:THR:CG2	2.21	0.54
1:D:215:ILE:O	1:D:219:GLU:HG2	2.08	0.53
1:B:65:VAL:HG11	1:B:95:ILE:HD11	1.89	0.53
1:D:198:ALA:HB1	3:D:430:JPM:C7	2.39	0.53
1:C:76:GLY:HA3	4:C:326:HOH:O	2.09	0.53
1:A:46:LEU:HD12	1:A:49:ARG:NH2	2.23	0.53
1:A:45:ARG:HE	1:A:49:ARG:HH21	1.57	0.53
1:A:67:ASN:HD21	1:A:69:GLU:HB2	1.73	0.53
1:C:95:ILE:HD11	1:C:122:ILE:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:ARG:HE	1:C:232:MET:CE	2.19	0.52
1:B:194:ILE:O	1:B:200:SER:HB3	2.09	0.52
1:A:101:THR:HG21	1:A:112:PRO:HD2	1.92	0.52
1:A:100:GLN:H	1:A:100:GLN:NE2	2.08	0.51
1:D:4:LEU:CB	1:D:32:GLN:HG3	2.40	0.51
1:B:101:THR:CG2	1:B:111:ALA:HA	2.39	0.51
1:C:30:GLN:OE1	1:C:55:PRO:HD2	2.09	0.51
1:D:199:MET:O	1:D:200:SER:CB	2.57	0.51
1:D:254:THR:HG21	4:D:276:HOH:O	2.09	0.51
1:C:11:LEU:HA	1:C:37:VAL:O	2.11	0.51
1:B:4:LEU:H	1:B:32:GLN:NE2	2.05	0.51
1:B:196:THR:HG22	1:B:199:MET:O	2.11	0.51
1:A:45:ARG:NH2	1:A:49:ARG:HH22	2.09	0.51
1:B:23:PHE:CE2	1:B:54:LEU:HD13	2.46	0.51
1:B:227:PRO:HD2	1:B:262:GLY:O	2.10	0.51
1:A:195:ARG:HH11	1:A:195:ARG:CG	2.21	0.50
1:B:78:VAL:O	1:B:82:ILE:HG12	2.11	0.50
1:D:178:GLU:HA	1:D:181:LYS:HE2	1.93	0.50
1:D:198:ALA:HB1	3:D:430:JPM:C8	2.41	0.50
1:D:95:ILE:CD1	1:D:122:ILE:CG2	2.87	0.50
1:A:45:ARG:NE	1:A:49:ARG:HH21	2.10	0.49
1:D:67:ASN:HD22	1:D:70:HIS:H	1.60	0.49
1:A:211:ALA:CA	1:A:214:GLN:HB2	2.25	0.49
1:C:197:LEU:O	1:C:200:SER:O	2.29	0.49
1:A:117:SER:OG	1:B:117:SER:OG	2.27	0.49
1:A:65:VAL:HG13	1:A:126:SER:CB	2.42	0.49
1:D:101:THR:HG21	1:D:112:PRO:HD2	1.95	0.49
1:A:46:LEU:HD12	1:A:49:ARG:HH22	1.77	0.49
1:A:66:GLN:HE21	1:A:121:HIS:CD2	2.31	0.49
1:B:236:THR:HG22	1:B:240:LYS:HE3	1.94	0.48
1:D:10:ILE:HG12	1:D:90:GLY:HA3	1.93	0.48
1:D:97:PHE:O	1:D:119:GLY:HA2	2.13	0.48
1:A:65:VAL:HG13	1:A:126:SER:HB3	1.95	0.48
1:B:194:ILE:O	1:B:200:SER:CB	2.61	0.48
1:C:43:ARG:NE	4:C:319:HOH:O	2.47	0.48
1:A:113:TYR:CE2	1:B:121:HIS:HB2	2.48	0.48
1:C:154:ALA:HB2	1:D:173:ARG:HB3	1.94	0.48
1:D:225:ARG:HD2	1:D:267:GLN:O	2.14	0.48
1:C:26:ALA:O	1:C:30:GLN:HG3	2.14	0.48
1:A:153:ARG:HH21	1:C:153:ARG:NH2	2.12	0.47
1:D:66:GLN:HE21	1:D:121:HIS:CD2	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:LEU:N	1:D:32:GLN:HG3	2.29	0.47
1:A:65:VAL:CG1	1:A:126:SER:CB	2.93	0.47
1:A:185:ARG:HA	1:A:254:THR:CG2	2.44	0.47
1:C:193:PRO:HA	2:C:320:NAD:O7N	2.15	0.47
1:D:186:SER:N	1:D:254:THR:HG22	2.15	0.47
1:D:11:LEU:HD13	1:D:11:LEU:C	2.40	0.47
1:D:98:MET:HE3	1:D:99:PRO:HD2	1.96	0.47
1:D:249:TRP:O	1:D:250:LEU:HD13	2.15	0.47
1:A:185:ARG:CA	1:A:254:THR:HG23	2.44	0.46
1:D:49:ARG:NE	4:D:293:HOH:O	2.40	0.46
1:D:185:ARG:HA	1:D:254:THR:HG23	1.96	0.46
1:C:67:ASN:HD22	1:C:69:GLU:H	1.63	0.46
1:C:41:PHE:C	1:C:41:PHE:CD1	2.93	0.46
1:D:196:THR:HG23	1:D:198:ALA:N	2.29	0.46
1:C:46:LEU:HD12	1:C:46:LEU:C	2.40	0.46
1:C:185:ARG:CG	1:C:254:THR:HG23	2.46	0.46
1:A:52:ASP:HB2	1:A:53:ARG:HH21	1.80	0.45
1:A:11:LEU:HD21	1:A:39:THR:CG2	2.46	0.45
1:D:4:LEU:HB3	1:D:32:GLN:CG	2.45	0.45
1:A:65:VAL:HB	2:A:300:NAD:N1A	2.31	0.45
1:A:220:GLU:O	1:A:224:GLN:HG3	2.17	0.45
1:C:236:THR:O	1:C:240:LYS:HG3	2.16	0.45
1:A:65:VAL:CG1	1:A:126:SER:HB3	2.47	0.45
1:A:211:ALA:HA	1:A:214:GLN:CB	2.26	0.45
1:C:46:LEU:O	1:C:50:ILE:HG12	2.16	0.45
1:A:105:ILE:HD12	1:A:105:ILE:HA	1.76	0.45
1:C:234:ASP:OD1	1:C:236:THR:CG2	2.63	0.45
1:A:52:ASP:HB2	1:A:53:ARG:HE	1.82	0.45
1:C:198:ALA:HB1	3:C:420:JPM:C7	2.47	0.45
1:B:259:TYR:O	1:C:253:THR:HB	2.17	0.44
1:A:67:ASN:C	1:A:67:ASN:ND2	2.71	0.44
1:A:49:ARG:O	1:A:53:ARG:CZ	2.65	0.44
1:A:187:ASN:ND2	1:A:256:ASP:H	2.15	0.44
1:B:65:VAL:CG2	1:B:126:SER:HB2	2.48	0.44
1:A:74:LEU:HD13	1:A:134:LEU:HD21	2.00	0.44
1:A:210:GLU:O	1:A:211:ALA:HB3	2.17	0.44
1:B:23:PHE:CZ	1:B:54:LEU:HD13	2.52	0.44
1:A:5:LEU:HB3	1:A:34:ALA:HB2	1.98	0.44
1:A:190:ALA:HB3	1:A:259:TYR:CD2	2.53	0.44
1:C:67:ASN:ND2	1:C:69:GLU:H	2.16	0.44
1:D:185:ARG:HA	1:D:254:THR:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:ALA:HB1	3:B:410:JPM:C7	2.48	0.44
1:C:43:ARG:NH1	4:C:309:HOH:O	2.51	0.44
1:D:199:MET:HB2	3:D:430:JPM:H5	1.98	0.44
1:A:106:ASN:HA	1:A:107:PRO:HD3	1.89	0.43
1:B:3:GLY:O	1:B:6:ASP:HB2	2.17	0.43
1:D:150:ASP:HA	1:D:151:PRO:HD3	1.90	0.43
1:C:74:LEU:HD13	1:C:134:LEU:HD21	2.00	0.43
1:C:67:ASN:HD22	1:C:69:GLU:N	2.16	0.43
1:B:97:PHE:O	1:B:119:GLY:HA2	2.19	0.43
1:C:109:PHE:HB3	1:D:132:LYS:HD2	2.00	0.43
1:B:98:MET:HE1	1:B:116:VAL:CA	2.35	0.43
1:A:196:THR:HG23	1:A:198:ALA:N	2.29	0.42
1:B:87:LYS:HE3	1:B:137:ILE:C	2.45	0.42
1:D:63:LEU:HD13	1:D:74:LEU:HG	2.01	0.42
1:A:195:ARG:HG3	1:A:195:ARG:NH1	2.25	0.42
1:A:248:ASP:O	1:A:251:PRO:HG3	2.20	0.42
1:C:219:GLU:HG2	1:C:232:MET:SD	2.60	0.42
1:C:66:GLN:HE21	1:C:121:HIS:CD2	2.37	0.42
1:B:167:ALA:O	1:B:171:VAL:HG23	2.19	0.42
1:D:87:LYS:NZ	4:D:319:HOH:O	2.51	0.42
1:B:41:PHE:CD1	1:B:41:PHE:C	2.95	0.42
1:C:199:MET:HE2	1:C:199:MET:HB3	1.77	0.42
1:B:249:TRP:C	1:B:251:PRO:HD3	2.45	0.42
1:B:153:ARG:HA	1:B:153:ARG:HD3	1.94	0.42
1:A:145:VAL:HA	1:A:187:ASN:O	2.20	0.41
1:D:186:SER:H	1:D:254:THR:CG2	2.17	0.41
1:A:45:ARG:NH2	1:A:49:ARG:NH2	2.68	0.41
1:C:105:ILE:O	1:C:105:ILE:HG13	2.20	0.41
1:A:67:ASN:ND2	1:A:70:HIS:H	2.19	0.41
1:C:145:VAL:HG11	1:C:242:VAL:HG13	2.02	0.41
1:C:201:ALA:HB1	1:C:202:ILE:HD13	2.03	0.41
1:B:78:VAL:HG11	1:B:88:LEU:HD11	2.02	0.41
1:B:98:MET:HE2	1:B:102:GLY:HA3	2.02	0.41
1:B:101:THR:HG21	1:B:112:PRO:CD	2.41	0.41
1:C:249:TRP:C	1:C:251:PRO:HD3	2.46	0.41
1:D:193:PRO:HA	2:D:330:NAD:O7N	2.21	0.41
1:D:199:MET:O	1:D:200:SER:OG	2.37	0.41
1:B:257:ILE:C	1:B:258:ILE:HD12	2.46	0.41
1:D:11:LEU:HD21	1:D:39:THR:HG23	2.03	0.41
1:C:95:ILE:CD1	1:C:122:ILE:CG2	2.99	0.41
1:B:39:THR:HA	1:B:61:LEU:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ARG:HA	1:B:254:THR:HG23	2.02	0.40
1:B:193:PRO:HA	2:B:310:NAD:O7N	2.21	0.40
1:C:195:ARG:HH21	1:C:219:GLU:HG3	1.85	0.40
1:D:98:MET:HE2	1:D:102:GLY:HA3	2.03	0.40
1:D:219:GLU:HB2	1:D:232:MET:SD	2.61	0.40
1:A:109:PHE:HB3	1:B:132:LYS:HG3	2.03	0.40
1:C:4:LEU:N	1:C:32:GLN:HE21	1.98	0.40
1:A:149:PHE:CZ	1:A:222:TRP:CH2	3.09	0.40
1:A:195:ARG:CG	1:A:195:ARG:NH1	2.83	0.40
1:A:11:LEU:HD21	1:A:39:THR:HG23	2.03	0.40
1:D:95:ILE:HD13	2:D:330:NAD:C4A	2.50	0.40
1:D:185:ARG:CA	1:D:254:THR:CG2	2.98	0.40
1:B:198:ALA:HB1	3:B:410:JPM:C8	2.52	0.40
1:C:2:THR:HA	1:C:3:GLY:HA3	1.90	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%)	251 (94%)	14 (5%)	1 (0%)	30	38
1	B	245/269 (91%)	229 (94%)	16 (6%)	0	100	100
1	C	257/269 (96%)	242 (94%)	15 (6%)	0	100	100
1	D	253/269 (94%)	235 (93%)	18 (7%)	0	100	100
All	All	1021/1076 (95%)	957 (94%)	63 (6%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	ARG

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	203/205 (99%)	175 (86%)	28 (14%)	3	4
1	B	192/205 (94%)	166 (86%)	26 (14%)	4	4
1	C	200/205 (98%)	178 (89%)	22 (11%)	6	7
1	D	198/205 (97%)	173 (87%)	25 (13%)	4	5
All	All	793/820 (97%)	692 (87%)	101 (13%)	4	5

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	6	ASP
1	A	35	GLN
1	A	53	ARG
1	A	54	LEU
1	A	65	VAL
1	A	67	ASN
1	A	74	LEU
1	A	79	THR
1	A	95	ILE
1	A	101	THR
1	A	105	ILE
1	A	162	THR
1	A	168	LEU
1	A	170	SER
1	A	188	LEU
1	A	195	ARG
1	A	199	MET
1	A	202	ILE
1	A	203	VAL
1	A	217	LEU
1	A	218	LEU
1	A	233	LYS
1	A	236	THR

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Mol	Chain	Res	Type
1	A	238	VAL
1	A	250	LEU
1	A	253	THR
1	A	254	THR
1	B	5	LEU
1	B	6	ASP
1	B	11	LEU
1	B	43	ARG
1	B	49	ARG
1	B	54	LEU
1	B	57	LYS
1	B	65	VAL
1	B	67	ASN
1	B	74	LEU
1	B	95	ILE
1	B	100	GLN
1	B	101	THR
1	B	161	MET
1	B	168	LEU
1	B	188	LEU
1	B	196	THR
1	B	197	LEU
1	B	199	MET
1	B	200	SER
1	B	224	GLN
1	B	238	VAL
1	B	250	LEU
1	B	253	THR
1	B	254	THR
1	B	269	LEU
1	C	5	LEU
1	C	11	LEU
1	C	19	SER
1	C	45	ARG
1	C	53	ARG
1	C	54	LEU
1	C	65	VAL
1	C	67	ASN
1	C	69	GLU
1	C	74	LEU
1	C	79	THR
1	C	95	ILE

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Mol	Chain	Res	Type
1	C	100	GLN
1	C	168	LEU
1	C	170	SER
1	C	188	LEU
1	C	197	LEU
1	C	236	THR
1	C	238	VAL
1	C	250	LEU
1	C	253	THR
1	C	254	THR
1	D	5	LEU
1	D	6	ASP
1	D	9	ARG
1	D	11	LEU
1	D	43	ARG
1	D	54	LEU
1	D	57	LYS
1	D	65	VAL
1	D	67	ASN
1	D	69	GLU
1	D	74	LEU
1	D	95	ILE
1	D	101	THR
1	D	105	ILE
1	D	130	MET
1	D	168	LEU
1	D	170	SER
1	D	188	LEU
1	D	196	THR
1	D	197	LEU
1	D	216	GLN
1	D	236	THR
1	D	238	VAL
1	D	250	LEU
1	D	254	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	67	ASN
1	A	86	ASN

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Mol	Chain	Res	Type
1	A	100	GLN
1	A	121	HIS
1	A	187	ASN
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	106	ASN
1	B	187	ASN
1	B	265	HIS
1	C	32	GLN
1	C	48	GLN
1	C	67	ASN
1	C	86	ASN
1	C	100	GLN
1	C	121	HIS
1	C	224	GLN
1	C	265	HIS
1	D	32	GLN
1	D	67	ASN
1	D	86	ASN
1	D	100	GLN
1	D	121	HIS
1	D	216	GLN
1	D	224	GLN
1	D	265	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
3	JPM	C	420	-	25,25,25	2.71	3 (12%)	34,34,34	1.24	3 (8%)
2	NAD	D	330	-	46,48,48	1.75	6 (13%)	64,73,73	1.81	12 (18%)
3	JPM	B	410	-	25,25,25	2.84	2 (8%)	34,34,34	1.29	4 (11%)
3	JPM	A	400	-	25,25,25	2.81	4 (16%)	34,34,34	1.36	5 (14%)
3	JPM	D	430	-	25,25,25	2.92	2 (8%)	34,34,34	1.11	4 (11%)
2	NAD	B	310	-	46,48,48	1.77	6 (13%)	64,73,73	1.76	11 (17%)
2	NAD	C	320	-	46,48,48	1.80	6 (13%)	64,73,73	1.96	14 (21%)
2	NAD	A	300	-	46,48,48	1.76	6 (13%)	64,73,73	1.85	13 (20%)

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	JPM	C	420	-	-	0/8/8/8	0/3/3/3
2	NAD	D	330	-	-	10/30/62/62	0/5/5/5
3	JPM	B	410	-	-	0/8/8/8	0/3/3/3
3	JPM	A	400	-	-	0/8/8/8	0/3/3/3
3	JPM	D	430	-	-	0/8/8/8	0/3/3/3
2	NAD	B	310	-	-	11/30/62/62	0/5/5/5
2	NAD	C	320	-	-	6/30/62/62	0/5/5/5
2	NAD	A	300	-	-	5/30/62/62	0/5/5/5

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	410	JPM	C11-CL5	-9.94	1.51	1.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	430	JPM	C7-CL1	-9.94	1.50	1.73
3	D	430	JPM	C11-CL5	-9.67	1.51	1.74
3	A	400	JPM	C11-CL5	-9.66	1.51	1.74
3	C	420	JPM	C11-CL5	-9.60	1.52	1.74
3	B	410	JPM	C7-CL1	-9.29	1.51	1.73
3	A	400	JPM	C7-CL1	-9.22	1.51	1.73
2	B	310	NAD	O7N-C7N	9.04	1.41	1.24
2	A	300	NAD	O7N-C7N	8.87	1.40	1.24
2	C	320	NAD	O7N-C7N	8.73	1.40	1.24
2	D	330	NAD	O7N-C7N	8.62	1.40	1.24
3	C	420	JPM	C7-CL1	-8.38	1.53	1.73
2	C	320	NAD	PA-O3	4.60	1.64	1.59
2	B	310	NAD	C2N-N1N	3.70	1.39	1.35
2	A	300	NAD	C2A-N3A	3.13	1.39	1.33
2	A	300	NAD	C2A-N1A	3.03	1.39	1.33
2	D	330	NAD	C2A-N1A	2.83	1.39	1.33
2	A	300	NAD	C2N-N1N	2.75	1.38	1.35
2	C	320	NAD	C2A-N1A	2.74	1.38	1.33
2	C	320	NAD	C2A-N3A	2.73	1.38	1.33
2	D	330	NAD	C2A-N3A	2.70	1.38	1.33
2	A	300	NAD	C8A-N7A	2.69	1.36	1.31
2	B	310	NAD	PA-O3	2.49	1.62	1.59
2	B	310	NAD	C2A-N3A	2.47	1.38	1.33
2	D	330	NAD	PN-O3	2.43	1.62	1.59
2	C	320	NAD	O4D-C1D	2.37	1.44	1.40
2	D	330	NAD	C8A-N7A	2.35	1.36	1.31
2	D	330	NAD	PA-O3	2.31	1.62	1.59
3	C	420	JPM	C10-C11	2.24	1.42	1.38
2	B	310	NAD	PN-O3	2.15	1.61	1.59
3	A	400	JPM	C12-C11	2.13	1.41	1.38
2	B	310	NAD	C2A-N1A	2.10	1.37	1.33
3	A	400	JPM	C12-C7	2.07	1.42	1.38
2	A	300	NAD	O4D-C1D	2.06	1.43	1.40
2	C	320	NAD	PN-O3	2.05	1.61	1.59

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	310	NAD	N3A-C2A-N1A	-6.59	118.60	128.58
2	A	300	NAD	N3A-C2A-N1A	-6.34	118.99	128.58
2	C	320	NAD	N3A-C2A-N1A	-6.33	118.99	128.58
2	D	330	NAD	N3A-C2A-N1A	-5.78	119.83	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	320	NAD	N9A-C8A-N7A	-4.82	107.09	113.94
2	A	300	NAD	O4B-C1B-N9A	4.79	117.29	108.09
2	D	330	NAD	C3N-C7N-N7N	4.63	123.44	117.74
2	D	330	NAD	O4B-C1B-N9A	4.61	116.94	108.09
2	C	320	NAD	C5A-N7A-C8A	4.36	110.30	103.45
2	A	300	NAD	C5A-C4A-N3A	-4.34	120.74	126.72
2	B	310	NAD	C5A-C4A-N3A	-4.32	120.77	126.72
2	A	300	NAD	N9A-C8A-N7A	-4.20	107.98	113.94
2	C	320	NAD	O4B-C1B-N9A	4.11	115.99	108.09
2	C	320	NAD	C5A-C4A-N3A	-4.02	121.19	126.72
2	B	310	NAD	C2A-N3A-C4A	3.83	121.17	111.83
3	B	410	JPM	C7-C12-C11	3.79	123.01	118.72
2	B	310	NAD	O4B-C1B-N9A	3.76	115.32	108.09
2	D	330	NAD	C5A-C4A-N3A	-3.74	121.57	126.72
3	A	400	JPM	C8-O1-C3	3.73	127.00	118.09
2	B	310	NAD	N9A-C8A-N7A	-3.67	108.72	113.94
2	A	300	NAD	C2A-N3A-C4A	3.57	120.55	111.83
2	C	320	NAD	C4A-C5A-N7A	-3.56	106.52	110.58
2	D	330	NAD	O7N-C7N-C3N	-3.55	115.25	119.60
2	A	300	NAD	C5A-N7A-C8A	3.55	109.03	103.45
2	C	320	NAD	C2A-N3A-C4A	3.55	120.49	111.83
2	D	330	NAD	N9A-C8A-N7A	-3.53	108.93	113.94
3	B	410	JPM	C8-O1-C3	3.51	126.46	118.09
2	C	320	NAD	C3N-C7N-N7N	3.36	121.88	117.74
2	D	330	NAD	C5A-N7A-C8A	3.18	108.44	103.45
3	A	400	JPM	C12-C11-CL5	3.13	123.09	119.17
2	A	300	NAD	C3N-C7N-N7N	3.11	121.57	117.74
2	B	310	NAD	C5A-N7A-C8A	3.11	108.33	103.45
3	C	420	JPM	C7-C12-C11	3.06	122.17	118.72
3	A	400	JPM	C9-C10-C11	3.02	122.28	119.24
2	B	310	NAD	N3A-C4A-N9A	3.01	132.29	127.17
2	C	320	NAD	C4B-O4B-C1B	-2.99	102.87	109.47
2	D	330	NAD	C2A-N3A-C4A	2.98	119.10	111.83
3	A	400	JPM	C10-C11-C12	-2.94	117.69	121.53
3	B	410	JPM	C10-C11-C12	-2.91	117.72	121.53
2	B	310	NAD	C3N-C7N-N7N	2.78	121.17	117.74
3	D	430	JPM	C8-O1-C3	2.75	124.66	118.09
2	C	320	NAD	C4A-N9A-C8A	2.74	108.61	105.74
2	A	300	NAD	N3A-C4A-N9A	2.73	131.81	127.17
3	C	420	JPM	C10-C11-C12	-2.70	118.00	121.53
2	A	300	NAD	C4A-C5A-N7A	-2.70	107.50	110.58
2	D	330	NAD	N3A-C4A-N9A	2.65	131.68	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	430	JPM	C10-C11-C12	-2.60	118.13	121.53
2	C	320	NAD	N3A-C4A-N9A	2.45	131.34	127.17
2	D	330	NAD	O2A-PA-O3	2.41	113.78	107.27
2	C	320	NAD	O3-PA-O1A	-2.40	103.47	110.70
2	B	310	NAD	C6N-N1N-C2N	-2.38	119.85	121.88
3	D	430	JPM	C7-C12-C11	2.36	121.39	118.72
3	D	430	JPM	C9-C10-C11	2.35	121.61	119.24
2	C	320	NAD	O7N-C7N-N7N	-2.29	119.30	122.62
2	A	300	NAD	C5B-C4B-C3B	-2.26	107.08	115.21
2	A	300	NAD	O3-PN-O1N	-2.24	103.97	110.70
3	A	400	JPM	C12-C7-CL1	2.23	122.11	118.45
2	B	310	NAD	O2N-PN-O1N	2.23	122.83	112.44
2	D	330	NAD	C4A-C5A-N7A	-2.20	108.07	110.58
2	A	300	NAD	C4A-N9A-C8A	2.20	108.05	105.74
2	D	330	NAD	O5B-C5B-C4B	-2.18	101.57	108.99
2	A	300	NAD	O5B-C5B-C4B	-2.15	101.67	108.99
2	C	320	NAD	O2N-PN-O3	2.12	113.00	107.27
2	B	310	NAD	C4A-C5A-N7A	-2.07	108.22	110.58
3	C	420	JPM	C2-C1-C6	-2.03	118.70	120.81
3	B	410	JPM	C10-C11-CL5	2.03	122.36	119.36

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	B	310	NAD	C5B-O5B-PA-O1A
2	B	310	NAD	C5B-O5B-PA-O3
2	B	310	NAD	PN-O3-PA-O5B
2	B	310	NAD	C5D-O5D-PN-O3
2	B	310	NAD	C5D-O5D-PN-O1N
2	B	310	NAD	C5D-O5D-PN-O2N
2	B	310	NAD	O4D-C1D-N1N-C2N
2	C	320	NAD	C5D-O5D-PN-O3
2	C	320	NAD	C5D-O5D-PN-O1N
2	C	320	NAD	C5D-O5D-PN-O2N
2	C	320	NAD	O4D-C1D-N1N-C2N
2	D	330	NAD	C5D-O5D-PN-O3
2	D	330	NAD	C5D-O5D-PN-O1N
2	D	330	NAD	C5D-O5D-PN-O2N

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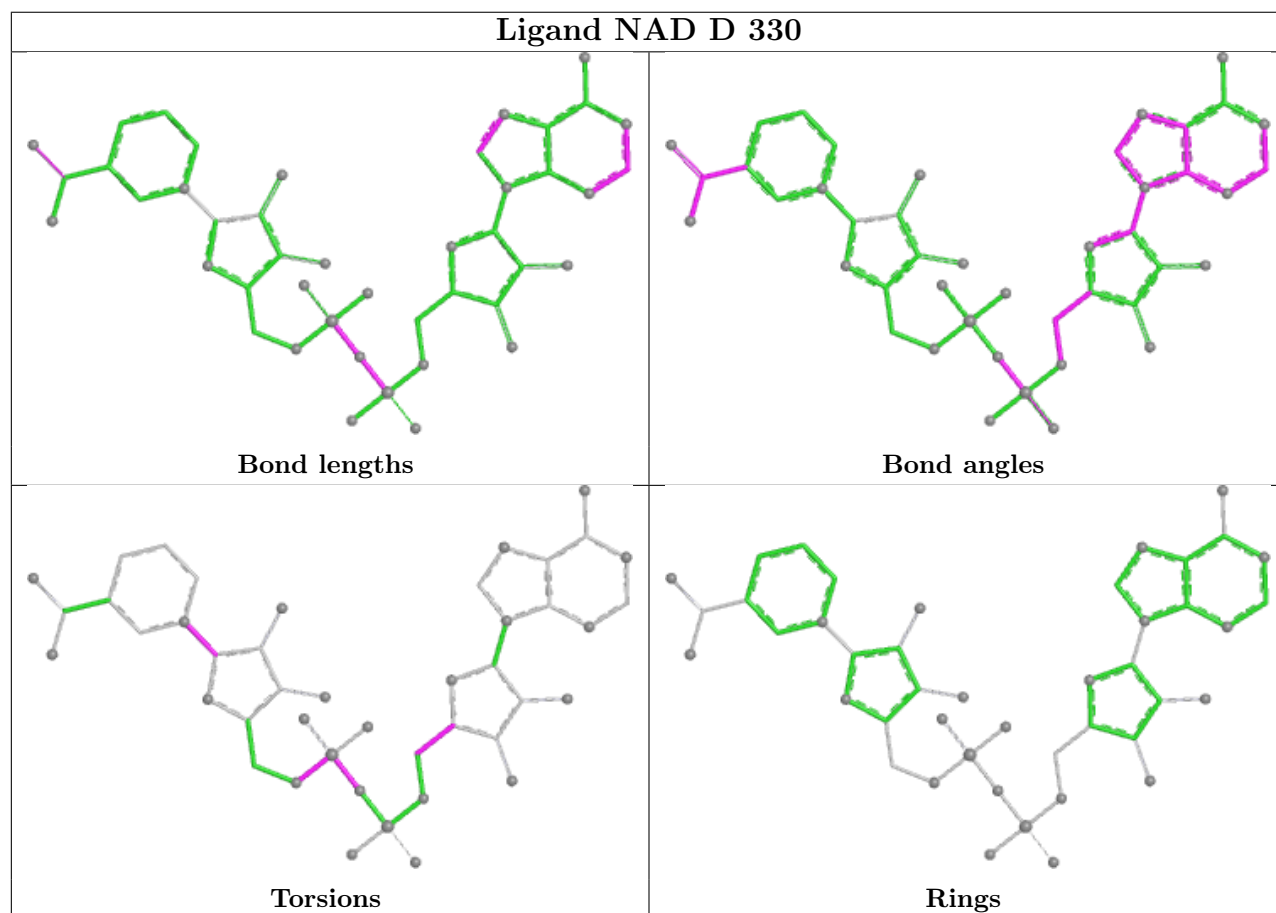
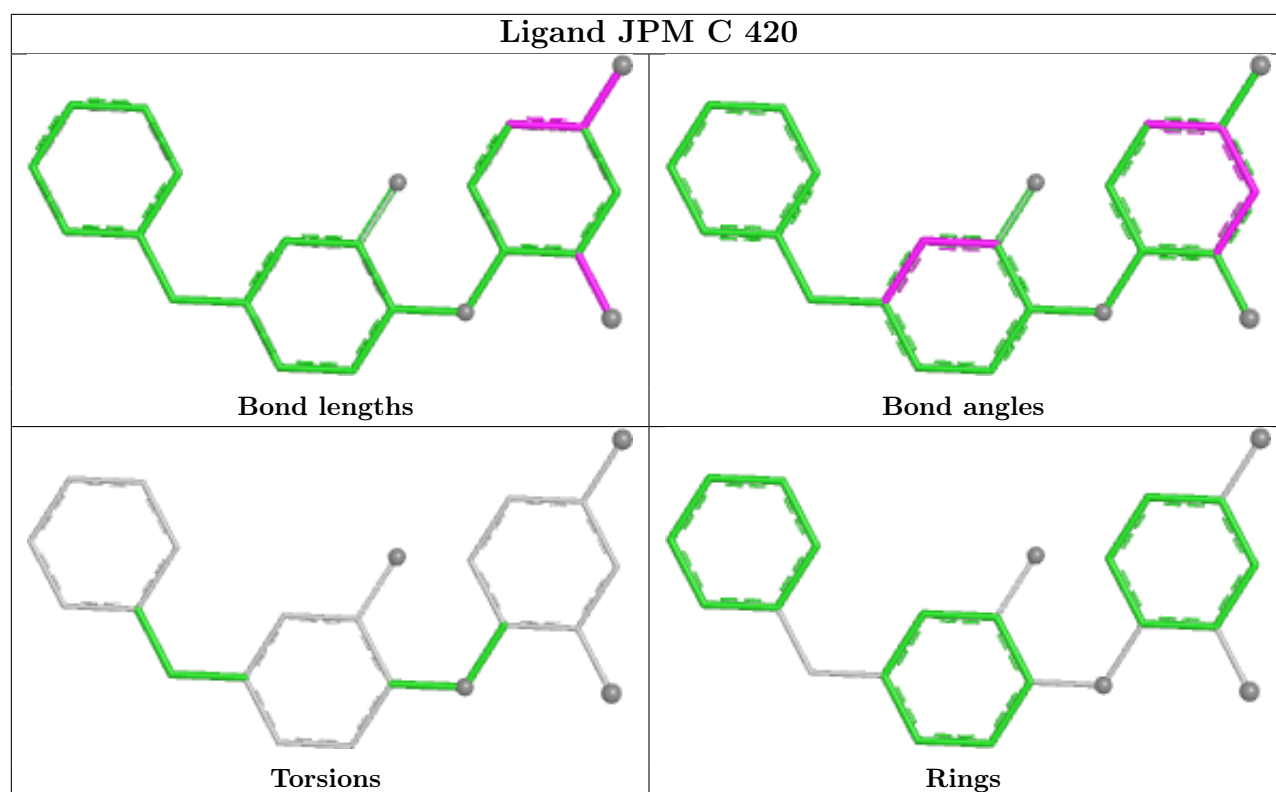
Mol	Chain	Res	Type	Atoms
2	D	330	NAD	O4D-C1D-N1N-C2N
2	D	330	NAD	O4D-C1D-N1N-C6N
2	D	330	NAD	C2D-C1D-N1N-C6N
2	C	320	NAD	PN-O3-PA-O5B
2	B	310	NAD	C5B-O5B-PA-O2A
2	D	330	NAD	C2D-C1D-N1N-C2N
2	A	300	NAD	O4B-C4B-C5B-O5B
2	B	310	NAD	O4B-C4B-C5B-O5B
2	D	330	NAD	O4B-C4B-C5B-O5B
2	A	300	NAD	O4D-C1D-N1N-C6N
2	B	310	NAD	O4D-C1D-N1N-C6N
2	C	320	NAD	O4D-C1D-N1N-C6N
2	D	330	NAD	PA-O3-PN-O1N
2	D	330	NAD	PA-O3-PN-O2N
2	B	310	NAD	C3B-C4B-C5B-O5B

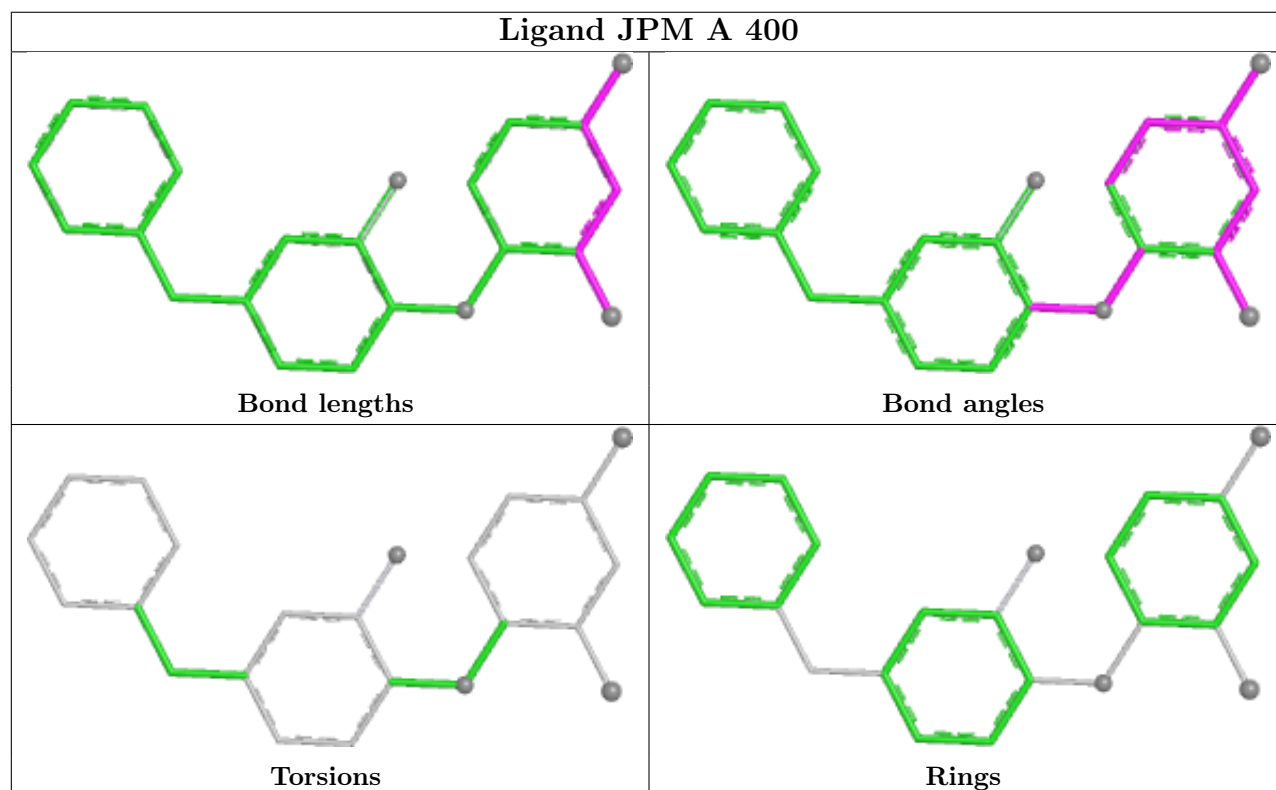
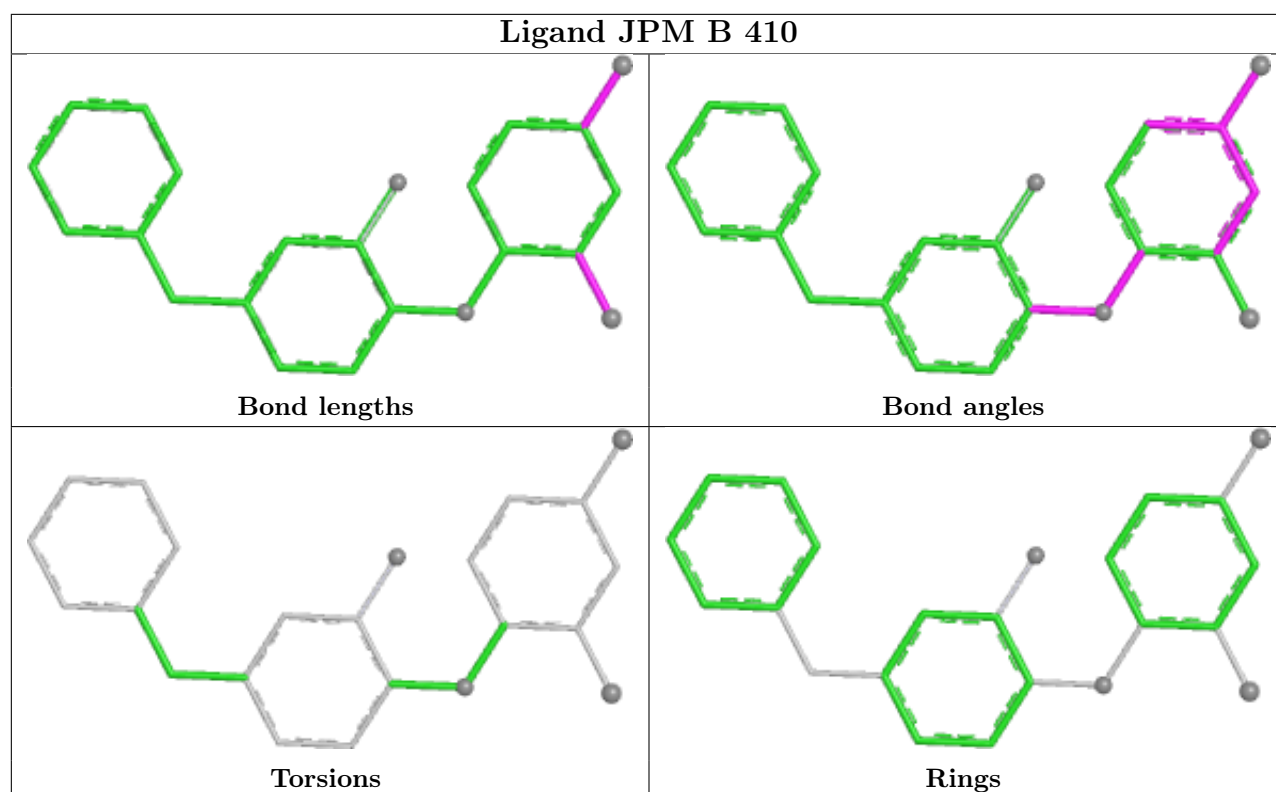
There are no ring outliers.

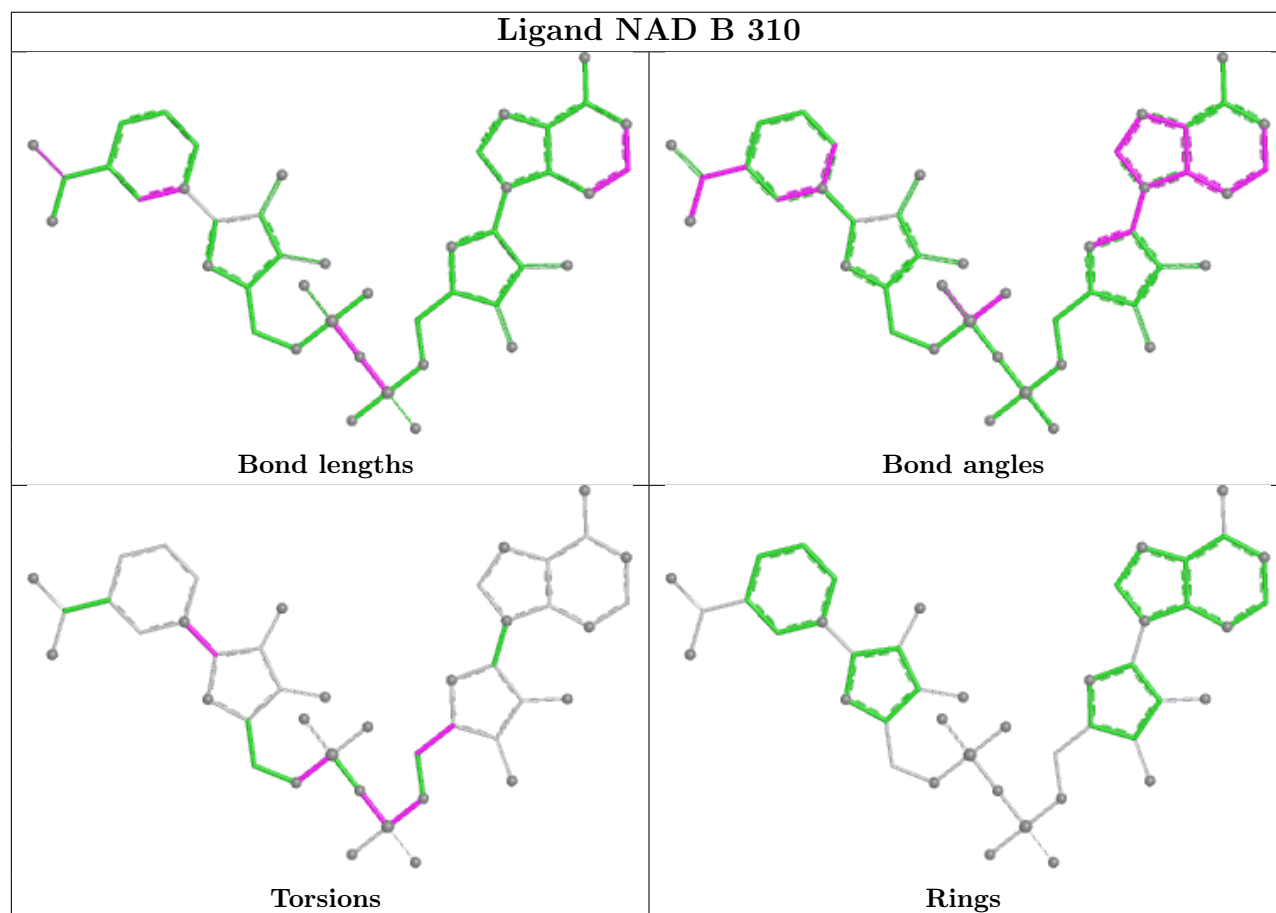
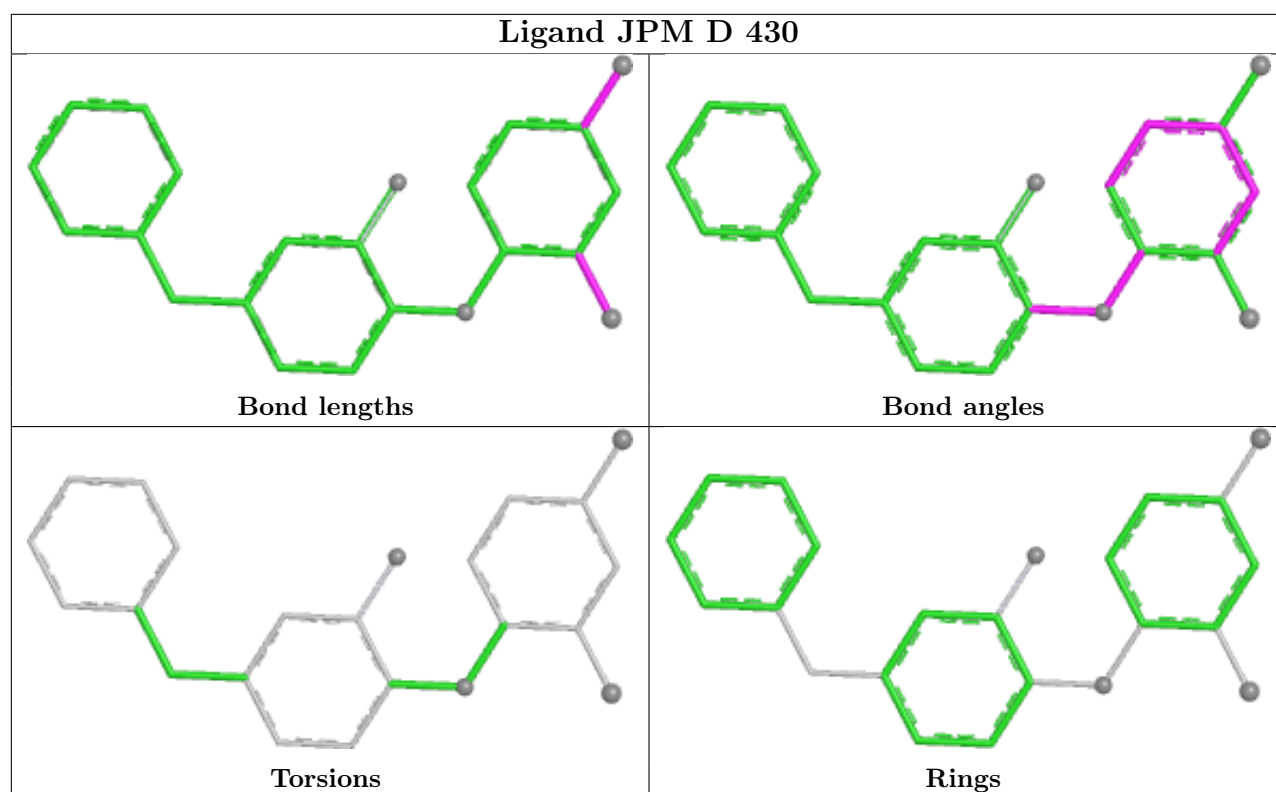
7 monomers are involved in 14 short contacts:

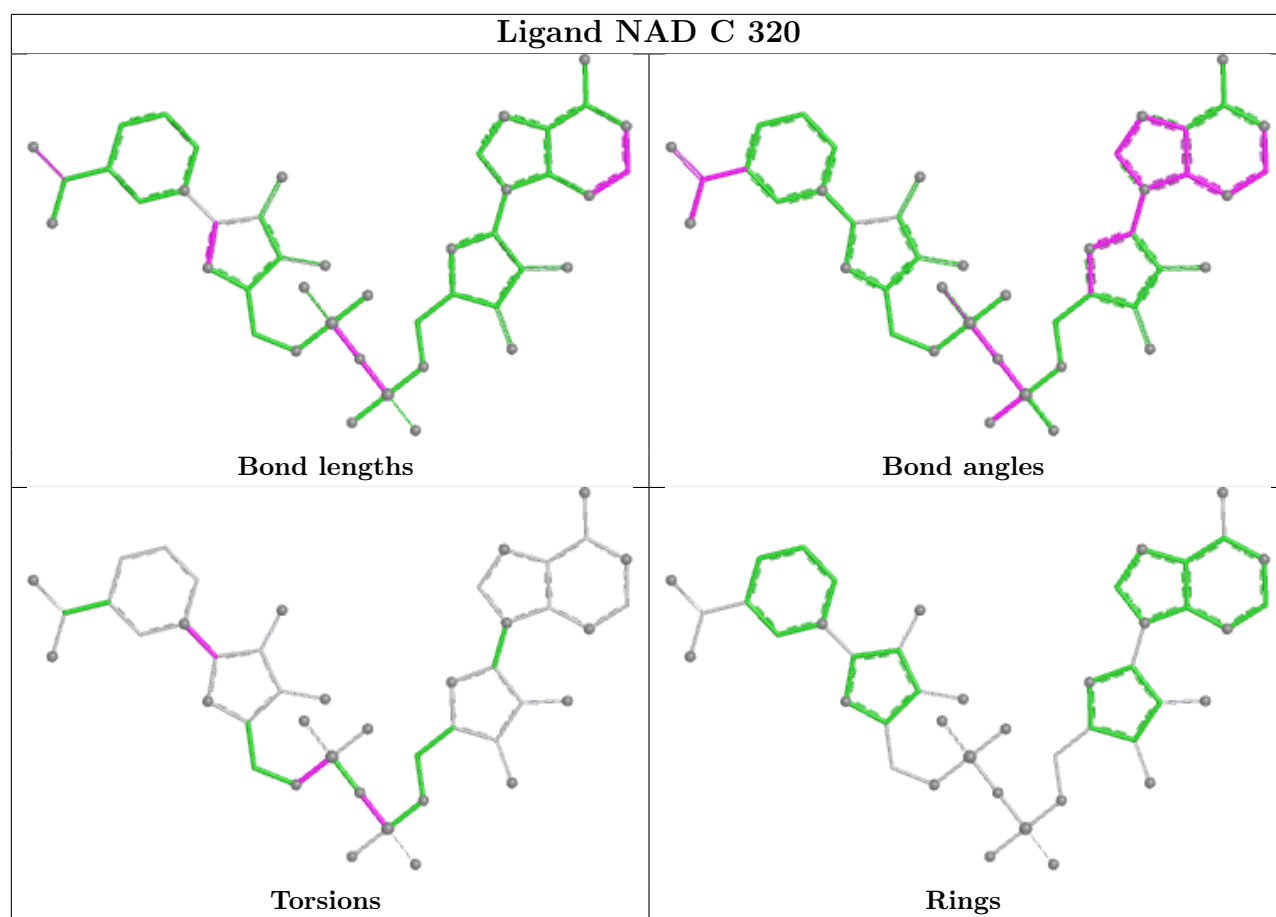
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	420	JPM	1	0
2	D	330	NAD	3	0
3	B	410	JPM	2	0
3	D	430	JPM	3	0
2	B	310	NAD	2	0
2	C	320	NAD	1	0
2	A	300	NAD	2	0

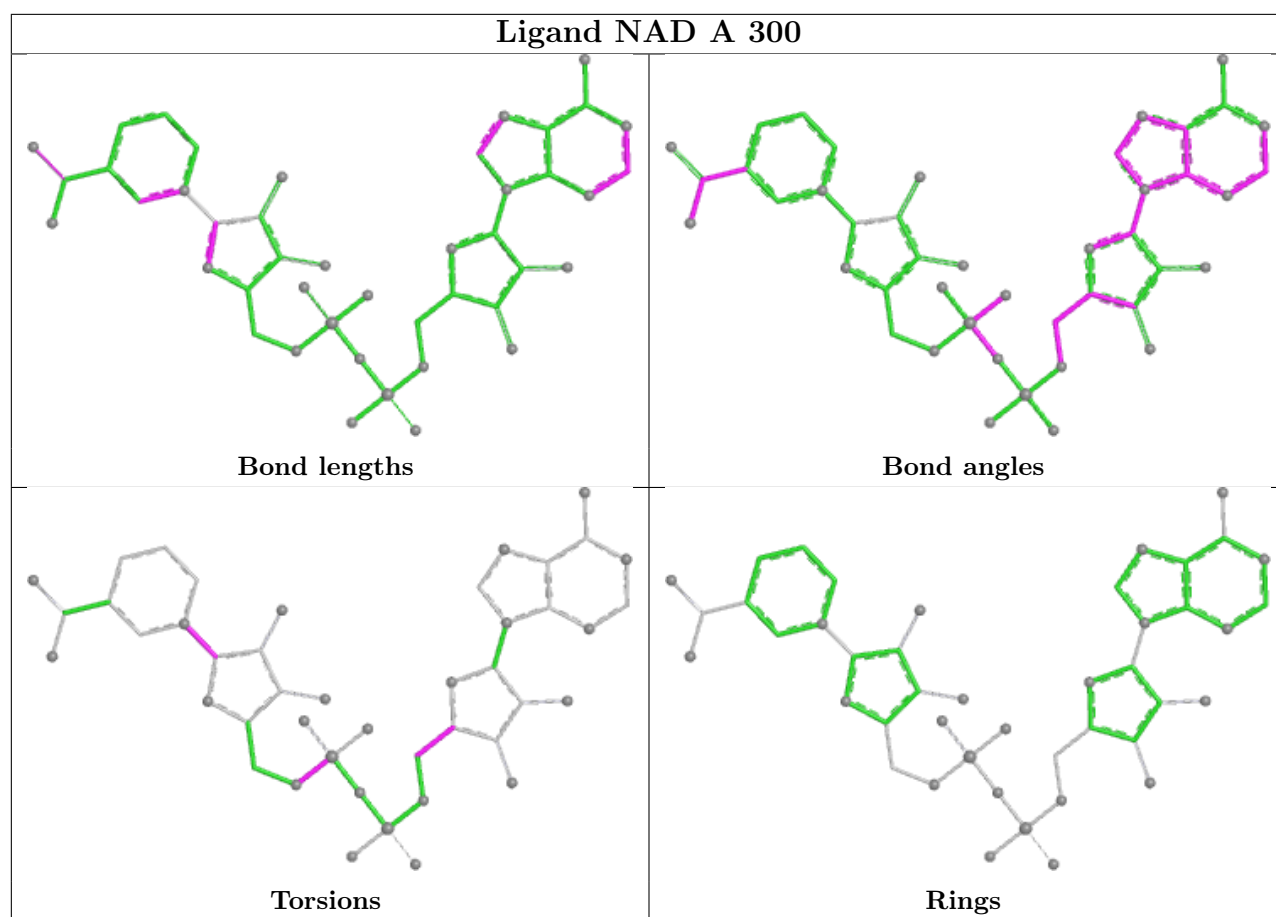
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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	268/269 (99%)	3.68	208 (77%) 0 0	27, 37, 57, 71	0
1	B	249/269 (92%)	3.55	203 (81%) 0 0	27, 36, 53, 66	0
1	C	261/269 (97%)	3.45	210 (80%) 0 0	29, 38, 55, 74	0
1	D	257/269 (95%)	3.45	207 (80%) 0 0	30, 40, 59, 66	0
All	All	1035/1076 (96%)	3.53	828 (80%) 0 0	27, 38, 57, 74	0

All (828) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	229	GLY	16.7
1	C	242	VAL	13.2
1	B	64	ASP	12.2
1	A	72	ALA	10.9
1	A	221	GLY	10.8
1	D	58	ALA	10.6
1	B	12	VAL	10.4
1	D	94	SER	9.9
1	B	126	SER	9.9
1	C	201	ALA	9.7
1	B	176	ALA	9.3
1	C	229	GLY	9.2
1	B	198	ALA	9.2
1	B	241	THR	9.2
1	D	11	LEU	9.2
1	B	196	THR	9.0
1	D	244	ALA	8.7
1	C	202	ILE	8.7
1	C	260	ALA	8.7
1	A	136	PRO	8.7
1	A	4	LEU	8.6

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Mol	Chain	Res	Type	RSRZ
1	A	144	ILE	8.5
1	A	244	ALA	8.5
1	A	146	GLY	8.3
1	A	226	ALA	8.1
1	D	198	ALA	8.1
1	C	246	LEU	8.1
1	C	19	SER	8.1
1	D	65	VAL	8.1
1	D	258	ILE	8.0
1	A	131	ALA	8.0
1	A	176	ALA	8.0
1	C	212	GLY	7.9
1	A	186	SER	7.8
1	B	242	VAL	7.8
1	C	185	ARG	7.8
1	A	122	ILE	7.7
1	A	7	GLY	7.7
1	B	65	VAL	7.6
1	A	178	GLU	7.6
1	B	13	SER	7.6
1	B	111	ALA	7.5
1	C	101	THR	7.4
1	D	113	TYR	7.4
1	D	155	MET	7.4
1	B	200	SER	7.3
1	A	177	ARG	7.3
1	B	21	ILE	7.2
1	A	172	ASN	7.2
1	A	267	GLN	7.2
1	D	182	TYR	7.0
1	D	109	PHE	6.9
1	A	129	SER	6.9
1	B	256	ASP	6.9
1	C	163	VAL	6.9
1	A	33	GLY	6.9
1	A	71	LEU	6.9
1	A	151	PRO	6.9
1	D	252	ALA	6.8
1	B	186	SER	6.8
1	C	58	ALA	6.7
1	B	252	ALA	6.7
1	D	142	GLY	6.7

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Mol	Chain	Res	Type	RSRZ
1	C	198	ALA	6.7
1	C	196	THR	6.6
1	D	154	ALA	6.6
1	A	135	LEU	6.6
1	C	76	GLY	6.6
1	C	170	SER	6.6
1	B	22	ALA	6.6
1	A	157	ALA	6.5
1	B	152	SER	6.5
1	A	150	ASP	6.5
1	D	38	LEU	6.5
1	A	123	SER	6.5
1	A	228	ILE	6.5
1	B	119	GLY	6.5
1	C	81	ALA	6.4
1	C	211	ALA	6.4
1	B	66	GLN	6.4
1	A	73	SER	6.3
1	D	262	GLY	6.3
1	A	160	TRP	6.3
1	C	247	SER	6.3
1	A	253	THR	6.3
1	D	95	ILE	6.3
1	C	142	GLY	6.3
1	A	268	LEU	6.2
1	C	192	GLY	6.2
1	B	25	ILE	6.2
1	B	92	VAL	6.2
1	D	256	ASP	6.2
1	C	127	TYR	6.1
1	B	76	GLY	6.1
1	A	218	LEU	6.1
1	C	251	PRO	6.1
1	A	61	LEU	6.1
1	B	129	SER	6.1
1	D	17	THR	6.0
1	C	223	ASP	6.0
1	B	10	ILE	6.0
1	D	21	ILE	6.0
1	B	114	ALA	6.0
1	C	20	SER	5.9
1	A	197	LEU	5.9

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Mol	Chain	Res	Type	RSRZ
1	B	189	VAL	5.9
1	C	152	SER	5.9
1	B	171	VAL	5.9
1	C	103	MET	5.9
1	A	179	ALA	5.9
1	C	191	ALA	5.9
1	B	35	GLN	5.8
1	C	151	PRO	5.8
1	B	160	TRP	5.8
1	D	90	GLY	5.8
1	D	54	LEU	5.8
1	B	28	VAL	5.7
1	A	152	SER	5.7
1	A	51	THR	5.7
1	C	249	TRP	5.7
1	B	158	TYR	5.7
1	B	116	VAL	5.7
1	D	56	ALA	5.7
1	D	250	LEU	5.7
1	A	195	ARG	5.6
1	A	54	LEU	5.6
1	B	15	ILE	5.6
1	D	183	GLY	5.6
1	A	22	ALA	5.5
1	A	154	ALA	5.5
1	A	220	GLU	5.5
1	B	70	HIS	5.5
1	D	162	THR	5.5
1	C	97	PHE	5.5
1	C	106	ASN	5.5
1	A	174	PHE	5.5
1	B	246	LEU	5.5
1	A	266	THR	5.4
1	B	230	TRP	5.4
1	B	26	ALA	5.4
1	B	75	ALA	5.4
1	B	175	VAL	5.4
1	C	158	TYR	5.4
1	A	145	VAL	5.4
1	D	190	ALA	5.3
1	C	46	LEU	5.3
1	C	30	GLN	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	110	ASP	5.3
1	B	162	THR	5.3
1	D	197	LEU	5.3
1	B	9	ARG	5.3
1	B	182	TYR	5.3
1	D	254	THR	5.3
1	C	75	ALA	5.3
1	A	18	ASP	5.3
1	A	215	ILE	5.3
1	D	257	ILE	5.2
1	C	131	ALA	5.2
1	D	4	LEU	5.2
1	D	184	VAL	5.2
1	A	23	PHE	5.2
1	A	187	ASN	5.2
1	A	55	PRO	5.2
1	C	236	THR	5.2
1	C	72	ALA	5.2
1	D	71	LEU	5.2
1	A	175	VAL	5.2
1	A	41	PHE	5.2
1	A	254	THR	5.2
1	D	179	ALA	5.1
1	B	52	ASP	5.1
1	C	231	ASN	5.1
1	A	3	GLY	5.1
1	A	212	GLY	5.1
1	D	84	ALA	5.1
1	B	150	ASP	5.1
1	D	163	VAL	5.1
1	D	8	LYS	5.1
1	D	260	ALA	5.1
1	D	100	GLN	5.1
1	A	28	VAL	5.1
1	D	166	SER	5.1
1	B	121	HIS	5.1
1	B	67	ASN	5.1
1	D	230	TRP	5.1
1	C	174	PHE	5.1
1	C	268	LEU	5.0
1	D	220	GLU	5.0
1	B	145	VAL	5.0

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Mol	Chain	Res	Type	RSRZ
1	C	241	THR	5.0
1	A	219	GLU	5.0
1	D	259	TYR	5.0
1	A	163	VAL	5.0
1	C	189	VAL	5.0
1	D	79	THR	5.0
1	A	155	MET	4.9
1	B	50	ILE	4.9
1	D	20	SER	4.9
1	A	208	GLY	4.9
1	D	158	TYR	4.9
1	A	138	MET	4.9
1	A	264	ALA	4.9
1	B	56	ALA	4.9
1	D	138	MET	4.9
1	A	20	SER	4.9
1	B	83	GLY	4.9
1	B	85	GLY	4.9
1	D	39	THR	4.9
1	A	53	ARG	4.9
1	C	160	TRP	4.9
1	D	23	PHE	4.9
1	A	94	SER	4.8
1	A	137	ILE	4.8
1	C	120	ILE	4.8
1	A	243	CYS	4.8
1	A	17	THR	4.8
1	C	253	THR	4.8
1	A	159	ASN	4.8
1	D	44	LEU	4.8
1	A	189	VAL	4.8
1	A	204	GLY	4.7
1	C	102	GLY	4.7
1	A	52	ASP	4.7
1	B	82	ILE	4.7
1	B	41	PHE	4.7
1	D	175	VAL	4.7
1	A	60	LEU	4.7
1	D	99	PRO	4.7
1	C	179	ALA	4.7
1	A	91	VAL	4.7
1	B	148	ASP	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	156	PRO	4.7
1	A	119	GLY	4.7
1	B	103	MET	4.7
1	A	217	LEU	4.6
1	D	215	ILE	4.6
1	C	230	TRP	4.6
1	C	23	PHE	4.6
1	A	21	ILE	4.6
1	A	88	LEU	4.6
1	A	188	LEU	4.6
1	C	34	ALA	4.6
1	A	246	LEU	4.6
1	C	125	TYR	4.5
1	C	187	ASN	4.5
1	D	59	PRO	4.5
1	C	183	GLY	4.5
1	D	249	TRP	4.5
1	C	248	ASP	4.5
1	D	88	LEU	4.5
1	A	97	PHE	4.5
1	C	252	ALA	4.5
1	D	111	ALA	4.5
1	D	101	THR	4.5
1	B	63	LEU	4.5
1	C	175	VAL	4.5
1	B	235	ALA	4.5
1	D	49	ARG	4.5
1	A	184	VAL	4.4
1	C	25	ILE	4.4
1	D	108	PHE	4.4
1	A	103	MET	4.4
1	D	224	GLN	4.4
1	C	136	PRO	4.4
1	C	257	ILE	4.4
1	A	26	ALA	4.4
1	B	269	LEU	4.4
1	B	183	GLY	4.4
1	B	32	GLN	4.4
1	B	131	ALA	4.4
1	B	54	LEU	4.4
1	B	93	HIS	4.4
1	B	125	TYR	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	10	ILE	4.4
1	D	180	GLY	4.4
1	C	117	SER	4.4
1	B	172	ASN	4.4
1	B	261	ASP	4.4
1	A	198	ALA	4.3
1	D	29	ALA	4.3
1	B	37	VAL	4.3
1	B	222	TRP	4.3
1	D	10	ILE	4.3
1	B	166	SER	4.3
1	A	134	LEU	4.3
1	D	116	VAL	4.3
1	D	174	PHE	4.3
1	B	36	LEU	4.3
1	B	109	PHE	4.3
1	A	59	PRO	4.3
1	A	38	LEU	4.3
1	A	39	THR	4.3
1	D	25	ILE	4.3
1	A	57	LYS	4.2
1	C	63	LEU	4.2
1	D	243	CYS	4.2
1	C	184	VAL	4.2
1	C	190	ALA	4.2
1	C	130	MET	4.2
1	B	243	CYS	4.2
1	D	42	ASP	4.2
1	C	60	LEU	4.2
1	B	184	VAL	4.2
1	D	145	VAL	4.2
1	B	113	TYR	4.2
1	D	57	LYS	4.2
1	A	74	LEU	4.2
1	A	249	TRP	4.2
1	C	109	PHE	4.2
1	C	149	PHE	4.2
1	C	156	PRO	4.1
1	B	134	LEU	4.1
1	C	222	TRP	4.1
1	A	24	HIS	4.1
1	C	16	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	143	SER	4.1
1	B	139	ASN	4.1
1	C	172	ASN	4.1
1	B	8	LYS	4.1
1	B	147	MET	4.1
1	D	112	PRO	4.1
1	A	125	TYR	4.1
1	D	97	PHE	4.1
1	A	108	PHE	4.1
1	D	146	GLY	4.1
1	C	162	THR	4.0
1	D	35	GLN	4.0
1	B	234	ASP	4.0
1	D	52	ASP	4.0
1	D	117	SER	4.0
1	D	171	VAL	4.0
1	D	149	PHE	4.0
1	D	147	MET	4.0
1	C	82	ILE	4.0
1	B	227	PRO	4.0
1	A	58	ALA	4.0
1	B	264	ALA	4.0
1	C	245	LEU	4.0
1	C	237	PRO	4.0
1	B	263	GLY	4.0
1	D	48	GLN	4.0
1	C	266	THR	4.0
1	C	261	ASP	4.0
1	A	82	ILE	4.0
1	D	15	ILE	4.0
1	B	136	PRO	3.9
1	D	193	PRO	3.9
1	A	92	VAL	3.9
1	A	214	GLN	3.9
1	D	191	ALA	3.9
1	C	178	GLU	3.9
1	A	67	ASN	3.9
1	D	115	ASP	3.9
1	C	68	GLU	3.9
1	C	132	LYS	3.9
1	B	143	SER	3.9
1	D	170	SER	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	193	PRO	3.9
1	B	224	GLN	3.9
1	B	142	GLY	3.9
1	B	239	ALA	3.9
1	C	154	ALA	3.9
1	C	258	ILE	3.9
1	D	16	ILE	3.9
1	D	127	TYR	3.9
1	C	250	LEU	3.9
1	D	231	ASN	3.9
1	D	251	PRO	3.8
1	C	48	GLN	3.8
1	B	199	MET	3.8
1	A	113	TYR	3.8
1	A	240	LYS	3.8
1	B	180	GLY	3.8
1	C	197	LEU	3.8
1	A	99	PRO	3.8
1	C	9	ARG	3.8
1	B	60	LEU	3.8
1	A	239	ALA	3.8
1	C	56	ALA	3.8
1	D	75	ALA	3.8
1	D	248	ASP	3.8
1	D	161	MET	3.8
1	B	23	PHE	3.8
1	A	128	ALA	3.7
1	C	18	ASP	3.7
1	D	159	ASN	3.7
1	D	223	ASP	3.7
1	D	13	SER	3.7
1	B	141	GLY	3.7
1	B	250	LEU	3.7
1	A	181	LYS	3.7
1	A	191	ALA	3.7
1	B	117	SER	3.7
1	C	37	VAL	3.7
1	D	130	MET	3.7
1	D	150	ASP	3.7
1	A	227	PRO	3.7
1	B	5	LEU	3.7
1	C	238	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	53	ARG	3.7
1	C	213	ALA	3.7
1	C	226	ALA	3.7
1	A	70	HIS	3.7
1	C	169	GLU	3.6
1	A	66	GLN	3.6
1	C	263	GLY	3.6
1	B	135	LEU	3.6
1	D	60	LEU	3.6
1	D	148	ASP	3.6
1	D	172	ASN	3.6
1	A	147	MET	3.6
1	C	7	GLY	3.6
1	C	119	GLY	3.6
1	A	269	LEU	3.6
1	C	11	LEU	3.6
1	B	127	TYR	3.6
1	A	224	GLN	3.6
1	B	48	GLN	3.6
1	A	153	ARG	3.6
1	D	85	GLY	3.6
1	B	11	LEU	3.6
1	C	254	THR	3.6
1	D	26	ALA	3.6
1	C	123	SER	3.6
1	A	100	GLN	3.6
1	B	47	ILE	3.6
1	C	21	ILE	3.6
1	D	192	GLY	3.6
1	A	11	LEU	3.6
1	B	6	ASP	3.6
1	A	259	TYR	3.5
1	B	122	ILE	3.5
1	B	228	ILE	3.5
1	C	38	LEU	3.5
1	D	86	ASN	3.5
1	A	156	PRO	3.5
1	B	31	GLU	3.5
1	C	116	VAL	3.5
1	D	87	LYS	3.5
1	C	50	ILE	3.5
1	C	180	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	44	LEU	3.5
1	A	77	ARG	3.5
1	D	32	GLN	3.5
1	D	165	LYS	3.5
1	A	105	ILE	3.5
1	B	137	ILE	3.5
1	B	229	GLY	3.5
1	D	50	ILE	3.5
1	D	121	HIS	3.5
1	B	237	PRO	3.5
1	D	227	PRO	3.5
1	A	203	VAL	3.5
1	A	81	ALA	3.5
1	B	128	ALA	3.5
1	C	143	SER	3.5
1	D	160	TRP	3.5
1	C	36	LEU	3.5
1	B	112	PRO	3.4
1	D	253	THR	3.4
1	D	233	LYS	3.4
1	A	75	ALA	3.4
1	B	81	ALA	3.4
1	D	164	ALA	3.4
1	A	180	GLY	3.4
1	A	50	ILE	3.4
1	A	185	ARG	3.4
1	D	6	ASP	3.4
1	A	98	MET	3.4
1	A	213	ALA	3.4
1	A	42	ASP	3.4
1	C	188	LEU	3.4
1	D	64	ASP	3.4
1	A	196	THR	3.4
1	C	22	ALA	3.4
1	D	200	SER	3.4
1	C	54	LEU	3.4
1	C	92	VAL	3.4
1	C	93	HIS	3.4
1	C	141	GLY	3.4
1	A	248	ASP	3.4
1	C	86	ASN	3.4
1	C	159	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	250	LEU	3.3
1	B	194	ILE	3.3
1	D	245	LEU	3.3
1	A	202	ILE	3.3
1	C	140	PRO	3.3
1	A	173	ARG	3.3
1	D	216	GLN	3.3
1	C	64	ASP	3.3
1	D	98	MET	3.3
1	D	187	ASN	3.3
1	B	71	LEU	3.3
1	B	257	ILE	3.3
1	B	258	ILE	3.3
1	D	73	SER	3.3
1	C	26	ALA	3.3
1	D	114	ALA	3.3
1	C	44	LEU	3.3
1	C	227	PRO	3.3
1	C	87	LYS	3.3
1	D	51	THR	3.3
1	B	174	PHE	3.3
1	C	108	PHE	3.3
1	B	179	ALA	3.2
1	C	264	ALA	3.2
1	D	96	GLY	3.2
1	C	220	GLU	3.2
1	D	120	ILE	3.2
1	A	111	ALA	3.2
1	D	261	ASP	3.2
1	A	118	LYS	3.2
1	D	63	LEU	3.2
1	C	215	ILE	3.2
1	B	39	THR	3.2
1	C	13	SER	3.2
1	B	91	VAL	3.2
1	B	87	LYS	3.2
1	D	33	GLY	3.2
1	B	100	GLN	3.2
1	D	47	ILE	3.2
1	A	34	ALA	3.2
1	C	176	ALA	3.2
1	C	244	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	158	TYR	3.2
1	D	242	VAL	3.2
1	B	79	THR	3.2
1	B	146	GLY	3.1
1	B	244	ALA	3.1
1	D	37	VAL	3.1
1	B	19	SER	3.1
1	B	265	HIS	3.1
1	A	231	ASN	3.1
1	B	84	ALA	3.1
1	B	164	ALA	3.1
1	D	67	ASN	3.1
1	D	235	ALA	3.1
1	A	37	VAL	3.1
1	C	145	VAL	3.1
1	A	46	LEU	3.1
1	A	43	ARG	3.1
1	D	173	ARG	3.1
1	A	232	MET	3.1
1	B	266	THR	3.1
1	C	265	HIS	3.1
1	B	262	GLY	3.1
1	A	237	PRO	3.1
1	D	140	PRO	3.1
1	D	151	PRO	3.1
1	B	177	ARG	3.1
1	C	233	LYS	3.1
1	A	257	ILE	3.1
1	B	105	ILE	3.1
1	D	194	ILE	3.1
1	D	152	SER	3.1
1	C	259	TYR	3.0
1	D	105	ILE	3.0
1	B	27	ARG	3.0
1	A	133	ALA	3.0
1	B	251	PRO	3.0
1	A	116	VAL	3.0
1	D	103	MET	3.0
1	A	48	GLN	3.0
1	A	222	TRP	3.0
1	D	66	GLN	3.0
1	D	247	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	45	ARG	3.0
1	C	139	ASN	3.0
1	B	156	PRO	3.0
1	B	163	VAL	3.0
1	B	89	ASP	3.0
1	B	96	GLY	3.0
1	A	130	MET	3.0
1	C	138	MET	3.0
1	C	235	ALA	3.0
1	D	46	LEU	3.0
1	D	93	HIS	3.0
1	C	228	ILE	3.0
1	D	137	ILE	3.0
1	A	132	LYS	3.0
1	B	102	GLY	3.0
1	A	199	MET	3.0
1	D	199	MET	3.0
1	A	140	PRO	3.0
1	B	74	LEU	2.9
1	C	77	ARG	2.9
1	C	267	GLN	2.9
1	C	144	ILE	2.9
1	A	31	GLU	2.9
1	B	7	GLY	2.9
1	D	62	GLU	2.9
1	D	212	GLY	2.9
1	B	29	ALA	2.9
1	C	164	ALA	2.9
1	C	24	HIS	2.9
1	D	144	ILE	2.9
1	D	241	THR	2.9
1	C	255	GLY	2.9
1	D	139	ASN	2.9
1	D	125	TYR	2.9
1	C	112	PRO	2.9
1	D	72	ALA	2.9
1	A	194	ILE	2.9
1	A	90	GLY	2.8
1	A	93	HIS	2.8
1	D	239	ALA	2.8
1	C	210	GLU	2.8
1	B	138	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	161	MET	2.8
1	B	248	ASP	2.8
1	C	67	ASN	2.8
1	B	185	ARG	2.8
1	D	19	SER	2.8
1	C	32	GLN	2.8
1	A	149	PHE	2.8
1	A	164	ALA	2.8
1	C	31	GLU	2.8
1	A	78	VAL	2.8
1	C	177	ARG	2.8
1	D	18	ASP	2.8
1	C	199	MET	2.8
1	D	92	VAL	2.8
1	C	173	ARG	2.8
1	A	83	GLY	2.8
1	B	40	GLY	2.8
1	C	224	GLN	2.8
1	A	161	MET	2.8
1	B	133	ALA	2.8
1	C	157	ALA	2.8
1	C	153	ARG	2.8
1	B	253	THR	2.7
1	C	146	GLY	2.7
1	D	141	GLY	2.7
1	B	165	LYS	2.7
1	A	207	LEU	2.7
1	A	12	VAL	2.7
1	B	238	VAL	2.7
1	D	89	ASP	2.7
1	D	122	ILE	2.7
1	A	13	SER	2.7
1	A	233	LYS	2.7
1	C	217	LEU	2.7
1	D	264	ALA	2.7
1	D	186	SER	2.7
1	B	195	ARG	2.7
1	C	12	VAL	2.7
1	D	28	VAL	2.7
1	A	258	ILE	2.7
1	C	3	GLY	2.7
1	C	122	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	112	PRO	2.7
1	C	161	MET	2.7
1	C	71	LEU	2.7
1	A	56	ALA	2.6
1	B	167	ALA	2.6
1	B	260	ALA	2.6
1	C	35	GLN	2.6
1	B	132	LYS	2.6
1	B	149	PHE	2.6
1	A	209	GLU	2.6
1	A	9	ARG	2.6
1	B	20	SER	2.6
1	C	121	HIS	2.6
1	C	168	LEU	2.6
1	D	188	LEU	2.6
1	A	230	TRP	2.6
1	B	108	PHE	2.6
1	A	238	VAL	2.6
1	A	142	GLY	2.6
1	B	90	GLY	2.6
1	C	14	GLY	2.6
1	B	151	PRO	2.6
1	C	55	PRO	2.6
1	C	105	ILE	2.6
1	B	268	LEU	2.6
1	C	218	LEU	2.6
1	D	30	GLN	2.6
1	D	217	LEU	2.6
1	D	68	GLU	2.6
1	A	148	ASP	2.6
1	B	30	GLN	2.6
1	C	181	LYS	2.6
1	B	38	LEU	2.6
1	B	153	ARG	2.6
1	D	185	ARG	2.6
1	A	190	ALA	2.6
1	B	115	ASP	2.6
1	C	110	ASP	2.6
1	A	205	GLY	2.6
1	C	79	THR	2.6
1	D	196	THR	2.6
1	C	134	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	195	ARG	2.5
1	A	14	GLY	2.5
1	D	255	GLY	2.5
1	B	57	LYS	2.5
1	D	53	ARG	2.5
1	C	148	ASP	2.5
1	C	57	LYS	2.5
1	A	79	THR	2.5
1	A	162	THR	2.5
1	C	2	THR	2.5
1	C	51	THR	2.5
1	D	24	HIS	2.5
1	C	78	VAL	2.5
1	D	143	SER	2.5
1	C	45	ARG	2.5
1	C	49	ARG	2.5
1	C	182	TYR	2.5
1	C	155	MET	2.5
1	C	42	ASP	2.5
1	B	221	GLY	2.5
1	A	236	THR	2.5
1	C	69	GLU	2.5
1	B	18	ASP	2.5
1	B	58	ALA	2.5
1	C	124	ALA	2.5
1	D	176	ALA	2.5
1	C	214	GLN	2.5
1	D	14	GLY	2.5
1	B	101	THR	2.4
1	C	27	ARG	2.4
1	C	28	VAL	2.4
1	B	157	ALA	2.4
1	C	167	ALA	2.4
1	D	22	ALA	2.4
1	D	34	ALA	2.4
1	D	81	ALA	2.4
1	A	69	GLU	2.4
1	B	3	GLY	2.4
1	A	25	ILE	2.4
1	C	8	LYS	2.4
1	C	232	MET	2.4
1	A	76	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	263	GLY	2.4
1	B	254	THR	2.4
1	C	73	SER	2.4
1	B	144	ILE	2.4
1	D	189	VAL	2.4
1	B	61	LEU	2.4
1	D	9	ARG	2.4
1	B	68	GLU	2.4
1	A	206	ALA	2.4
1	B	226	ALA	2.4
1	B	188	LEU	2.4
1	D	135	LEU	2.4
1	B	77	ARG	2.4
1	D	219	GLU	2.4
1	C	99	PRO	2.3
1	C	70	HIS	2.3
1	A	182	TYR	2.3
1	B	33	GLY	2.3
1	B	34	ALA	2.3
1	B	173	ARG	2.3
1	A	30	GLN	2.3
1	A	210	GLU	2.3
1	B	78	VAL	2.3
1	C	91	VAL	2.3
1	D	31	GLU	2.3
1	A	86	ASN	2.3
1	C	262	GLY	2.3
1	D	76	GLY	2.3
1	D	222	TRP	2.3
1	B	232	MET	2.3
1	D	110	ASP	2.3
1	C	98	MET	2.3
1	A	127	TYR	2.3
1	C	29	ALA	2.3
1	D	181	LYS	2.3
1	B	197	LEU	2.2
1	D	12	VAL	2.3
1	C	234	ASP	2.2
1	A	29	ALA	2.2
1	A	211	ALA	2.2
1	A	166	SER	2.2
1	A	47	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	88	LEU	2.2
1	C	269	LEU	2.2
1	C	80	GLU	2.2
1	B	51	THR	2.2
1	A	126	SER	2.2
1	B	247	SER	2.2
1	C	47	ILE	2.2
1	A	49	ARG	2.2
1	D	55	PRO	2.2
1	C	96	GLY	2.2
1	B	17	THR	2.2
1	D	128	ALA	2.2
1	A	234	ASP	2.2
1	D	91	VAL	2.2
1	D	104	GLY	2.2
1	D	2	THR	2.2
1	D	195	ARG	2.1
1	A	115	ASP	2.1
1	B	86	ASN	2.1
1	B	99	PRO	2.1
1	B	140	PRO	2.1
1	C	216	GLN	2.1
1	C	85	GLY	2.1
1	B	190	ALA	2.1
1	B	236	THR	2.1
1	D	82	ILE	2.1
1	B	178	GLU	2.1
1	C	59	PRO	2.1
1	D	3	GLY	2.1
1	D	7	GLY	2.1
1	A	241	THR	2.1
1	A	114	ALA	2.1
1	C	186	SER	2.1
1	B	155	MET	2.1
1	D	61	LEU	2.1
1	D	74	LEU	2.1
1	D	238	VAL	2.1
1	B	97	PHE	2.1
1	A	104	GLY	2.1
1	D	266	THR	2.1
1	A	10	ILE	2.1
1	C	113	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	41	PHE	2.1
1	C	240	LYS	2.0
1	A	265	HIS	2.0
1	B	95	ILE	2.0
1	A	102	GLY	2.0
1	A	64	ASP	2.0
1	B	106	ASN	2.0
1	B	187	ASN	2.0
1	D	177	ARG	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](#)

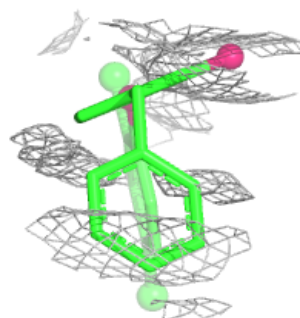
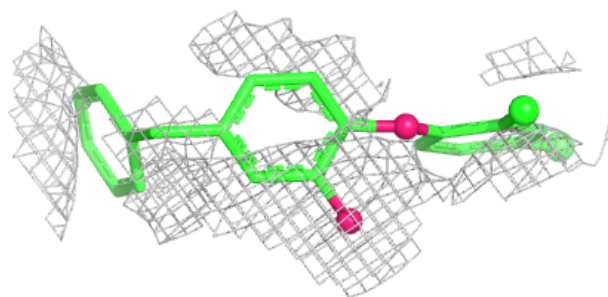
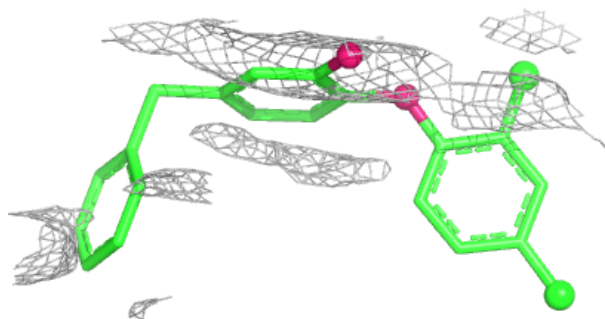
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	JPM	A	400	23/23	0.25	0.23	21,32,43,44	0
2	NAD	D	330	44/44	0.34	0.22	39,42,45,47	0
2	NAD	B	310	44/44	0.46	0.24	36,41,44,44	0
3	JPM	D	430	23/23	0.46	0.21	32,41,43,43	0
3	JPM	B	410	23/23	0.50	0.19	36,42,48,49	0
3	JPM	C	420	23/23	0.52	0.21	21,34,39,41	0
2	NAD	C	320	44/44	0.55	0.23	28,34,37,38	0
2	NAD	A	300	44/44	0.73	0.12	28,33,37,38	0

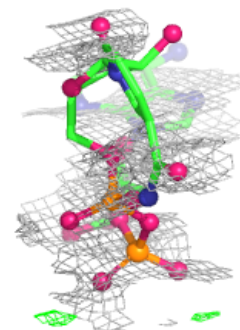
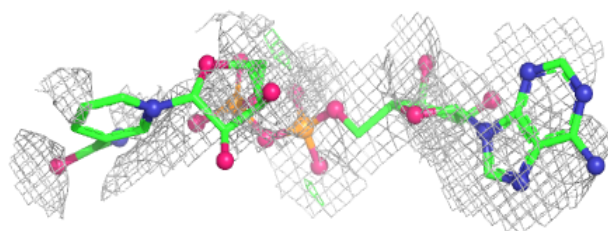
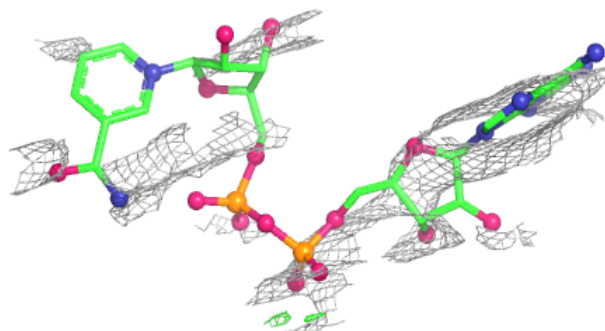
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around JPM 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)

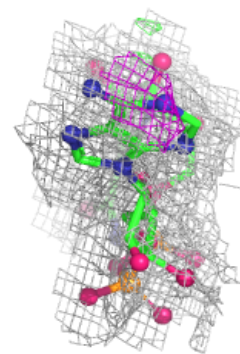
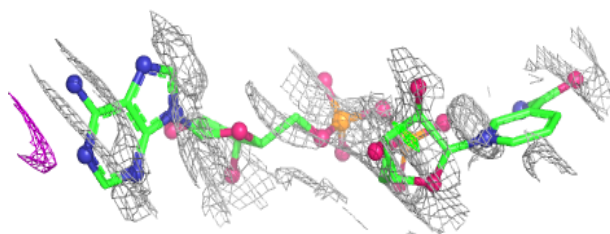
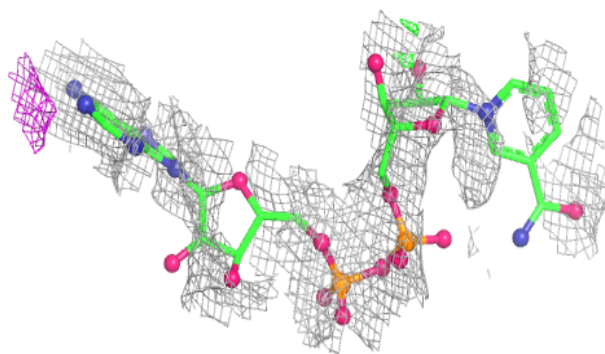
**Electron density around NAD D 330:**

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

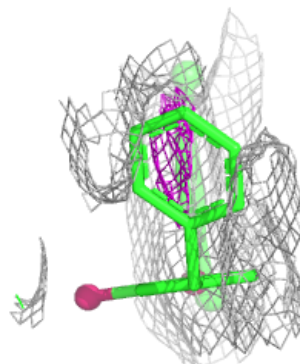
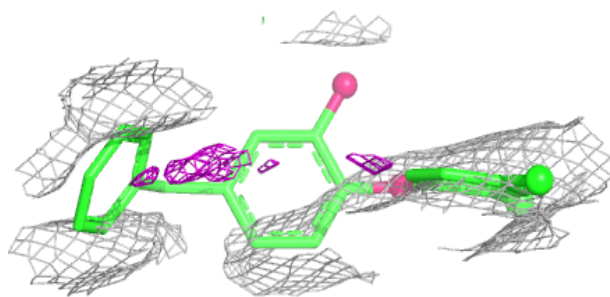
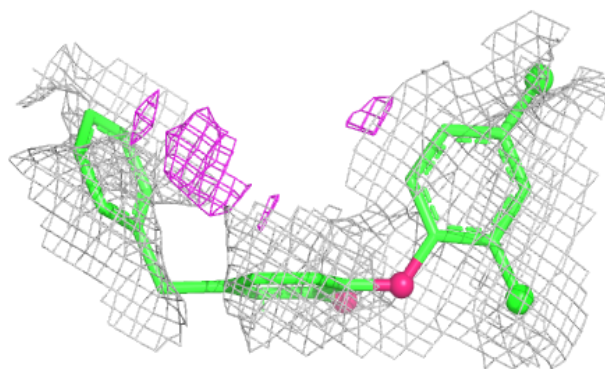


Electron density around NAD B 310:

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

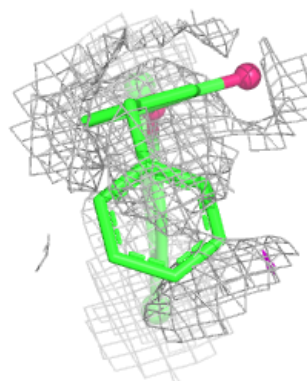
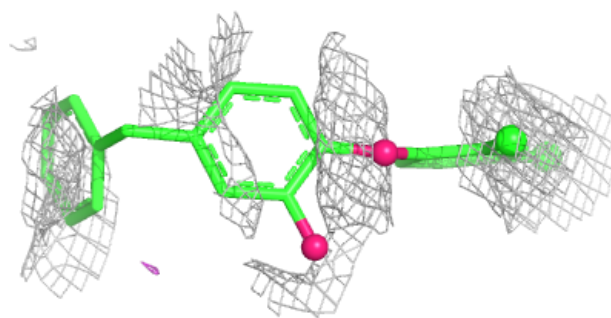
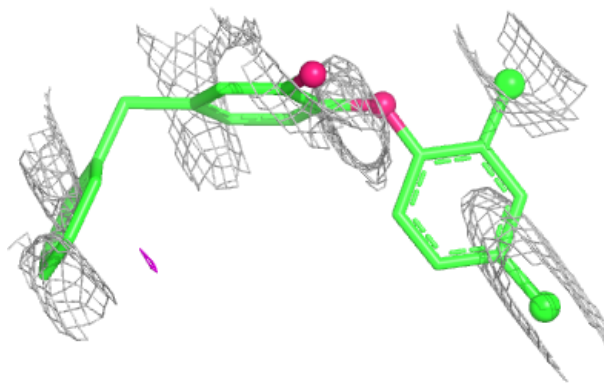
**Electron density around JPM D 430:**

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

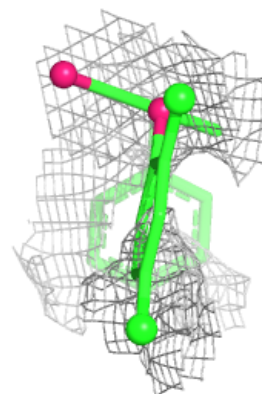
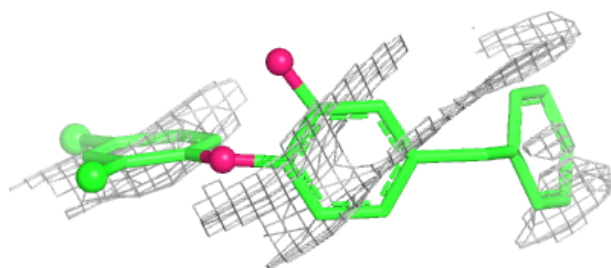
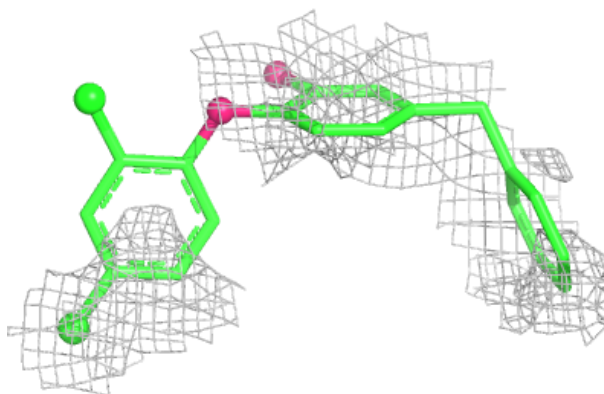


Electron density around JPM B 410:

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

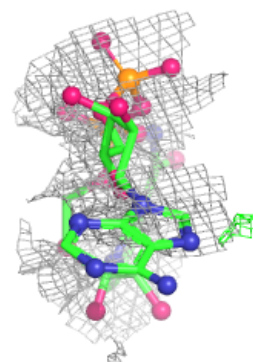
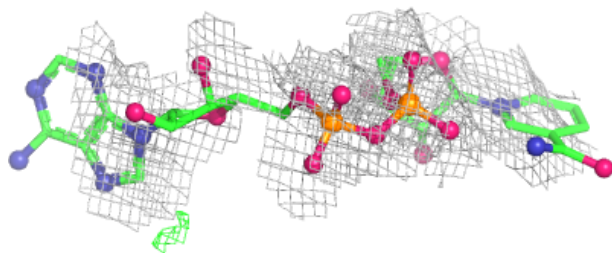
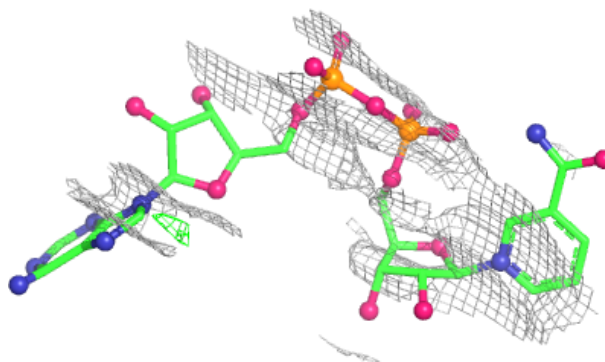
**Electron density around JPM C 420:**

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

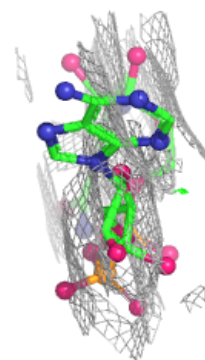
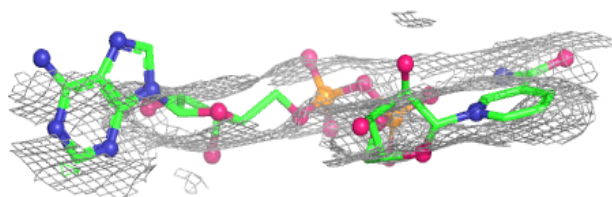
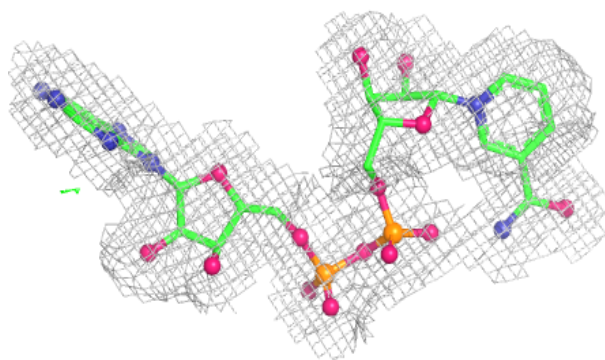


Electron density around NAD C 320:

$2mF_o-DF_c$ (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.