



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:00 AM UTC

PDB ID : 1ZRQ / pdb_00001zrq
Title : Escherichia coli Methylenetetrahydrofolate Reductase (reduced) complexed with NADH, pH 6.0
Authors : Pejchal, R.; Sargeant, R.; Ludwig, M.L.
Deposited on : 2005-05-19
Resolution : 2.20 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

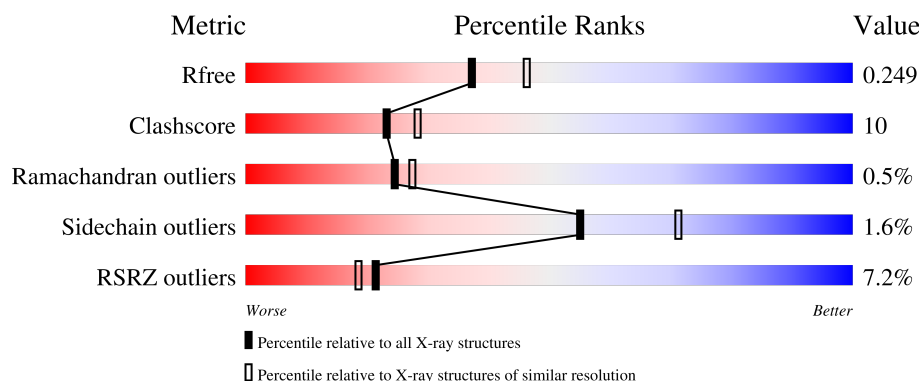
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	304	15% 71% 19% • 8%
1	B	304	3% 75% 19% • 6%
1	C	304	2% 67% 19% • 12%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7024 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 5,10-methylenetetrahydrofolate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2147	1361	372	403	11			
1	B	287	Total	C	N	O	S	0	0	0
			2223	1410	388	414	11			
1	C	268	Total	C	N	O	S	0	0	0
			2081	1322	361	387	11			

There are 24 discrepancies between the modelled and reference sequences:

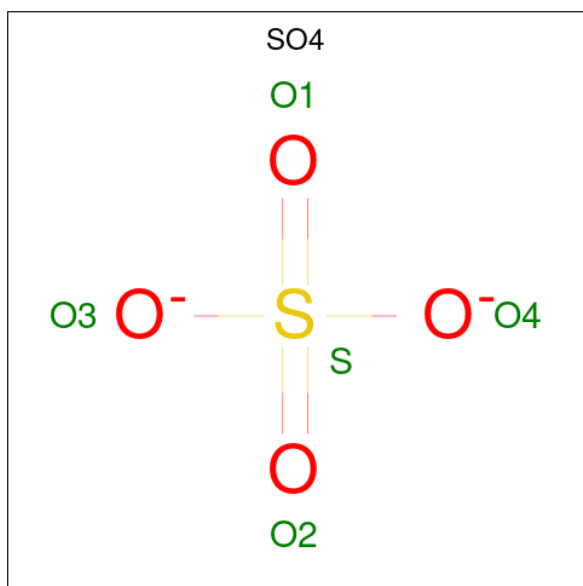
Chain	Residue	Modelled	Actual	Comment	Reference
A	297	LEU	-	cloning artifact	UNP P00394
A	298	GLU	-	cloning artifact	UNP P00394
A	299	HIS	-	expression tag	UNP P00394
A	300	HIS	-	expression tag	UNP P00394
A	301	HIS	-	expression tag	UNP P00394
A	302	HIS	-	expression tag	UNP P00394
A	303	HIS	-	expression tag	UNP P00394
A	304	HIS	-	expression tag	UNP P00394
B	297	LEU	-	cloning artifact	UNP P00394
B	298	GLU	-	cloning artifact	UNP P00394
B	299	HIS	-	expression tag	UNP P00394
B	300	HIS	-	expression tag	UNP P00394
B	301	HIS	-	expression tag	UNP P00394
B	302	HIS	-	expression tag	UNP P00394
B	303	HIS	-	expression tag	UNP P00394
B	304	HIS	-	expression tag	UNP P00394
C	297	LEU	-	cloning artifact	UNP P00394
C	298	GLU	-	cloning artifact	UNP P00394
C	299	HIS	-	expression tag	UNP P00394
C	300	HIS	-	expression tag	UNP P00394
C	301	HIS	-	expression tag	UNP P00394
C	302	HIS	-	expression tag	UNP P00394
C	303	HIS	-	expression tag	UNP P00394

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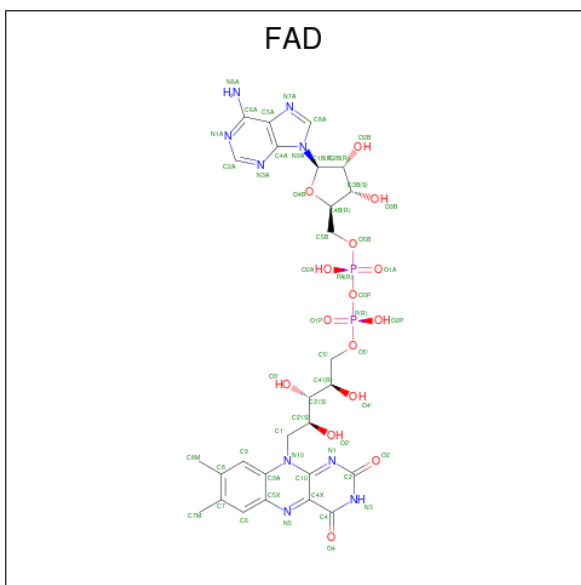
Chain	Residue	Modelled	Actual	Comment	Reference
C	304	HIS	-	expression tag	UNP P00394

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



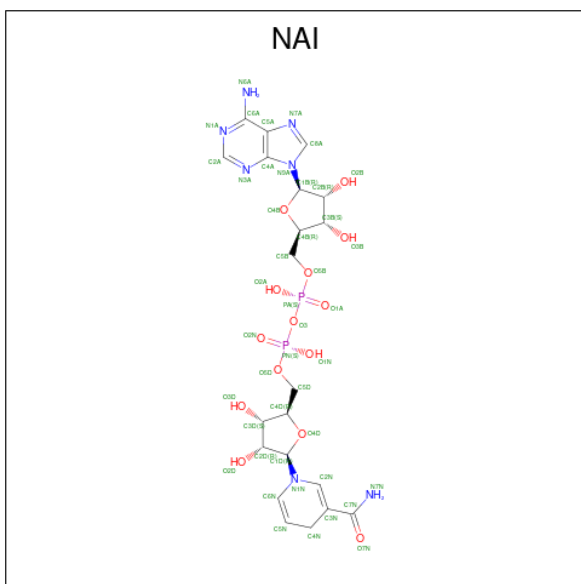
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 4 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $\text{C}_{21}\text{H}_{29}\text{N}_7\text{O}_{14}\text{P}_2$).



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

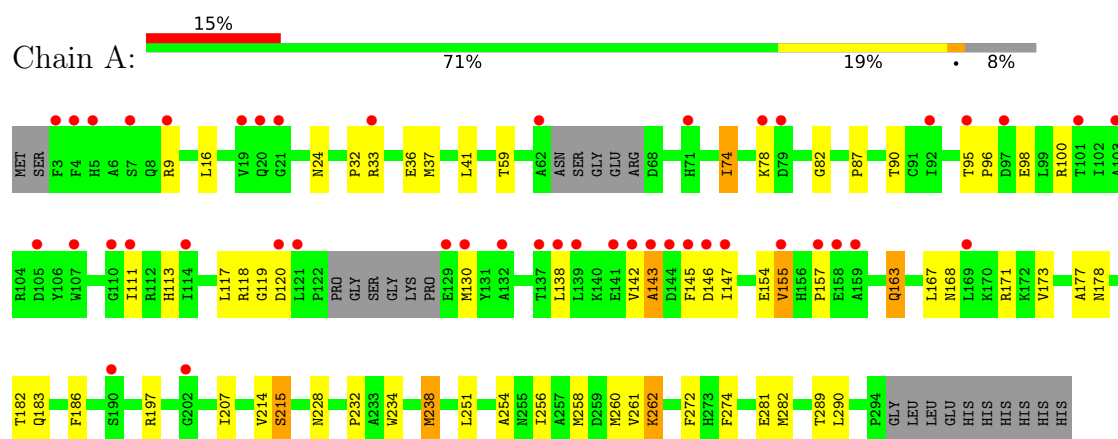
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	46	Total	O	0	0
			46	46		
5	B	104	Total	O	0	0
			104	104		
5	C	112	Total	O	0	0
			112	112		

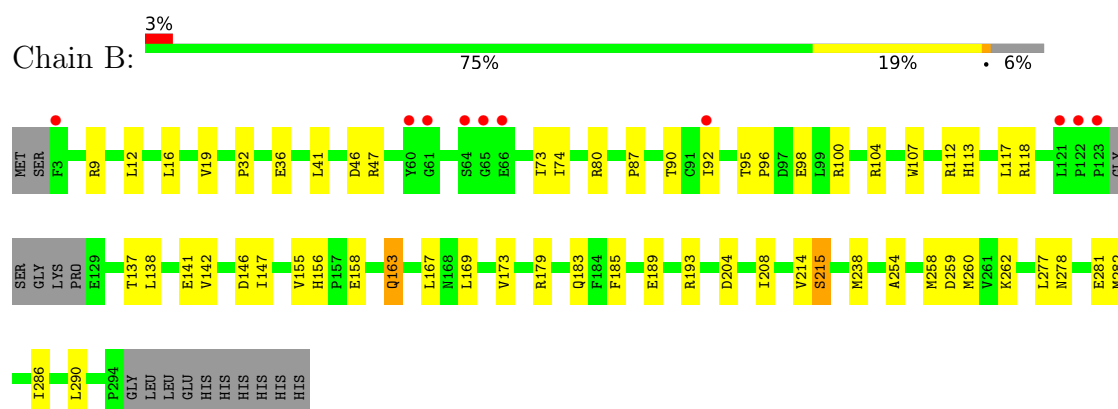
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

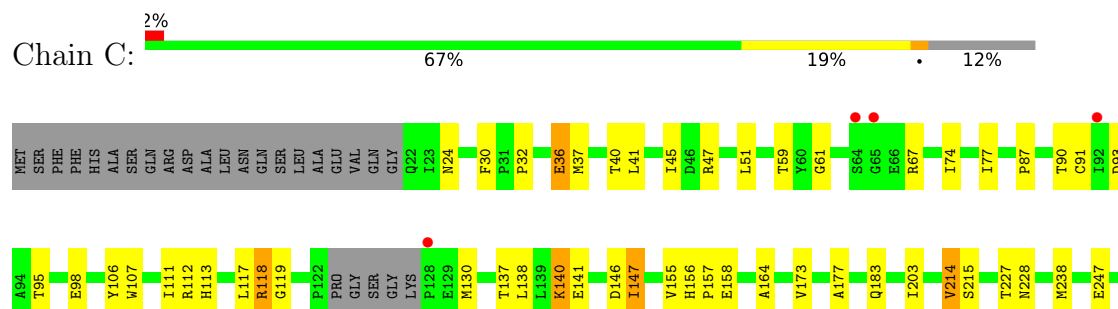
- Molecule 1: 5,10-methylenetetrahydrofolate reductase

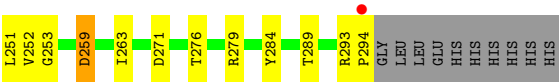


- Molecule 1: 5,10-methylenetetrahydrofolate reductase



- Molecule 1: 5,10-methylenetetrahydrofolate reductase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	102.19Å 128.16Å 96.86Å 90.00° 120.94° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.20) 99.8 (20.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.219 , 0.252 0.217 , 0.249	Depositor DCC
R_{free} test set	5516 reflections (10.19%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.368	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7024	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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: FAD, NAI, SO4

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	0.37	0/2189	0.84	5/2975 (0.2%)
1	B	0.34	0/2269	0.84	6/3078 (0.2%)
1	C	0.33	0/2125	0.85	5/2884 (0.2%)
All	All	0.35	0/6583	0.84	16/8937 (0.2%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	146	ASP	N-CA-C	-7.58	96.89	109.46
1	B	183	GLN	N-CA-C	-7.39	100.78	110.53
1	A	183	GLN	N-CA-C	-7.37	100.11	110.50
1	C	183	GLN	N-CA-C	-7.36	100.81	110.53
1	C	147	ILE	N-CA-C	7.08	118.02	108.11
1	B	215	SER	N-CA-C	-6.96	105.32	113.88
1	A	214	VAL	N-CA-C	6.74	117.56	107.51
1	C	146	ASP	N-CA-C	-6.63	98.41	108.96
1	C	214	VAL	N-CA-C	6.15	116.72	107.80
1	B	281	GLU	N-CA-C	6.09	118.42	111.11
1	B	214	VAL	N-CA-C	6.08	116.37	107.37
1	A	74	ILE	O-C-N	5.85	127.65	121.91
1	A	215	SER	N-CA-C	-5.84	106.69	113.88
1	C	215	SER	N-CA-C	-5.84	106.77	114.31
1	B	147	ILE	N-CA-C	5.58	115.92	108.11
1	A	274	PHE	N-CA-C	5.22	117.75	109.24

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	2147	0	2058	50	0
1	B	2223	0	2163	43	0
1	C	2081	0	2025	48	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	A	53	0	31	0	0
3	B	53	0	31	0	0
3	C	53	0	31	0	0
4	A	44	0	27	1	0
4	B	44	0	27	1	0
4	C	44	0	27	5	0
5	A	46	0	0	3	0
5	B	104	0	0	1	0
5	C	112	0	0	2	1
All	All	7024	0	6420	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 10.

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:A:16:LEU:HD22	1:A:262:LYS:HG2	1.42	1.00
1:A:261:VAL:HG21	1:A:290:LEU:HD11	1.55	0.88
1:A:261:VAL:HG22	1:A:290:LEU:HD21	1.57	0.84
1:B:163:GLN:HE21	1:B:163:GLN:H	1.28	0.80
1:A:186:PHE:HA	1:A:260:MET:HE1	1.66	0.77
1:A:173:VAL:HA	1:A:177:ALA:HB3	1.68	0.75
1:A:74:ILE:HG13	1:A:87:PRO:HB3	1.68	0.74
1:A:146:ASP:HB3	1:A:178:ASN:HD22	1.56	0.71
1:C:238:MET:HE3	1:C:252:VAL:HG13	1.72	0.71
1:A:261:VAL:HG23	1:A:272:PHE:CE2	2.26	0.70
1:B:163:GLN:H	1:B:163:GLN:NE2	1.90	0.70
1:C:61:GLY:HA3	4:C:497:NAI:O1N	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:LYS:O	1:A:82:GLY:HA2	1.92	0.69
1:B:16:LEU:O	1:B:19:VAL:HG12	1.96	0.66
1:B:90:THR:HA	1:B:117:LEU:O	1.96	0.64
1:A:9:ARG:HE	1:C:263:ILE:HG13	1.63	0.64
1:A:154:GLU:O	1:A:155:VAL:HG22	1.96	0.64
1:B:32:PRO:HD3	1:B:41:LEU:HD22	1.81	0.63
1:C:137:THR:O	1:C:141:GLU:HG3	1.98	0.63
1:B:92:ILE:HG12	1:B:118:ARG:O	1.99	0.63
1:B:189:GLU:HB3	1:B:193:ARG:NH2	2.14	0.63
1:A:16:LEU:HD22	1:A:262:LYS:CG	2.25	0.62
1:C:173:VAL:HA	1:C:177:ALA:HB3	1.81	0.62
1:A:143:ALA:HB3	1:A:145:PHE:CE1	2.36	0.61
1:B:137:THR:O	1:B:141:GLU:HG3	2.01	0.60
1:C:112:ARG:HH11	1:C:112:ARG:HG3	1.66	0.59
1:C:30:PHE:CG	4:C:497:NAI:H4B	2.36	0.59
1:A:157:PRO:HG3	1:A:228:ASN:HB2	1.84	0.59
1:A:90:THR:HA	1:A:117:LEU:O	2.04	0.58
1:B:95:THR:OG1	1:B:98:GLU:HG3	2.03	0.58
1:A:96:PRO:HG3	1:A:130:MET:HE1	1.84	0.58
1:A:261:VAL:CG2	1:A:290:LEU:HD21	2.31	0.57
1:C:36:GLU:H	1:C:36:GLU:CD	2.12	0.57
1:C:74:ILE:HG13	1:C:87:PRO:HB3	1.84	0.57
1:C:95:THR:OG1	1:C:98:GLU:HG3	2.04	0.57
1:A:96:PRO:O	1:A:100:ARG:HG3	2.05	0.56
1:A:33:ARG:N	1:A:33:ARG:HD3	2.20	0.56
1:B:32:PRO:HD2	1:B:73:ILE:HD11	1.87	0.56
1:C:30:PHE:CD2	4:C:497:NAI:H4B	2.41	0.56
1:C:140:LYS:HD3	1:C:147:ILE:HD12	1.87	0.55
1:C:140:LYS:NZ	1:C:140:LYS:HB3	2.21	0.55
1:B:138:LEU:C	1:B:138:LEU:HD23	2.31	0.54
1:A:59:THR:HG21	4:A:495:NAI:O3B	2.07	0.54
1:B:107:TRP:CE3	1:B:112:ARG:HD2	2.41	0.54
1:C:24:ASN:HB2	1:C:271:ASP:OD1	2.08	0.54
4:B:496:NAI:H2N	5:B:577:HOH:O	2.08	0.54
1:A:163:GLN:O	1:A:167:LEU:HG	2.09	0.53
1:C:59:THR:HG21	4:C:497:NAI:H5N	1.90	0.53
1:B:46:ASP:OD1	1:B:80:ARG:HD3	2.08	0.53
1:B:193:ARG:HH21	1:B:193:ARG:HG3	1.74	0.53
1:B:238:MET:HE2	1:B:238:MET:HA	1.91	0.53
1:B:163:GLN:NE2	1:B:163:GLN:N	2.57	0.53
1:B:16:LEU:HD11	1:B:290:LEU:HD23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:THR:HG22	1:C:238:MET:HE1	1.92	0.52
1:C:138:LEU:HD23	1:C:138:LEU:O	2.10	0.52
1:B:32:PRO:HD3	1:B:41:LEU:CD2	2.39	0.52
1:A:147:ILE:O	1:A:178:ASN:N	2.43	0.52
1:B:74:ILE:HG13	1:B:87:PRO:HB3	1.92	0.51
1:A:32:PRO:HD3	1:A:41:LEU:HD22	1.91	0.51
1:C:59:THR:CG2	4:C:497:NAI:H5N	2.41	0.51
1:A:138:LEU:O	1:A:142:VAL:HG23	2.10	0.51
1:A:232:PRO:HB2	1:A:234:TRP:CD1	2.46	0.51
1:B:215:SER:HB3	1:B:282:MET:SD	2.51	0.51
1:C:32:PRO:HB3	1:C:37:MET:HG3	1.92	0.50
1:A:111:ILE:HD12	1:A:111:ILE:N	2.26	0.50
1:C:90:THR:HA	1:C:117:LEU:O	2.11	0.50
1:C:138:LEU:HD23	1:C:138:LEU:C	2.37	0.50
1:A:254:ALA:O	1:A:258:MET:HG3	2.12	0.49
1:A:261:VAL:CG2	1:A:290:LEU:HD11	2.36	0.49
1:B:9:ARG:HD2	1:B:9:ARG:O	2.13	0.49
1:C:32:PRO:HD3	1:C:41:LEU:HD22	1.95	0.48
1:C:107:TRP:CZ3	1:C:112:ARG:HG2	2.48	0.48
1:A:32:PRO:HB3	1:A:37:MET:HG3	1.95	0.48
1:A:118:ARG:HD2	1:A:119:GLY:O	2.13	0.48
1:C:156:HIS:HD1	1:C:158:GLU:H	1.61	0.48
1:B:12:LEU:HG	1:B:262:LYS:HG2	1.96	0.47
1:C:259:ASP:O	1:C:263:ILE:HG12	2.14	0.47
1:A:146:ASP:CB	1:A:178:ASN:HD22	2.25	0.47
1:B:179:ARG:HD3	1:B:208:ILE:HD12	1.95	0.47
1:A:238:MET:HA	1:A:238:MET:HE3	1.96	0.47
1:A:32:PRO:C	1:A:33:ARG:HD3	2.40	0.47
1:B:47:ARG:HH11	1:B:47:ARG:HG2	1.81	0.46
1:B:104:ARG:HG2	1:B:142:VAL:HG13	1.96	0.46
1:C:106:TYR:HD1	1:C:111:ILE:HG13	1.81	0.46
1:A:24:ASN:HA	5:A:650:HOH:O	2.14	0.46
1:A:182:THR:CG2	1:A:207:ILE:HG22	2.46	0.45
1:A:281:GLU:HG2	1:C:247:GLU:HG2	1.97	0.45
1:C:157:PRO:HB3	1:C:228:ASN:ND2	2.31	0.45
1:B:96:PRO:O	1:B:100:ARG:HG3	2.15	0.45
1:C:156:HIS:CE1	1:C:158:GLU:HB2	2.52	0.45
1:A:251:LEU:HD23	1:C:251:LEU:HD23	1.99	0.45
1:C:107:TRP:CE3	1:C:112:ARG:HG2	2.51	0.44
1:A:36:GLU:H	1:A:36:GLU:CD	2.26	0.44
1:B:36:GLU:H	1:B:36:GLU:CD	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:SER:HB3	1:A:282:MET:SD	2.57	0.44
1:C:47:ARG:HH11	1:C:47:ARG:HG2	1.82	0.44
1:B:167:LEU:HD12	1:B:167:LEU:HA	1.82	0.44
1:B:96:PRO:CB	1:B:100:ARG:HH12	2.31	0.44
1:B:156:HIS:CE1	1:B:158:GLU:HB2	2.53	0.43
1:B:185:PHE:O	1:B:260:MET:HE1	2.17	0.43
1:B:163:GLN:HE21	1:B:163:GLN:N	2.04	0.43
1:A:95:THR:OG1	1:A:98:GLU:HG3	2.19	0.43
1:A:238:MET:HG2	1:A:256:ILE:HD11	2.00	0.43
1:A:238:MET:HE2	1:C:289:THR:HA	2.00	0.43
1:A:168:ASN:O	1:A:171:ARG:HB3	2.19	0.42
1:C:276:THR:HB	1:C:279:ARG:O	2.19	0.42
1:A:87:PRO:HD2	1:A:113:HIS:O	2.19	0.42
1:C:45:ILE:HD13	1:C:77:ILE:HG12	2.02	0.42
1:C:40:THR:CG2	1:C:279:ARG:HH11	2.32	0.42
1:A:120:ASP:HB2	5:A:639:HOH:O	2.19	0.42
1:B:277:LEU:O	1:B:278:ASN:HB2	2.18	0.42
1:C:51:LEU:HD11	1:C:284:TYR:CD1	2.54	0.42
1:C:227:THR:HB	5:C:614:HOH:O	2.19	0.42
1:A:171:ARG:HD2	5:A:605:HOH:O	2.20	0.42
1:B:87:PRO:HD2	1:B:113:HIS:O	2.20	0.42
1:B:282:MET:O	1:B:286:ILE:HG13	2.20	0.42
1:A:258:MET:O	1:A:261:VAL:HG12	2.20	0.41
1:C:293:ARG:HB3	1:C:294:PRO:HD2	2.02	0.41
1:A:33:ARG:N	1:A:33:ARG:CD	2.83	0.41
1:A:232:PRO:HB2	1:A:234:TRP:NE1	2.35	0.41
1:B:254:ALA:O	1:B:258:MET:HG3	2.21	0.41
1:C:87:PRO:HD2	1:C:113:HIS:O	2.21	0.41
1:B:169:LEU:O	1:B:173:VAL:HG23	2.21	0.41
1:C:47:ARG:HG2	1:C:47:ARG:NH1	2.35	0.41
1:C:91:CYS:SG	1:C:130:MET:HG3	2.61	0.41
1:C:118:ARG:HD2	1:C:119:GLY:O	2.21	0.41
1:B:47:ARG:HG2	1:B:47:ARG:NH1	2.35	0.41
1:C:214:VAL:O	1:C:253:GLY:HA3	2.20	0.41
1:B:9:ARG:HD2	1:B:9:ARG:C	2.47	0.40
1:B:100:ARG:O	1:B:104:ARG:HG3	2.21	0.40
1:C:67:ARG:HG2	5:C:622:HOH:O	2.20	0.40
1:C:112:ARG:HG3	1:C:112:ARG:NH1	2.35	0.40
1:B:193:ARG:NH2	1:B:193:ARG:HG3	2.36	0.40
1:B:204:ASP:HB2	1:C:164:ALA:HB2	2.02	0.40
1:C:173:VAL:HG21	1:C:203:ILE:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:ARG:HG3	1:B:9:ARG:HH21	1.87	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:C:622:HOH:O	5:C:622:HOH:O[2_557]	1.52	0.68

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	275/304 (90%)	265 (96%)	8 (3%)	2 (1%)	18	19
1	B	283/304 (93%)	277 (98%)	5 (2%)	1 (0%)	30	34
1	C	264/304 (87%)	254 (96%)	9 (3%)	1 (0%)	30	34
All	All	822/912 (90%)	796 (97%)	22 (3%)	4 (0%)	24	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	VAL
1	C	155	VAL
1	A	143	ALA
1	B	155	VAL

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	219/258 (85%)	215 (98%)	4 (2%)	51	68
1	B	231/258 (90%)	229 (99%)	2 (1%)	70	84
1	C	217/258 (84%)	212 (98%)	5 (2%)	44	59
All	All	667/774 (86%)	656 (98%)	11 (2%)	55	71

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	GLN
1	A	197	ARG
1	A	238	MET
1	A	262	LYS
1	B	163	GLN
1	B	259	ASP
1	C	36	GLU
1	C	93	ASP
1	C	118	ARG
1	C	140	LYS
1	C	259	ASP

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

Mol	Chain	Res	Type
1	A	13	ASN
1	A	14	GLN
1	A	24	ASN
1	A	108	ASN
1	A	163	GLN
1	A	178	ASN
1	B	14	GLN
1	B	109	ASN
1	B	163	GLN
1	B	219	GLN
1	B	228	ASN
1	B	237	GLN
1	C	108	ASN
1	C	219	GLN
1	C	228	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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	$\# Z > 2$
4	NAI	C	497	-	47,48,48	1.47	10 (21%)	64,73,73	1.52	9 (14%)
2	SO4	A	900	-	4,4,4	0.37	0	6,6,6	0.06	0
4	NAI	B	496	-	47,48,48	1.51	10 (21%)	64,73,73	1.50	10 (15%)
2	SO4	C	902	-	4,4,4	0.37	0	6,6,6	0.08	0
3	FAD	B	396	-	58,58,58	1.57	8 (13%)	85,89,89	1.30	11 (12%)
3	FAD	A	395	-	58,58,58	1.57	9 (15%)	85,89,89	1.43	9 (10%)
3	FAD	C	397	-	58,58,58	1.66	10 (17%)	85,89,89	1.28	9 (10%)
4	NAI	A	495	-	47,48,48	1.51	10 (21%)	64,73,73	1.50	10 (15%)
2	SO4	B	901	-	4,4,4	0.38	0	6,6,6	0.06	0
2	SO4	A	899	-	4,4,4	0.37	0	6,6,6	0.06	0

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
4	NAI	C	497	-	-	5/29/72/72	0/5/5/5
4	NAI	B	496	-	-	4/29/72/72	0/5/5/5
3	FAD	B	396	-	-	1/34/50/50	0/6/6/6
3	FAD	A	395	-	-	6/34/50/50	0/6/6/6
3	FAD	C	397	-	-	2/34/50/50	0/6/6/6
4	NAI	A	495	-	-	4/29/72/72	0/5/5/5

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	395	FAD	C10-N10	5.42	1.49	1.37
3	C	397	FAD	C10-N10	5.21	1.48	1.37
3	C	397	FAD	C9A-N10	5.13	1.50	1.41
3	B	396	FAD	C10-N10	5.10	1.48	1.37
3	C	397	FAD	C4X-N5	4.83	1.41	1.30
3	B	396	FAD	C4X-N5	4.75	1.41	1.30
4	B	496	NAI	C4N-C3N	-4.59	1.41	1.50
4	A	495	NAI	C4N-C3N	-4.54	1.41	1.50
3	B	396	FAD	C9A-N10	4.45	1.48	1.41
4	C	497	NAI	C4N-C3N	-4.35	1.41	1.50
3	A	395	FAD	C9A-N10	4.20	1.48	1.41
3	A	395	FAD	C4X-N5	4.17	1.39	1.30
3	A	395	FAD	C9-C9A	3.57	1.45	1.39
3	C	397	FAD	C9-C9A	3.45	1.45	1.39
3	B	396	FAD	C6-C5X	3.44	1.45	1.40
3	B	396	FAD	C9-C9A	3.40	1.45	1.39
3	C	397	FAD	C6-C5X	3.30	1.45	1.40
4	A	495	NAI	PN-O3	3.30	1.63	1.59
4	B	496	NAI	PN-O3	3.26	1.63	1.59
4	B	496	NAI	C5A-N7A	-3.12	1.33	1.39
4	A	495	NAI	C5A-N7A	-3.09	1.33	1.39
3	A	395	FAD	C6-C5X	3.09	1.44	1.40
4	B	496	NAI	C4N-C5N	-3.03	1.41	1.49
4	A	495	NAI	C4N-C5N	-3.01	1.41	1.49
3	C	397	FAD	C8-C7	3.01	1.48	1.40
3	A	395	FAD	C8-C7	3.01	1.48	1.40
4	C	497	NAI	C5A-N7A	-2.97	1.33	1.39
4	C	497	NAI	C4N-C5N	-2.90	1.41	1.49
4	A	495	NAI	C4A-N9A	-2.87	1.31	1.37
4	B	496	NAI	C4A-N9A	-2.87	1.31	1.37
3	B	396	FAD	C8-C7	2.84	1.47	1.40
4	C	497	NAI	C4A-N9A	-2.75	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	397	FAD	P-O3P	2.72	1.62	1.59
4	C	497	NAI	O4D-C1D	2.66	1.48	1.42
3	A	395	FAD	C5'-C4'	2.62	1.55	1.51
4	C	497	NAI	PN-O3	2.61	1.62	1.59
4	A	495	NAI	O4D-C1D	2.55	1.47	1.42
4	B	496	NAI	O4D-C1D	2.51	1.47	1.42
4	B	496	NAI	C6N-C5N	2.49	1.40	1.33
3	C	397	FAD	C10-N1	2.48	1.38	1.33
4	A	495	NAI	C6N-C5N	2.47	1.40	1.33
4	C	497	NAI	C6N-C5N	2.34	1.40	1.33
3	C	397	FAD	C8M-C8	2.31	1.55	1.51
3	B	396	FAD	C9A-C5X	2.27	1.44	1.41
4	C	497	NAI	C7N-C3N	2.26	1.53	1.48
4	C	497	NAI	O4B-C1B	2.21	1.47	1.42
4	B	496	NAI	C7N-C3N	2.14	1.53	1.48
3	A	395	FAD	P-O3P	2.14	1.61	1.59
4	A	495	NAI	C7N-C3N	2.11	1.53	1.48
3	A	395	FAD	C9A-C5X	2.10	1.44	1.41
4	A	495	NAI	C6N-N1N	2.09	1.42	1.37
3	C	397	FAD	C9A-C5X	2.08	1.44	1.41
4	A	495	NAI	O4B-C1B	2.05	1.46	1.42
4	C	497	NAI	C6N-N1N	2.05	1.42	1.37
3	B	396	FAD	C7M-C7	2.03	1.54	1.51
4	B	496	NAI	C6N-N1N	2.03	1.42	1.37
4	B	496	NAI	O4B-C1B	2.01	1.46	1.42

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	497	NAI	N3A-C2A-N1A	-5.54	120.20	128.58
4	A	495	NAI	N3A-C2A-N1A	-5.42	120.38	128.58
4	B	496	NAI	N3A-C2A-N1A	-5.42	120.38	128.58
3	A	395	FAD	C5'-C4'-C3'	5.15	121.94	112.22
4	C	497	NAI	C5A-C4A-N3A	-4.49	120.54	126.72
4	A	495	NAI	C5A-C4A-N3A	-4.48	120.54	126.72
4	B	496	NAI	C5A-C4A-N3A	-4.44	120.61	126.72
3	A	395	FAD	C5X-C9A-N10	-3.81	114.52	117.97
3	A	395	FAD	C9-C9A-N10	3.71	126.85	121.85
3	C	397	FAD	C5X-C9A-N10	-3.70	114.62	117.97
4	A	495	NAI	N9A-C8A-N7A	-3.69	108.70	113.94
4	C	497	NAI	N9A-C8A-N7A	-3.69	108.70	113.94
4	B	496	NAI	N9A-C8A-N7A	-3.68	108.71	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	495	NAI	C2A-N3A-C4A	3.66	120.78	111.83
4	B	496	NAI	C2A-N3A-C4A	3.65	120.75	111.83
4	C	497	NAI	C2A-N3A-C4A	3.65	120.75	111.83
3	C	397	FAD	C9-C9A-N10	3.64	126.75	121.85
3	A	395	FAD	C4'-C3'-C2'	3.61	119.58	113.57
3	A	395	FAD	C9A-C5X-N5	3.57	126.24	122.45
3	B	396	FAD	O2-C2-N3	3.53	125.35	118.58
3	A	395	FAD	O2'-C2'-C3'	3.23	116.81	109.25
3	B	396	FAD	C5X-C9A-N10	-3.23	115.05	117.97
3	B	396	FAD	C9-C9A-N10	3.12	126.05	121.85
3	B	396	FAD	O5'-C5'-C4'	2.98	117.30	109.36
3	C	397	FAD	O5'-C5'-C4'	2.96	117.28	109.36
3	B	396	FAD	C9A-C5X-N5	2.93	125.57	122.45
4	C	497	NAI	N3A-C4A-N9A	2.86	132.02	127.17
4	C	497	NAI	C5A-N7A-C8A	2.69	107.67	103.45
4	A	495	NAI	N3A-C4A-N9A	2.67	131.72	127.17
4	B	496	NAI	N3A-C4A-N9A	2.67	131.71	127.17
3	C	397	FAD	C9A-C5X-N5	2.64	125.26	122.45
4	A	495	NAI	C5A-N7A-C8A	2.57	107.49	103.45
4	B	496	NAI	C5A-N7A-C8A	2.56	107.48	103.45
4	C	497	NAI	C4A-N9A-C8A	2.56	108.42	105.74
4	A	495	NAI	C4A-C5A-N7A	-2.48	107.74	110.58
4	B	496	NAI	C4A-N9A-C8A	2.48	108.34	105.74
4	A	495	NAI	C4A-N9A-C8A	2.47	108.33	105.74
4	C	497	NAI	C4A-C5A-N7A	-2.46	107.77	110.58
4	B	496	NAI	C4A-C5A-N7A	-2.44	107.79	110.58
3	B	396	FAD	C5'-C4'-C3'	2.43	116.80	112.22
3	A	395	FAD	O5'-C5'-C4'	2.42	115.83	109.36
3	C	397	FAD	C5'-C4'-C3'	2.38	116.71	112.22
3	B	396	FAD	C8M-C8-C7	2.38	125.61	120.76
3	B	396	FAD	O5B-C5B-C4B	2.30	116.83	108.99
3	B	396	FAD	C10-N1-C2	2.30	121.83	116.85
4	A	495	NAI	C3N-C2N-N1N	-2.26	119.89	123.20
3	B	396	FAD	C8M-C8-C9	-2.24	115.62	119.57
4	B	496	NAI	C3N-C2N-N1N	-2.24	119.92	123.20
4	C	497	NAI	C3N-C2N-N1N	-2.23	119.92	123.20
3	C	397	FAD	O2B-C2B-C1B	2.20	117.67	110.10
3	B	396	FAD	N3-C2-N1	-2.16	114.91	119.50
3	A	395	FAD	C6-C5X-N5	-2.10	114.97	118.44
4	A	495	NAI	C2B-C1B-N9A	-2.09	108.10	113.30
3	A	395	FAD	C8M-C8-C7	2.08	125.00	120.76
3	C	397	FAD	C2B-C1B-N9A	2.07	118.46	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	397	FAD	O3B-C3B-C4B	-2.05	105.20	111.08
4	B	496	NAI	C2B-C1B-N9A	-2.04	108.22	113.30
3	C	397	FAD	C8M-C8-C7	2.03	124.92	120.76

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	495	NAI	C5B-O5B-PA-O2A
4	A	495	NAI	O4D-C1D-N1N-C2N
4	B	496	NAI	C5B-O5B-PA-O2A
4	B	496	NAI	O4D-C1D-N1N-C2N
4	C	497	NAI	C5B-O5B-PA-O2A
4	C	497	NAI	O4D-C1D-N1N-C2N
3	A	395	FAD	O3'-C3'-C4'-C5'
3	A	395	FAD	O2'-C2'-C3'-C4'
3	C	397	FAD	O2'-C2'-C3'-C4'
3	A	395	FAD	PA-O3P-P-O1P
3	A	395	FAD	C2'-C3'-C4'-C5'
4	A	495	NAI	C5B-O5B-PA-O3
4	B	496	NAI	C5B-O5B-PA-O3
4	C	497	NAI	C5B-O5B-PA-O1A
4	C	497	NAI	C5B-O5B-PA-O3
3	A	395	FAD	PA-O3P-P-O2P
3	B	396	FAD	O2'-C2'-C3'-C4'
4	C	497	NAI	C4D-C5D-O5D-PN
3	A	395	FAD	O4'-C4'-C5'-O5'
4	A	495	NAI	C4D-C5D-O5D-PN
4	B	496	NAI	C4D-C5D-O5D-PN
3	C	397	FAD	O2'-C2'-C3'-O3'

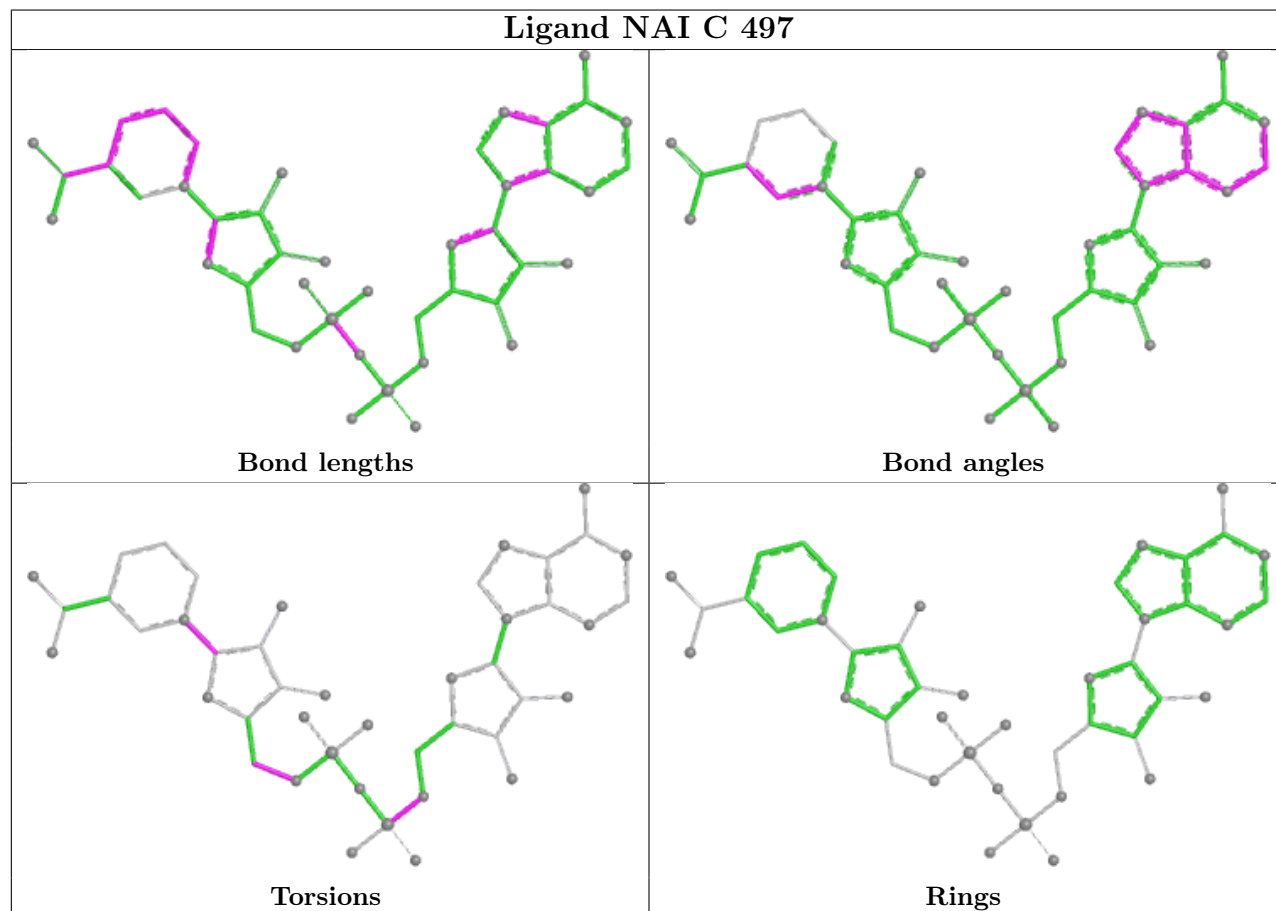
There are no ring outliers.

3 monomers are involved in 7 short contacts:

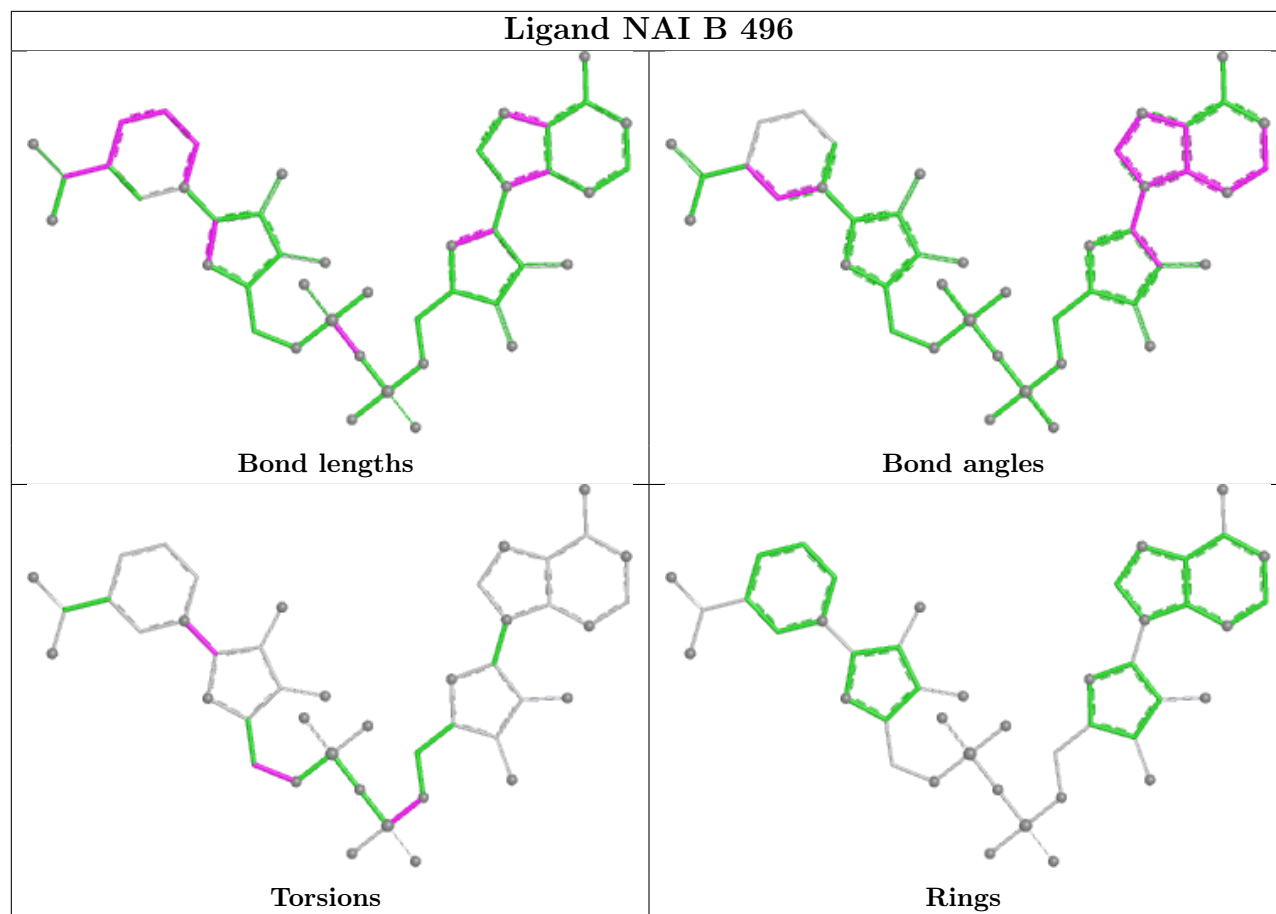
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	497	NAI	5	0
4	B	496	NAI	1	0
4	A	495	NAI	1	0

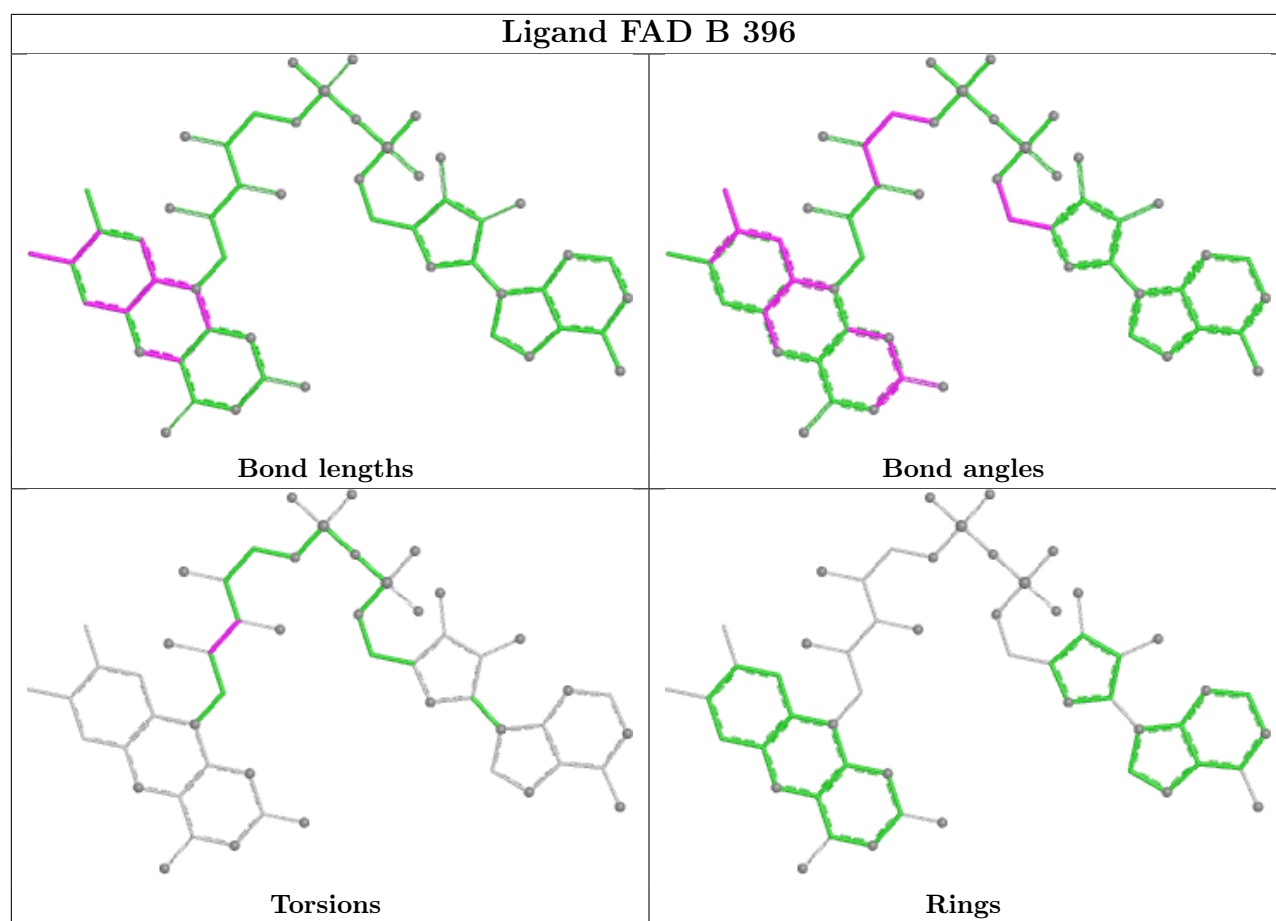
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

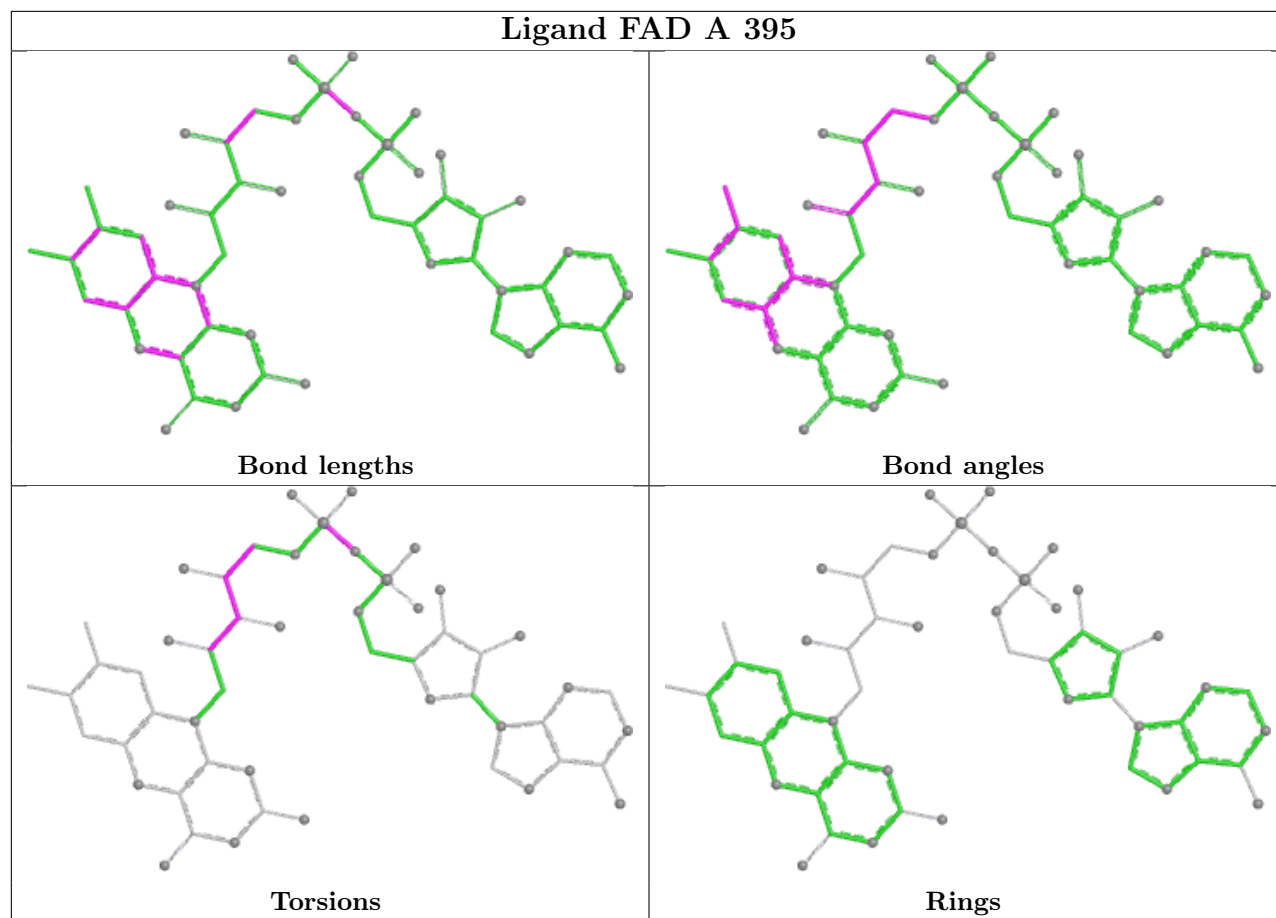
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

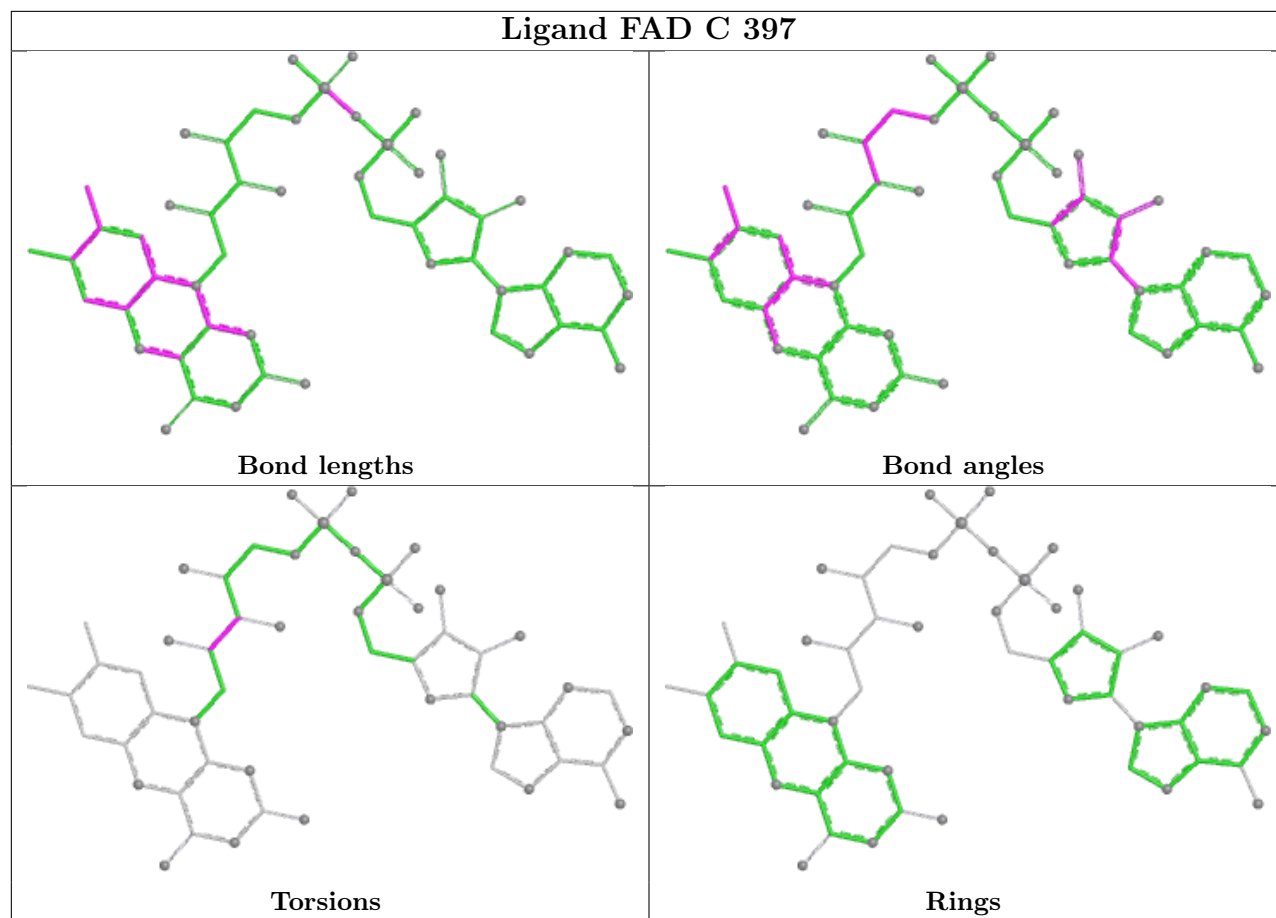


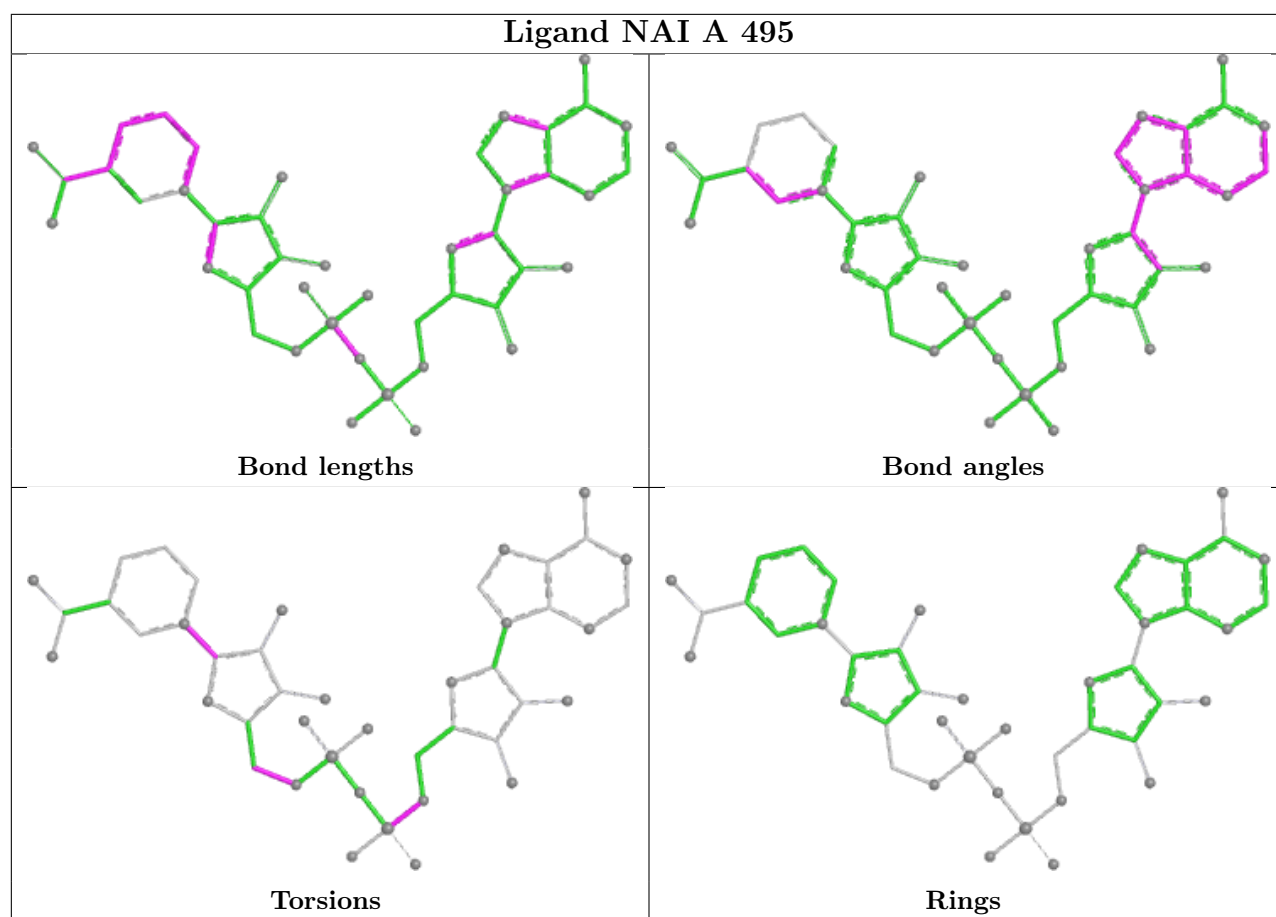
Ligand NAI B 496











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	281/304 (92%)	0.97	45 (16%) 5 3	20, 43, 65, 79	0
1	B	287/304 (94%)	0.12	10 (3%) 47 44	15, 29, 48, 66	0
1	C	268/304 (88%)	0.09	5 (1%) 66 63	16, 30, 45, 54	0
All	All	836/912 (91%)	0.40	60 (7%) 21 18	15, 33, 60, 79	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	PHE	5.0
1	A	142	VAL	4.9
1	A	145	PHE	4.7
1	B	121	LEU	3.8
1	A	121	LEU	3.7
1	A	147	ILE	3.7
1	A	19	VAL	3.6
1	A	62	ALA	3.6
1	A	78	LYS	3.4
1	A	120	ASP	3.3
1	A	139	LEU	3.3
1	B	122	PRO	3.2
1	A	138	LEU	3.1
1	A	95	THR	3.1
1	C	64	SER	3.1
1	B	65	GLY	3.1
1	C	128	PRO	3.0
1	B	92	ILE	3.0
1	C	92	ILE	2.9
1	A	7	SER	2.8
1	A	20	GLN	2.8
1	A	9	ARG	2.7
1	A	159	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	144	ASP	2.7
1	A	97	ASP	2.7
1	A	143	ALA	2.7
1	B	66	GLU	2.6
1	A	4	PHE	2.6
1	A	105	ASP	2.6
1	A	130	MET	2.6
1	B	123	PRO	2.5
1	A	114	ILE	2.5
1	A	107	TRP	2.5
1	A	21	GLY	2.5
1	A	202	GLY	2.5
1	C	65	GLY	2.5
1	A	111	ILE	2.4
1	A	146	ASP	2.4
1	A	110	GLY	2.4
1	A	141	GLU	2.4
1	A	103	ALA	2.4
1	B	64	SER	2.3
1	C	294	PRO	2.3
1	A	190	SER	2.3
1	B	3	PHE	2.2
1	A	132	ALA	2.2
1	A	158	GLU	2.2
1	A	129	GLU	2.2
1	A	101	THR	2.2
1	B	60	TYR	2.1
1	A	169	LEU	2.1
1	A	5	HIS	2.1
1	A	137	THR	2.1
1	A	79	ASP	2.1
1	A	157	PRO	2.1
1	A	155	VAL	2.1
1	A	71	HIS	2.0
1	A	92	ILE	2.0
1	A	33	ARG	2.0
1	B	61	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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](#)

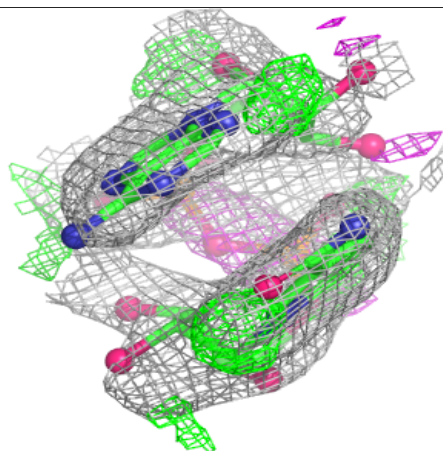
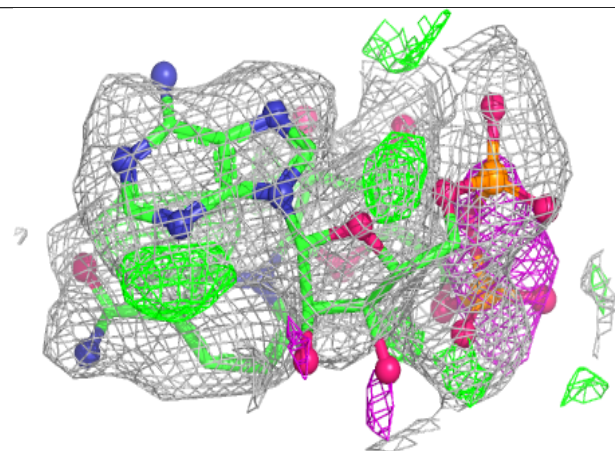
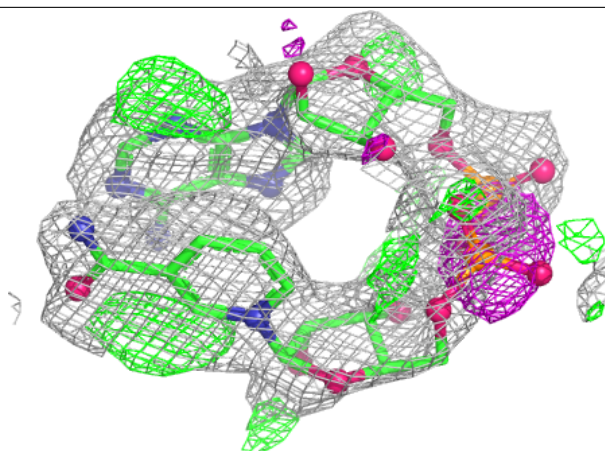
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	NAI	C	497	44/44	0.64	0.21	46,58,63,64	44
2	SO4	A	899	5/5	0.73	0.13	79,79,79,79	0
4	NAI	A	495	44/44	0.79	0.17	45,57,60,61	44
4	NAI	B	496	44/44	0.85	0.18	39,54,57,58	44
3	FAD	A	395	53/53	0.88	0.13	32,40,58,59	0
2	SO4	C	902	5/5	0.90	0.14	62,63,63,63	0
2	SO4	B	901	5/5	0.93	0.10	47,48,48,49	0
2	SO4	A	900	5/5	0.93	0.10	64,64,65,65	0
3	FAD	B	396	53/53	0.95	0.07	19,26,35,35	0
3	FAD	C	397	53/53	0.97	0.06	20,24,31,31	0

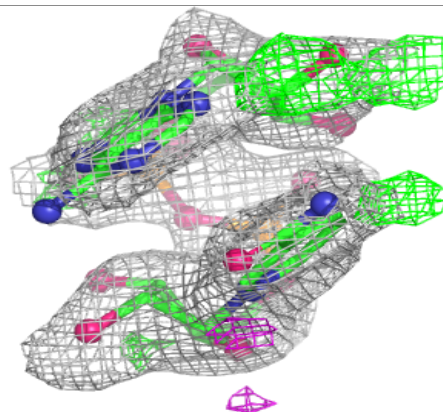
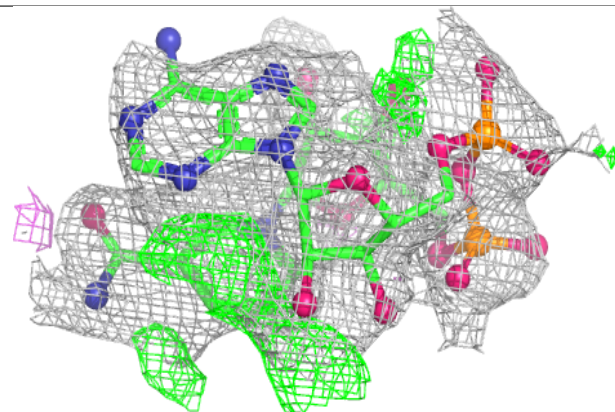
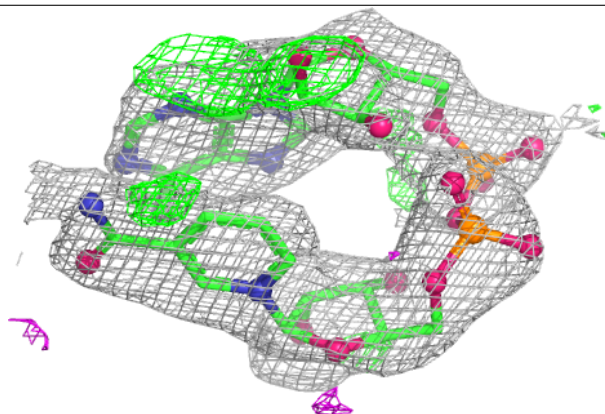
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAI C 497:

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

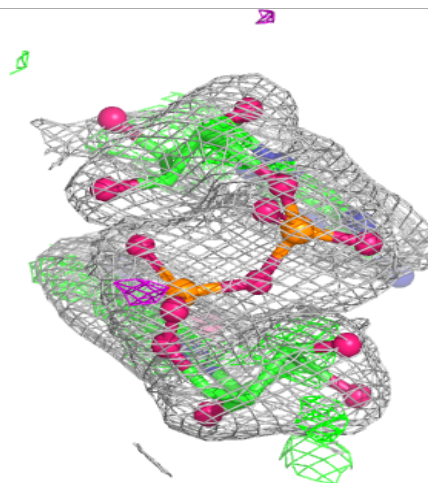
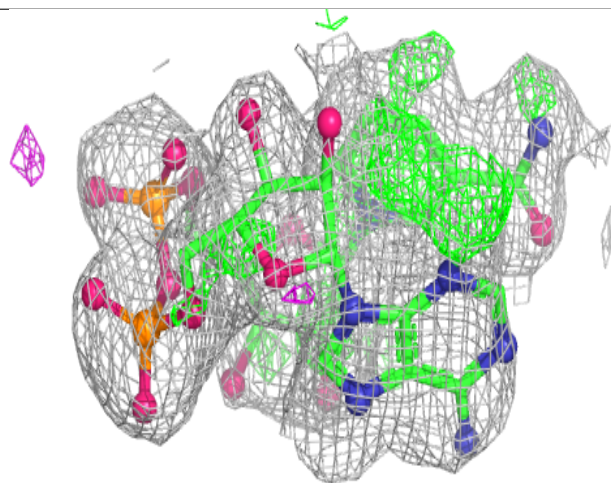
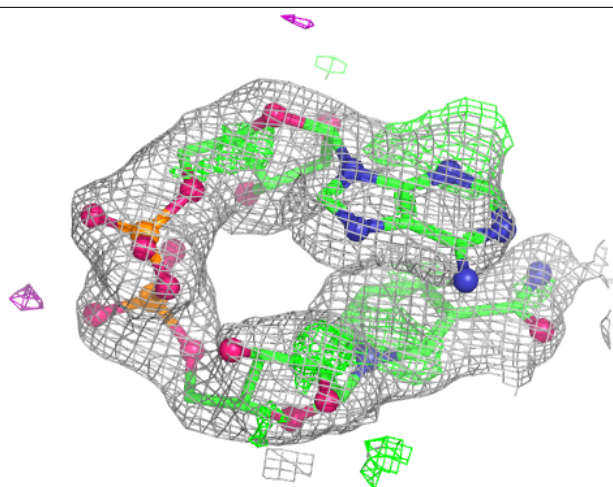
**Electron density around NAI A 495:**

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



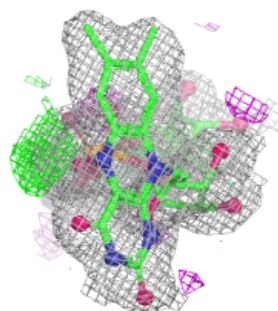
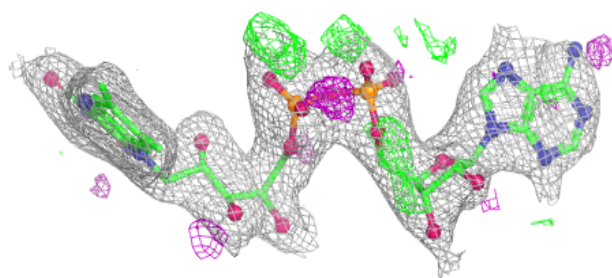
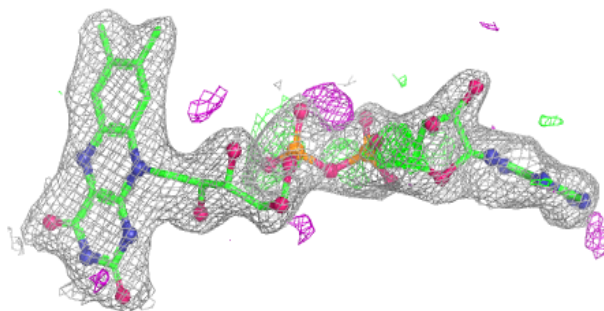
Electron density around NAI B 496:

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

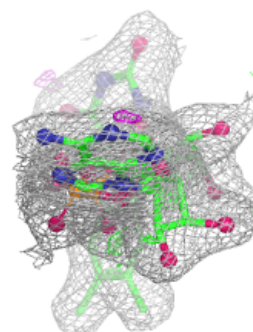
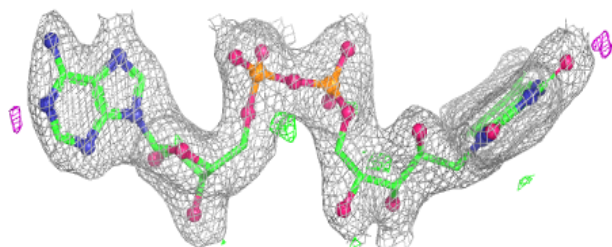
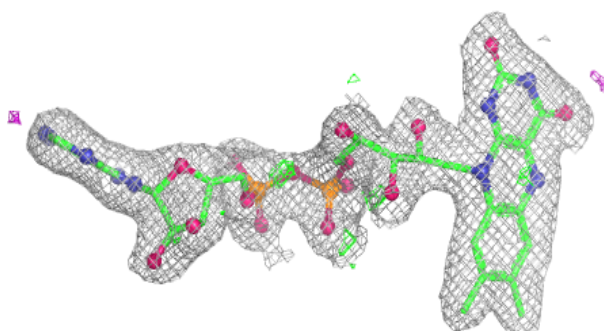


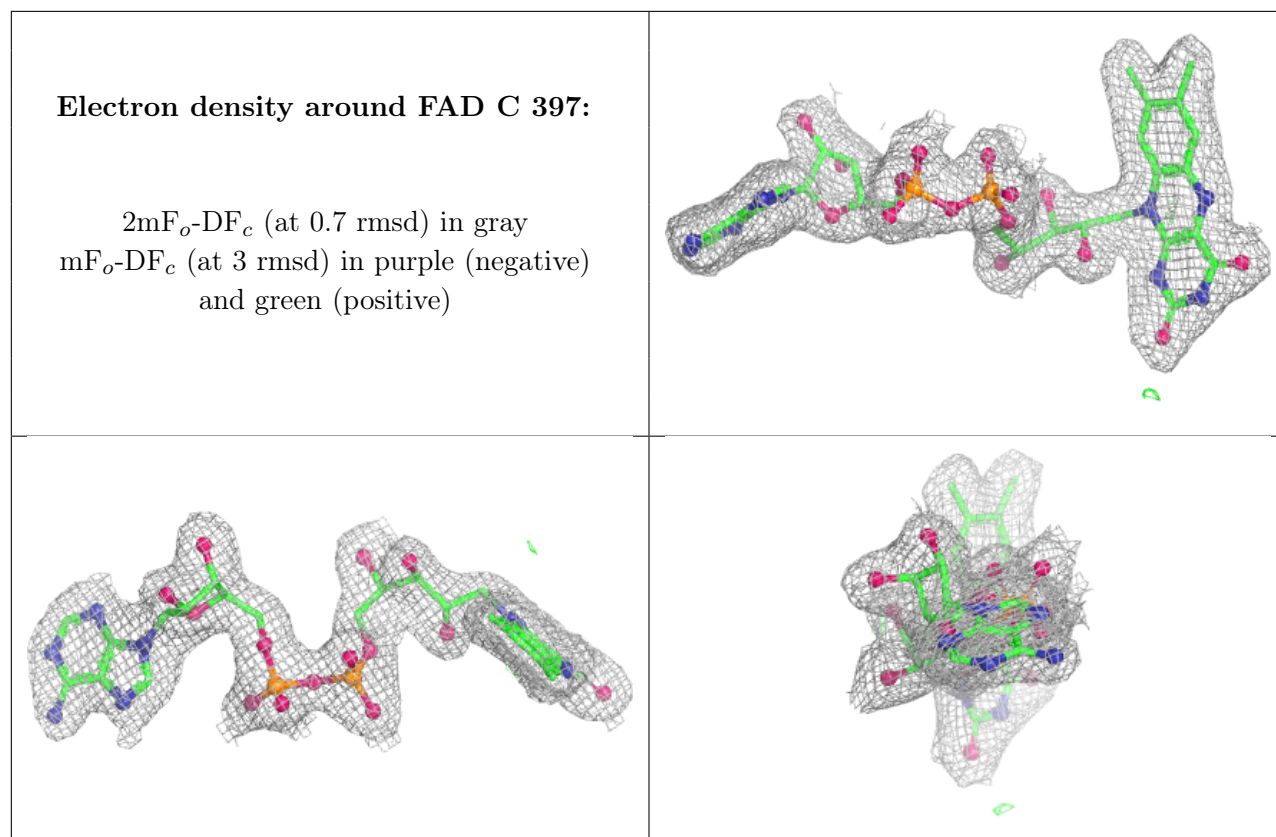
Electron density around FAD A 395:

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

**Electron density around FAD B 396:**

$2mF_o-DF_c$ (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.