



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 06:44 pm BST

PDB ID : 2WOI
Title : Trypanothione reductase from Trypanosoma brucei
Authors : Alphey, M.S.; Fairlamb, A.H.
Deposited on : 2009-07-24
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

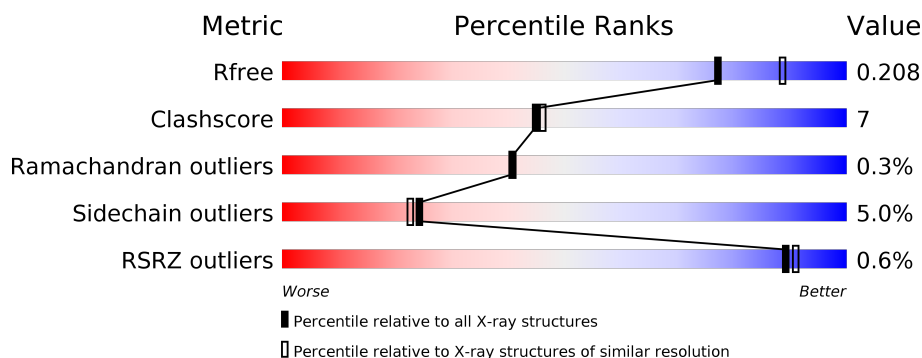
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	495	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>..</div> </div> </div>
1	B	495	<div> <div>80%</div> <div>17%</div> <div>..</div> </div>
1	C	495	<div> <div>83%</div> <div>12%</div> <div>..</div> </div>
1	D	495	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>..</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16312 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 TRYPANOTHIONE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	0	1	0
			3730	2372	636	702	20			
1	B	487	Total	C	N	O	S	0	2	0
			3703	2355	631	698	19			
1	C	484	Total	C	N	O	S	0	3	0
			3689	2346	626	698	19			
1	D	489	Total	C	N	O	S	0	2	0
			3718	2362	632	704	20			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q389T8
A	-1	SER	-	expression tag	UNP Q389T8
A	0	HIS	-	expression tag	UNP Q389T8
B	-2	GLY	-	expression tag	UNP Q389T8
B	-1	SER	-	expression tag	UNP Q389T8
B	0	HIS	-	expression tag	UNP Q389T8
C	-2	GLY	-	expression tag	UNP Q389T8
C	-1	SER	-	expression tag	UNP Q389T8
C	0	HIS	-	expression tag	UNP Q389T8
D	-2	GLY	-	expression tag	UNP Q389T8
D	-1	SER	-	expression tag	UNP Q389T8
D	0	HIS	-	expression tag	UNP Q389T8

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Na	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Na 1	0	0
4	D	2	Total 2	Na 2	0	0
4	C	1	Total 1	Na 1	0	0

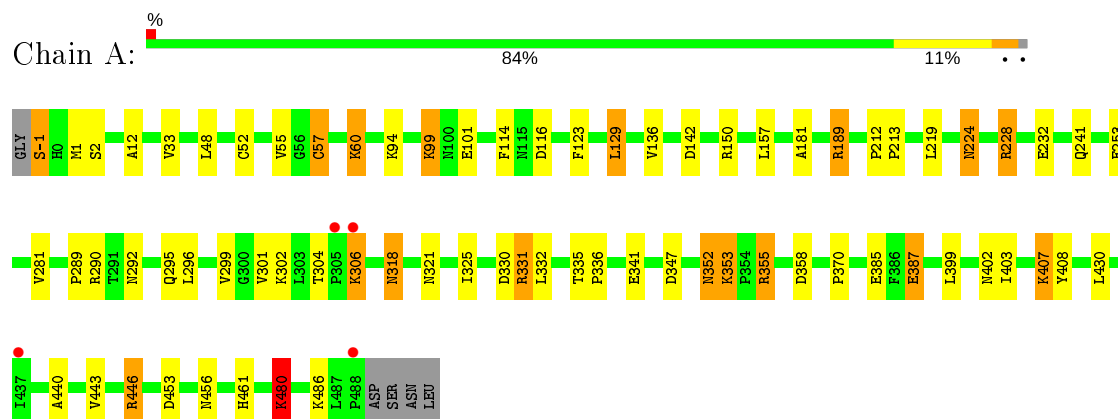
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	389	Total 389	O 389	0	0
5	B	281	Total 281	O 281	0	0
5	C	266	Total 266	O 266	0	0
5	D	313	Total 313	O 313	0	0

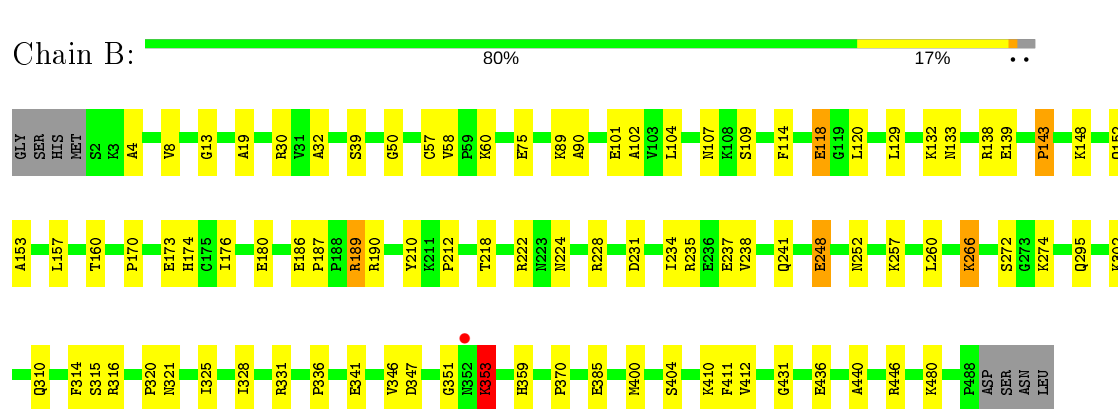
3 Residue-property plots [i](#)

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

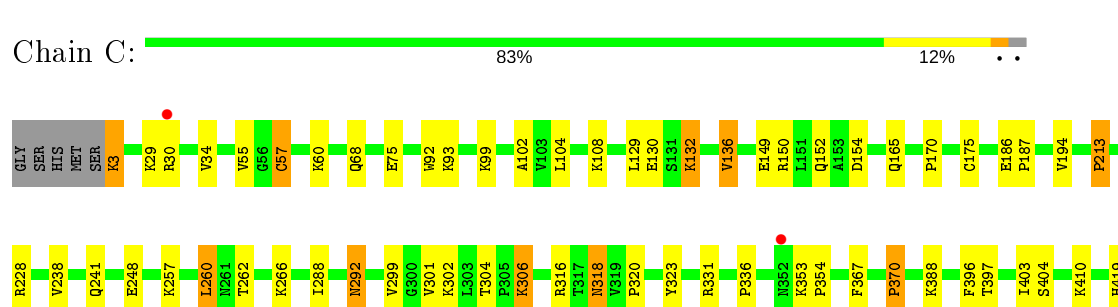
• Molecule 1: TRYPANOTHIONE REDUCTASE



• Molecule 1: TRYPANOTHIONE REDUCTASE

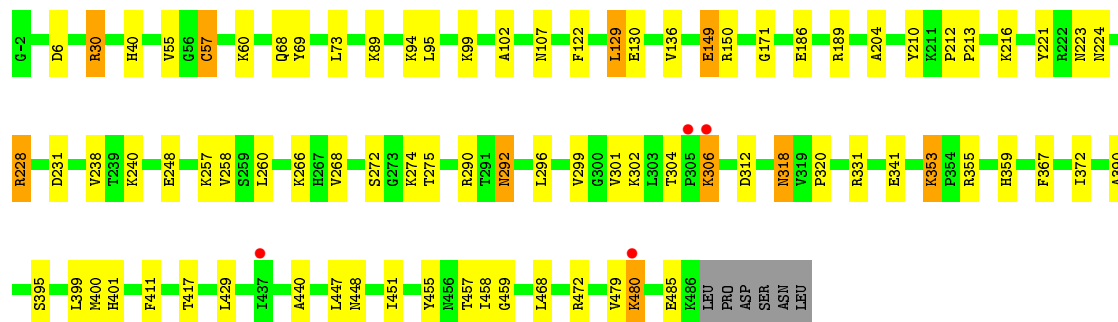
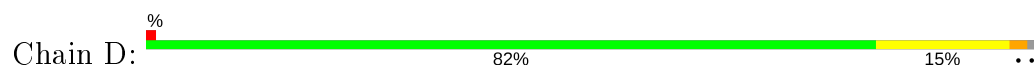


• Molecule 1: TRYPANOTHIONE REDUCTASE





• Molecule 1: TRYPANOTHIONE REDUCTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.80Å 63.62Å 169.82Å 90.00° 97.90° 90.00°	Depositor
Resolution (Å)	46.91 – 2.10 46.91 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.91-2.10) 99.8 (46.91-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.160 , 0.208 0.160 , 0.208	Depositor DCC
R_{free} test set	6297 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16312	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: NA, FAD, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.22	12/3812 (0.3%)	0.99	6/5170 (0.1%)
1	B	1.09	2/3786 (0.1%)	0.92	4/5135 (0.1%)
1	C	1.09	4/3775 (0.1%)	0.91	2/5123 (0.0%)
1	D	1.14	3/3802 (0.1%)	0.94	5/5157 (0.1%)
All	All	1.14	21/15175 (0.1%)	0.94	17/20585 (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	C	0	2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	281	VAL	CB-CG2	7.92	1.69	1.52
1	C	57	CYS	CB-SG	7.42	1.94	1.82
1	C	175	CYS	CB-SG	-7.33	1.69	1.82
1	A	52	CYS	CB-SG	-6.63	1.71	1.82
1	D	122	PHE	CE2-CZ	6.60	1.49	1.37
1	C	455	TYR	CD1-CE1	6.50	1.49	1.39
1	A	57	CYS	CB-SG	6.43	1.93	1.82
1	D	204	ALA	CA-CB	6.12	1.65	1.52
1	A	181	ALA	CA-CB	5.95	1.65	1.52
1	A	385	GLU	CG-CD	5.85	1.60	1.51
1	D	57	CYS	CB-SG	5.80	1.92	1.82
1	A	101	GLU	CG-CD	5.52	1.60	1.51
1	A	408	TYR	CD2-CE2	5.40	1.47	1.39
1	B	436	GLU	CG-CD	5.39	1.60	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	253	GLU	CG-CD	5.35	1.59	1.51
1	B	412	VAL	CB-CG1	5.27	1.64	1.52
1	A	443	VAL	CB-CG1	5.26	1.64	1.52
1	A	57	CYS	CA-CB	5.21	1.65	1.53
1	A	136	VAL	CB-CG2	-5.06	1.42	1.52
1	A	123	PHE	CD2-CE2	5.04	1.49	1.39
1	C	194	VAL	CB-CG2	5.04	1.63	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	290	ARG	NE-CZ-NH2	-8.55	116.03	120.30
1	D	312	ASP	CB-CG-OD1	7.46	125.01	118.30
1	D	149	GLU	CB-CA-C	-7.04	96.31	110.40
1	B	353	LYS	N-CA-C	-6.88	92.42	111.00
1	A	358	ASP	CB-CG-OD1	6.77	124.39	118.30
1	B	189	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	C	213	PRO	C-N-CA	-6.24	109.19	122.30
1	A	189	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	D	150	ARG	CG-CD-NE	-5.60	100.03	111.80
1	A	213	PRO	C-N-CA	-5.50	110.74	122.30
1	B	351	GLY	N-CA-C	-5.45	99.48	113.10
1	B	347	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	142	ASP	CB-CG-OD1	5.39	123.15	118.30
1	C	260	LEU	CB-CG-CD2	5.35	120.09	111.00
1	A	142	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	A	306	LYS	CD-CE-NZ	5.10	123.44	111.70
1	D	6	ASP	CB-CG-OD1	-5.03	113.78	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	484	MET	Peptide
1	C	485	GLU	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	3730	0	3745	55	0
1	B	3703	0	3708	60	1
1	C	3689	0	3692	46	0
1	D	3718	0	3718	50	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
2	C	53	0	31	1	0
2	D	53	0	31	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
5	A	389	0	0	17	0
5	B	281	0	0	22	1
5	C	266	0	0	8	1
5	D	313	0	0	11	2
All	All	16312	0	14987	196	3

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 7.

All (196) 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:224:ASN:HB2	5:A:2195:HOH:O	1.55	1.06
1:B:222:ARG:HD3	5:B:2125:HOH:O	1.60	0.99
1:B:190:ARG:HD2	5:B:2169:HOH:O	1.64	0.95
1:A:228:ARG:NH1	5:A:2199:HOH:O	1.98	0.94
1:B:118:GLU:OE2	5:B:2080:HOH:O	1.88	0.89
1:C:485:GLU:N	1:C:485:GLU:OE1	2.05	0.88
1:B:321:ASN:HB2	5:B:2191:HOH:O	1.73	0.87
1:C:292:ASN:HB2	5:C:2167:HOH:O	1.76	0.85
1:B:101:GLU:HG3	5:B:2012:HOH:O	1.75	0.85
1:C:228:ARG:NH2	5:C:2115:HOH:O	2.10	0.83
1:A:399:LEU:HD12	1:A:402:ASN:HD22	1.44	0.80
1:B:224:ASN:HD22	1:B:252:ASN:HD21	1.30	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:LYS:HG3	5:B:2051:HOH:O	1.83	0.79
1:A:403:ILE:HD11	1:B:102:ALA:HB2	1.67	0.75
1:C:370:PRO:HG2	1:C:430:LEU:HD11	1.69	0.75
1:A:399:LEU:HD21	1:B:58:VAL:HG13	1.70	0.74
1:B:174:HIS:CE1	5:B:2096:HOH:O	2.40	0.74
1:C:299:VAL:HG23	1:C:301:VAL:HG23	1.70	0.73
1:A:241:GLN:OE1	1:A:370:PRO:HG3	1.88	0.73
1:B:302:LYS:HD3	1:B:310:GLN:NE2	2.03	0.72
1:C:132:LYS:HE2	1:C:320:PRO:O	1.91	0.71
1:A:295:GLN:OE1	5:A:2267:HOH:O	2.07	0.70
1:B:266:LYS:N	1:B:266:LYS:HD2	2.05	0.70
1:C:301:VAL:HA	1:C:318:ASN:HD21	1.56	0.70
1:A:355:ARG:HG2	1:A:355:ARG:HH21	1.56	0.69
1:B:228:ARG:NH2	5:B:2122:HOH:O	2.26	0.67
1:A:-1:SER:CA	5:A:2001:HOH:O	2.43	0.66
1:A:399:LEU:CD2	1:B:58:VAL:HG13	2.26	0.66
1:C:92:TRP:HB3	1:C:187:PRO:HD3	1.78	0.65
1:B:8:VAL:HG22	1:B:32:ALA:HB3	1.79	0.65
1:D:302:LYS:H	1:D:318:ASN:HD21	1.45	0.64
1:D:455:TYR:CE2	1:D:472:ARG:HB2	2.33	0.63
1:A:289:PRO:HG3	1:A:330:ASP:HB2	1.80	0.63
1:B:138:ARG:HG3	5:B:2083:HOH:O	1.98	0.63
1:B:370:PRO:HD2	5:B:2226:HOH:O	1.98	0.63
1:D:318:ASN:H	1:D:318:ASN:HD22	1.46	0.62
1:A:440:ALA:HB3	1:B:440:ALA:HB3	1.82	0.62
1:C:397:THR:OG1	1:C:410:LYS:HD3	2.00	0.61
1:B:109:SER:HB2	5:B:2076:HOH:O	1.99	0.61
1:B:132:LYS:HB2	5:B:2085:HOH:O	2.01	0.60
1:B:316:ARG:HB3	5:B:2193:HOH:O	2.01	0.60
1:A:228:ARG:CZ	5:A:2199:HOH:O	2.44	0.60
1:B:228:ARG:NH2	5:B:2126:HOH:O	1.97	0.59
1:C:318:ASN:HD22	1:C:318:ASN:N	2.01	0.58
1:D:292:ASN:HB2	5:D:2214:HOH:O	2.01	0.58
1:D:341:GLU:OE2	1:D:359:HIS:HE1	1.87	0.58
1:A:318:ASN:H	1:A:318:ASN:HD22	1.52	0.58
1:D:353:LYS:HE2	1:D:353:LYS:HA	1.85	0.57
1:C:318:ASN:H	1:C:318:ASN:HD22	1.51	0.57
1:B:410:LYS:HE2	5:B:2136:HOH:O	2.04	0.56
1:B:302:LYS:HD3	1:B:310:GLN:HE22	1.70	0.56
1:D:302:LYS:H	1:D:318:ASN:ND2	2.03	0.56
1:D:240:LYS:NZ	5:D:2181:HOH:O	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-1:SER:HA	5:A:2001:HOH:O	2.04	0.56
1:D:355:ARG:HD3	5:D:2242:HOH:O	2.06	0.56
1:C:316:ARG:HG2	1:C:323:TYR:CD1	2.41	0.56
1:D:171:GLY:HA3	1:D:258:VAL:O	2.05	0.56
1:A:355:ARG:NH2	1:A:355:ARG:HG2	2.19	0.55
1:A:453:ASP:HA	1:B:446[A]:ARG:NH1	2.21	0.55
1:D:216:LYS:HE3	1:D:248[A]:GLU:HB2	1.88	0.55
1:A:224:ASN:ND2	5:A:2195:HOH:O	2.21	0.55
1:A:355:ARG:NH2	5:A:2310:HOH:O	2.38	0.55
1:A:352:ASN:HA	5:A:2305:HOH:O	2.06	0.55
1:C:102:ALA:HB1	1:D:399:LEU:HD11	1.89	0.55
1:B:133:ASN:HB3	1:B:153:ALA:O	2.07	0.54
1:D:304:THR:HG22	5:D:2225:HOH:O	2.06	0.54
1:B:139:GLU:OE1	1:B:148:LYS:HE3	2.07	0.54
1:C:130:GLU:HB2	1:C:136:VAL:CG2	2.38	0.54
1:C:316:ARG:HG2	1:C:323:TYR:CE1	2.43	0.54
1:A:335:THR:HB	1:A:336:PRO:HD3	1.90	0.53
1:D:221:TYR:CE2	1:D:223:ASN:HB2	2.44	0.53
1:D:448:ASN:ND2	5:D:2290:HOH:O	2.41	0.53
1:B:104:LEU:HA	1:B:107:ASN:HD22	1.73	0.53
1:A:302:LYS:H	1:A:318:ASN:ND2	2.07	0.53
5:C:2244:HOH:O	1:D:367:PHE:HE2	1.91	0.53
1:C:455:TYR:CZ	1:C:472:ARG:HD3	2.43	0.53
1:A:12:ALA:HB2	1:A:33:VAL:HG12	1.90	0.53
1:B:176:ILE:HB	1:B:180:GLU:HB2	1.92	0.52
1:C:336:PRO:HG2	1:D:459:GLY:O	2.09	0.52
1:D:40:HIS:H	1:D:107:ASN:HD21	1.57	0.52
1:D:429:LEU:HD21	1:D:468:LEU:HD21	1.92	0.52
1:A:370:PRO:HG2	1:A:430:LEU:HD11	1.91	0.52
1:D:130:GLU:HB2	1:D:136:VAL:HG23	1.91	0.52
1:A:301:VAL:HA	1:A:318:ASN:HD21	1.74	0.51
1:D:238:VAL:HG21	1:D:372:ILE:HD11	1.91	0.51
1:B:218:THR:HG23	1:B:248:GLU:HG2	1.92	0.51
1:A:292:ASN:HB2	5:A:2263:HOH:O	2.10	0.51
1:A:352:ASN:HA	5:A:2114:HOH:O	2.10	0.51
1:A:352:ASN:HB3	5:A:2114:HOH:O	2.11	0.51
1:A:321:ASN:OD1	1:A:321:ASN:N	2.45	0.50
1:B:314:PHE:O	1:B:315:SER:HB2	2.12	0.50
1:C:93:LYS:NZ	1:C:186[B]:GLU:OE2	2.45	0.50
1:D:149:GLU:CG	5:D:2122:HOH:O	2.59	0.50
1:B:157:LEU:HD11	1:B:325:ILE:HG12	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ILE:O	1:B:238:VAL:HG12	2.11	0.50
1:B:353:LYS:HB2	5:B:2206:HOH:O	2.12	0.50
1:B:173:GLU:H	1:B:173:GLU:CD	2.15	0.50
1:B:480:LYS:NZ	5:B:2273:HOH:O	2.43	0.49
1:D:479:VAL:O	1:D:480:LYS:C	2.50	0.49
1:C:446:ARG:HD2	1:D:457:THR:OG1	2.13	0.49
1:B:320:PRO:O	1:B:321:ASN:HB2	2.11	0.49
1:C:336:PRO:HB2	1:D:458:ILE:HG23	1.95	0.49
1:C:367:PHE:HE2	5:C:2264:HOH:O	1.96	0.48
1:A:446:ARG:HB3	1:A:446:ARG:HH11	1.78	0.48
1:A:456:ASN:HD22	1:B:446[A]:ARG:NH2	2.11	0.48
1:C:299:VAL:CG2	1:C:301:VAL:HG23	2.43	0.48
1:C:302:LYS:H	1:C:318:ASN:ND2	2.11	0.48
1:D:30:ARG:HD3	5:D:2099:HOH:O	2.12	0.48
1:C:165:GLN:HB2	1:C:288:ILE:HG23	1.96	0.48
1:D:68:GLN:NE2	5:D:2054:HOH:O	2.47	0.48
1:B:370:PRO:CD	5:B:2226:HOH:O	2.59	0.47
1:D:417:THR:HG21	1:D:451:ILE:HB	1.95	0.47
1:C:353:LYS:HA	1:C:354:PRO:HD2	1.78	0.47
1:C:93:LYS:NZ	1:C:186[B]:GLU:CD	2.68	0.47
1:D:40:HIS:H	1:D:107:ASN:ND2	2.12	0.47
1:A:189:ARG:HA	1:A:212:PRO:HD2	1.96	0.47
1:A:48:LEU:HD11	1:A:114:PHE:HE2	1.78	0.47
1:A:347:ASP:HB3	1:A:353:LYS:HG3	1.97	0.47
1:D:189:ARG:HA	1:D:212:PRO:HD2	1.96	0.47
1:D:69:TYR:O	1:D:73:LEU:HG	2.15	0.47
1:C:93:LYS:NZ	1:C:186[B]:GLU:OE1	2.45	0.46
1:D:213:PRO:HG3	5:D:2028:HOH:O	2.14	0.46
1:B:189:ARG:HA	1:B:212:PRO:HD2	1.97	0.46
1:C:170:PRO:HG2	1:C:257:LYS:HG3	1.97	0.46
1:C:29:LYS:HA	1:C:29:LYS:HD2	1.77	0.46
1:C:68:GLN:NE2	5:C:2026:HOH:O	2.45	0.46
1:D:129:LEU:HD22	1:D:296:LEU:HD23	1.97	0.46
1:C:92:TRP:CB	1:C:187:PRO:HD3	2.45	0.45
1:A:461:HIS:HB2	1:B:336:PRO:HG3	1.99	0.45
1:C:453:ASP:CG	1:D:447:LEU:HD21	2.37	0.45
1:C:241:GLN:OE1	1:C:370:PRO:HG3	2.16	0.45
1:A:407:LYS:HE2	5:A:2337:HOH:O	2.17	0.45
1:C:440:ALA:HB3	1:D:440:ALA:HB3	1.98	0.45
1:C:486:LYS:HA	5:C:2262:HOH:O	2.16	0.45
1:A:302:LYS:H	1:A:318:ASN:HD21	1.65	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:GLU:OE2	1:B:359:HIS:HE1	2.00	0.44
1:B:19:ALA:O	1:B:346:VAL:HG21	2.16	0.44
1:A:129:LEU:HD22	1:A:296:LEU:HD23	2.00	0.44
1:B:160:THR:OG1	1:B:328:ILE:HD12	2.17	0.44
1:B:186:GLU:HB2	1:B:187:PRO:HD2	1.99	0.44
1:D:228:ARG:HB3	1:D:228:ARG:HE	1.29	0.44
1:C:3:LYS:HA	5:C:2003:HOH:O	2.18	0.44
1:D:306:LYS:HE2	1:D:306:LYS:HB2	1.79	0.44
1:D:320:PRO:HA	5:D:2233:HOH:O	2.17	0.44
1:D:94:LYS:NZ	5:D:2076:HOH:O	2.51	0.44
1:B:370:PRO:N	5:B:2226:HOH:O	2.51	0.44
1:D:395:SER:HA	1:D:411:PHE:O	2.18	0.44
1:D:485:GLU:OE2	1:D:485:GLU:N	2.50	0.44
1:B:90:ALA:HB1	1:B:210:TYR:CD1	2.53	0.43
1:B:237:GLU:O	1:B:241:GLN:HG3	2.18	0.43
1:C:130:GLU:HB2	1:C:136:VAL:HG22	1.99	0.43
1:B:170:PRO:HG2	1:B:257:LYS:HB3	1.99	0.43
1:A:453:ASP:HA	1:B:446[A]:ARG:HH12	1.82	0.43
1:D:390:ALA:HB3	1:D:417:THR:OG1	2.19	0.43
1:B:370:PRO:HG2	5:B:2242:HOH:O	2.18	0.43
1:A:387:GLU:OE1	1:A:480:LYS:HE2	2.19	0.43
1:A:331[B]:ARG:HB3	1:A:332:LEU:H	1.54	0.43
1:A:94:LYS:CG	5:B:2051:HOH:O	2.56	0.43
1:B:359:HIS:HD2	5:B:2215:HOH:O	2.01	0.43
1:C:93:LYS:HZ2	1:C:186[B]:GLU:CD	2.22	0.43
1:B:143:PRO:HB3	1:B:295:GLN:NE2	2.34	0.43
1:D:299:VAL:HG23	1:D:301:VAL:HG23	1.99	0.43
1:D:95:LEU:HD22	1:D:210:TYR:CZ	2.54	0.42
1:B:75:GLU:HB3	1:B:404:SER:HB2	2.01	0.42
1:A:299:VAL:HG23	1:A:301:VAL:HG23	2.01	0.42
1:B:114:PHE:CE1	1:B:120:LEU:HG	2.54	0.42
1:D:353:LYS:HA	1:D:353:LYS:CE	2.49	0.42
1:B:411:PHE:CD1	1:B:431:GLY:HA3	2.55	0.42
1:C:306:LYS:HB2	1:C:306:LYS:HE3	1.63	0.42
1:A:224:ASN:CB	5:A:2195:HOH:O	2.35	0.42
1:A:60:LYS:HD2	1:A:60:LYS:C	2.40	0.42
1:B:13:GLY:HA2	1:B:50:GLY:HA3	2.02	0.42
1:A:12:ALA:HB2	1:A:33:VAL:CG1	2.50	0.42
1:B:302:LYS:CD	1:B:310:GLN:NE2	2.78	0.42
1:A:321:ASN:HB3	5:A:2144:HOH:O	2.20	0.42
1:B:4:ALA:HB2	1:B:152:GLN:HE21	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:419:HIS:HE1	5:C:2073:HOH:O	2.03	0.41
1:A:331[A]:ARG:NH1	1:A:341:GLU:OE2	2.46	0.41
1:C:304:THR:C	1:C:306:LYS:H	2.24	0.41
1:C:75:GLU:HB3	1:C:404:SER:HB2	2.03	0.41
1:D:268:VAL:O	1:D:275:THR:HA	2.20	0.41
1:D:400:MET:HG3	1:D:401:HIS:N	2.35	0.41
1:B:272:SER:OG	1:B:274[B]:LYS:HG3	2.21	0.41
1:A:304:THR:HG22	5:A:2275:HOH:O	2.20	0.41
1:A:99:LYS:C	1:A:99:LYS:HD2	2.41	0.41
1:B:231:ASP:O	1:B:235:ARG:HG3	2.21	0.41
1:A:219:LEU:HD23	1:A:219:LEU:C	2.41	0.41
1:A:157:LEU:HD11	1:A:325:ILE:HG12	2.02	0.41
1:C:34:VAL:HG12	2:C:998:FAD:H2A	2.03	0.41
1:C:396:PHE:N	1:C:396:PHE:CD1	2.89	0.40
1:C:403:ILE:HD11	1:D:102:ALA:HB2	2.02	0.40
1:A:2:SER:HB2	1:A:150:ARG:O	2.22	0.40
1:A:352:ASN:CB	5:A:2114:HOH:O	2.68	0.40
1:D:272:SER:OG	1:D:274:LYS:HE3	2.21	0.40
1:C:104:LEU:HG	1:C:108:LYS:HD2	2.03	0.40
1:D:455:TYR:CZ	1:D:472:ARG:HD3	2.57	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:2095:HOH:O	5:D:2126:HOH:O[1_556]	1.75	0.45
5:C:2001:HOH:O	5:D:2290:HOH:O[2_455]	2.11	0.09
1:B:118:GLU:OE1	1:B:446[A]:ARG:NH2[2_456]	2.15	0.05

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	489/495 (99%)	472 (96%)	15 (3%)	2 (0%)	34	32
1	B	487/495 (98%)	469 (96%)	17 (4%)	1 (0%)	47	49
1	C	485/495 (98%)	464 (96%)	20 (4%)	1 (0%)	47	49
1	D	489/495 (99%)	473 (97%)	15 (3%)	1 (0%)	47	49
All	All	1950/1980 (98%)	1878 (96%)	67 (3%)	5 (0%)	41	41

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	480	LYS
1	A	55	VAL
1	C	55	VAL
1	D	55	VAL
1	B	143	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	404/407 (99%)	381 (94%)	23 (6%)	20	18
1	B	399/407 (98%)	385 (96%)	14 (4%)	36	38
1	C	399/407 (98%)	374 (94%)	25 (6%)	18	15
1	D	402/407 (99%)	382 (95%)	20 (5%)	24	23
All	All	1604/1628 (98%)	1522 (95%)	82 (5%)	24	22

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	SER
1	A	1	MET
1	A	57	CYS
1	A	60	LYS
1	A	99	LYS
1	A	116	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	129	LEU
1	A	224	ASN
1	A	228	ARG
1	A	232	GLU
1	A	290	ARG
1	A	306	LYS
1	A	318	ASN
1	A	331[A]	ARG
1	A	331[B]	ARG
1	A	352	ASN
1	A	353	LYS
1	A	355	ARG
1	A	387	GLU
1	A	407	LYS
1	A	446	ARG
1	A	480	LYS
1	A	486	LYS
1	B	30	ARG
1	B	39	SER
1	B	57	CYS
1	B	60	LYS
1	B	89	LYS
1	B	118	GLU
1	B	129	LEU
1	B	248	GLU
1	B	260	LEU
1	B	266	LYS
1	B	331	ARG
1	B	353	LYS
1	B	385	GLU
1	B	400	MET
1	C	3	LYS
1	C	30	ARG
1	C	57	CYS
1	C	60	LYS
1	C	99	LYS
1	C	129	LEU
1	C	132	LYS
1	C	136	VAL
1	C	149	GLU
1	C	150	ARG
1	C	152	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	154	ASP
1	C	213	PRO
1	C	238	VAL
1	C	248	GLU
1	C	260	LEU
1	C	262	THR
1	C	266	LYS
1	C	292	ASN
1	C	306	LYS
1	C	318	ASN
1	C	331	ARG
1	C	370	PRO
1	C	388	LYS
1	C	485	GLU
1	D	30	ARG
1	D	57	CYS
1	D	60	LYS
1	D	89	LYS
1	D	99	LYS
1	D	129	LEU
1	D	186	GLU
1	D	224[A]	ASN
1	D	224[B]	ASN
1	D	228	ARG
1	D	231	ASP
1	D	257	LYS
1	D	260	LEU
1	D	266	LYS
1	D	292	ASN
1	D	306	LYS
1	D	318	ASN
1	D	331	ARG
1	D	353	LYS
1	D	480	LYS

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

Mol	Chain	Res	Type
1	A	318	ASN
1	A	402	ASN
1	A	456	ASN
1	B	107	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	252	ASN
1	B	310	GLN
1	B	359	HIS
1	C	107	ASN
1	C	318	ASN
1	C	359	HIS
1	D	68	GLN
1	D	107	ASN
1	D	292	ASN
1	D	295	GLN
1	D	318	ASN
1	D	359	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 11 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	C	998	-	51,58,58	1.64	7 (13%)	60,89,89	1.72	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	D	998	-	51,58,58	1.55	6 (11%)	60,89,89	1.92	9 (15%)
2	FAD	A	998	-	51,58,58	1.52	7 (13%)	60,89,89	2.15	17 (28%)
2	FAD	B	998	-	51,58,58	1.61	9 (17%)	60,89,89	2.05	11 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	C	998	-	-	5/30/50/50	0/6/6/6
2	FAD	D	998	-	-	5/30/50/50	0/6/6/6
2	FAD	A	998	-	-	5/30/50/50	0/6/6/6
2	FAD	B	998	-	-	5/30/50/50	0/6/6/6

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	998	FAD	C10-N1	5.67	1.40	1.33
2	B	998	FAD	C4X-N5	5.40	1.41	1.33
2	D	998	FAD	C4X-N5	5.29	1.40	1.33
2	C	998	FAD	C2A-N3A	4.53	1.39	1.32
2	B	998	FAD	C2A-N3A	3.98	1.38	1.32
2	B	998	FAD	C4X-C10	3.98	1.42	1.38
2	A	998	FAD	C1'-N10	3.92	1.52	1.48
2	A	998	FAD	C10-N1	3.91	1.38	1.33
2	B	998	FAD	C10-N1	3.67	1.38	1.33
2	C	998	FAD	C5X-N5	3.64	1.41	1.35
2	D	998	FAD	C5X-N5	3.60	1.41	1.35
2	C	998	FAD	C4X-N5	3.59	1.38	1.33
2	D	998	FAD	C10-N1	3.51	1.37	1.33
2	D	998	FAD	C2A-N3A	3.48	1.37	1.32
2	A	998	FAD	C5X-N5	3.45	1.41	1.35
2	D	998	FAD	C4-N3	3.35	1.38	1.33
2	A	998	FAD	C2A-N3A	3.35	1.37	1.32
2	B	998	FAD	C9A-N10	2.90	1.42	1.38
2	C	998	FAD	C1'-N10	2.89	1.51	1.48
2	A	998	FAD	C4X-N5	2.89	1.37	1.33
2	B	998	FAD	C5X-N5	2.86	1.40	1.35
2	D	998	FAD	C9A-N10	2.78	1.42	1.38
2	C	998	FAD	C2A-N1A	2.76	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	998	FAD	C4-N3	2.70	1.37	1.33
2	B	998	FAD	C2B-C1B	-2.43	1.50	1.53
2	B	998	FAD	C4A-N3A	2.31	1.38	1.35
2	B	998	FAD	C2A-N1A	2.28	1.38	1.33
2	C	998	FAD	C4-N3	2.14	1.36	1.33
2	A	998	FAD	C9A-C5X	-2.02	1.38	1.42

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	998	FAD	C4-N3-C2	7.73	121.67	115.14
2	B	998	FAD	C4-N3-C2	7.47	121.45	115.14
2	B	998	FAD	N3A-C2A-N1A	-7.38	117.14	128.68
2	C	998	FAD	C4-N3-C2	7.22	121.24	115.14
2	D	998	FAD	C4-N3-C2	6.54	120.66	115.14
2	D	998	FAD	C4X-N5-C5X	6.15	122.92	116.77
2	C	998	FAD	N3A-C2A-N1A	-5.77	119.66	128.68
2	D	998	FAD	C10-C4X-N5	-5.32	117.58	121.26
2	A	998	FAD	C1'-N10-C9A	5.15	122.34	118.29
2	B	998	FAD	C4X-N5-C5X	4.74	121.50	116.77
2	D	998	FAD	C4A-C5A-N7A	-4.63	104.57	109.40
2	A	998	FAD	C4X-C4-N3	-4.63	117.10	123.43
2	A	998	FAD	C4X-N5-C5X	4.60	121.36	116.77
2	A	998	FAD	C5X-C9A-N10	4.28	120.82	117.72
2	B	998	FAD	C1'-N10-C9A	4.26	121.65	118.29
2	D	998	FAD	N3A-C2A-N1A	-3.84	122.67	128.68
2	D	998	FAD	C4X-C4-N3	-3.79	118.25	123.43
2	A	998	FAD	N3A-C2A-N1A	-3.77	122.79	128.68
2	B	998	FAD	C4X-C4-N3	-3.66	118.43	123.43
2	A	998	FAD	C5A-C6A-N6A	3.44	125.57	120.35
2	B	998	FAD	O4B-C1B-C2B	-3.24	102.19	106.93
2	D	998	FAD	C4-C4X-N5	3.18	122.23	118.60
2	B	998	FAD	C10-C4X-N5	-3.15	119.08	121.26
2	A	998	FAD	C4A-C5A-N7A	-2.97	106.30	109.40
2	C	998	FAD	C4X-C4-N3	-2.81	119.59	123.43
2	A	998	FAD	C10-C4X-N5	-2.75	119.36	121.26
2	A	998	FAD	C4'-C3'-C2'	-2.71	107.73	113.36
2	C	998	FAD	C4X-N5-C5X	2.70	119.47	116.77
2	A	998	FAD	O2'-C2'-C1'	-2.64	103.23	109.59
2	B	998	FAD	C5X-C9A-N10	2.61	119.61	117.72
2	A	998	FAD	C4-C4X-C10	2.55	121.64	119.95
2	D	998	FAD	N6A-C6A-N1A	-2.52	113.35	118.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	998	FAD	C2A-N1A-C6A	2.50	123.03	118.75
2	C	998	FAD	O4B-C1B-C2B	-2.48	103.30	106.93
2	A	998	FAD	O4B-C1B-C2B	-2.45	103.35	106.93
2	A	998	FAD	C9A-C5X-N5	-2.40	118.61	122.36
2	A	998	FAD	O4'-C4'-C3'	2.38	114.89	109.10
2	C	998	FAD	O2'-C2'-C1'	-2.36	103.90	109.59
2	A	998	FAD	C5A-C6A-N1A	-2.30	115.14	120.35
2	B	998	FAD	C4-C4X-N5	2.29	121.22	118.60
2	C	998	FAD	C7M-C7-C6	-2.11	115.31	120.34
2	C	998	FAD	C1'-N10-C10	2.10	120.29	118.41
2	A	998	FAD	O2P-P-O1P	2.08	122.52	112.24
2	D	998	FAD	O4B-C1B-C2B	-2.07	103.90	106.93
2	B	998	FAD	C4A-C5A-N7A	-2.05	107.26	109.40

There are no chirality outliers.

All (20) torsion outliers are listed below:

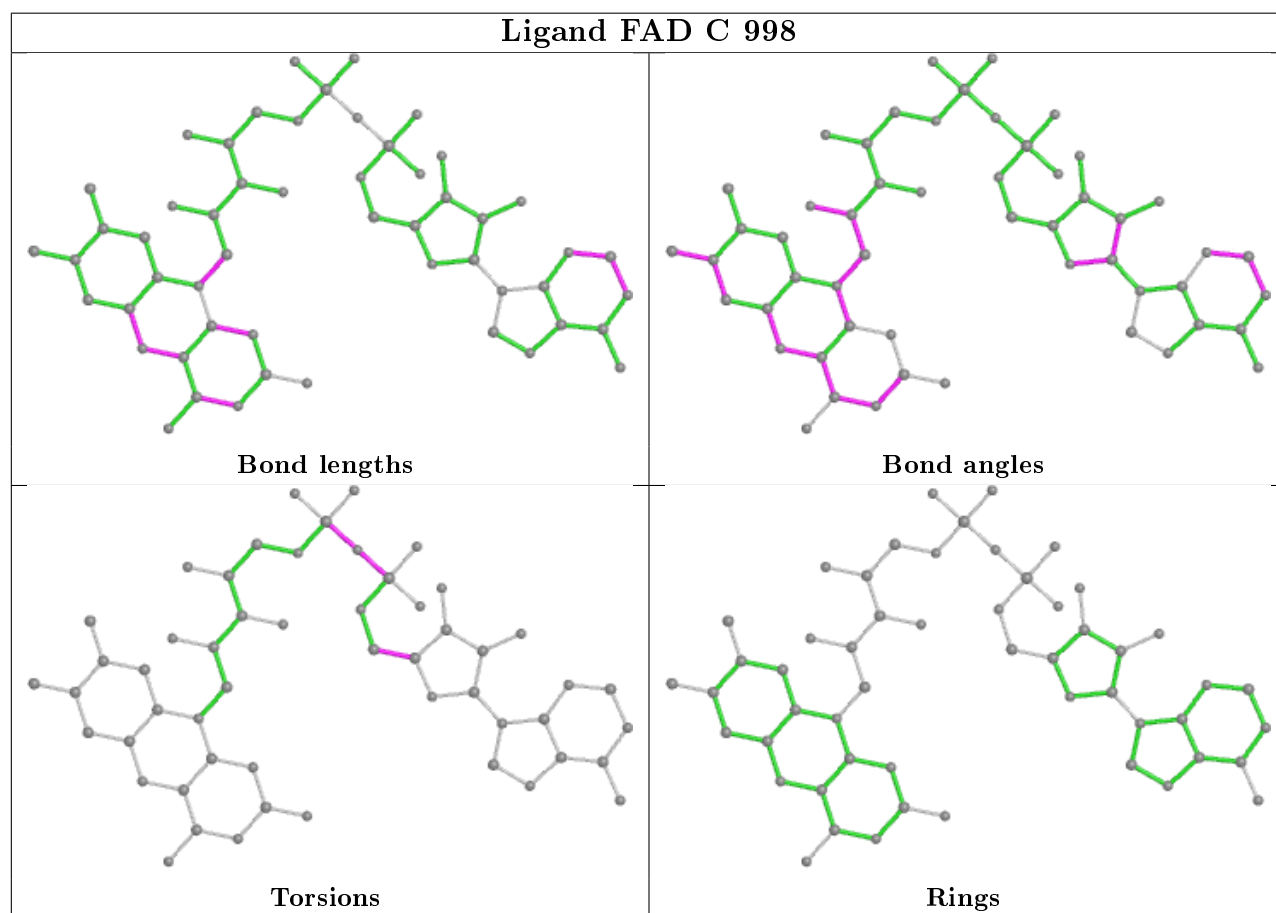
Mol	Chain	Res	Type	Atoms
2	C	998	FAD	O4B-C4B-C5B-O5B
2	C	998	FAD	PA-O3P-P-O5'
2	A	998	FAD	PA-O3P-P-O5'
2	B	998	FAD	PA-O3P-P-O5'
2	C	998	FAD	C3B-C4B-C5B-O5B
2	B	998	FAD	C3B-C4B-C5B-O5B
2	D	998	FAD	C3B-C4B-C5B-O5B
2	D	998	FAD	O4B-C4B-C5B-O5B
2	C	998	FAD	P-O3P-PA-O1A
2	A	998	FAD	O4B-C4B-C5B-O5B
2	D	998	FAD	PA-O3P-P-O5'
2	B	998	FAD	O4B-C4B-C5B-O5B
2	D	998	FAD	P-O3P-PA-O1A
2	A	998	FAD	P-O3P-PA-O1A
2	B	998	FAD	P-O3P-PA-O1A
2	C	998	FAD	P-O3P-PA-O2A
2	D	998	FAD	P-O3P-PA-O2A
2	B	998	FAD	P-O3P-PA-O2A
2	A	998	FAD	P-O3P-PA-O2A
2	A	998	FAD	C3B-C4B-C5B-O5B

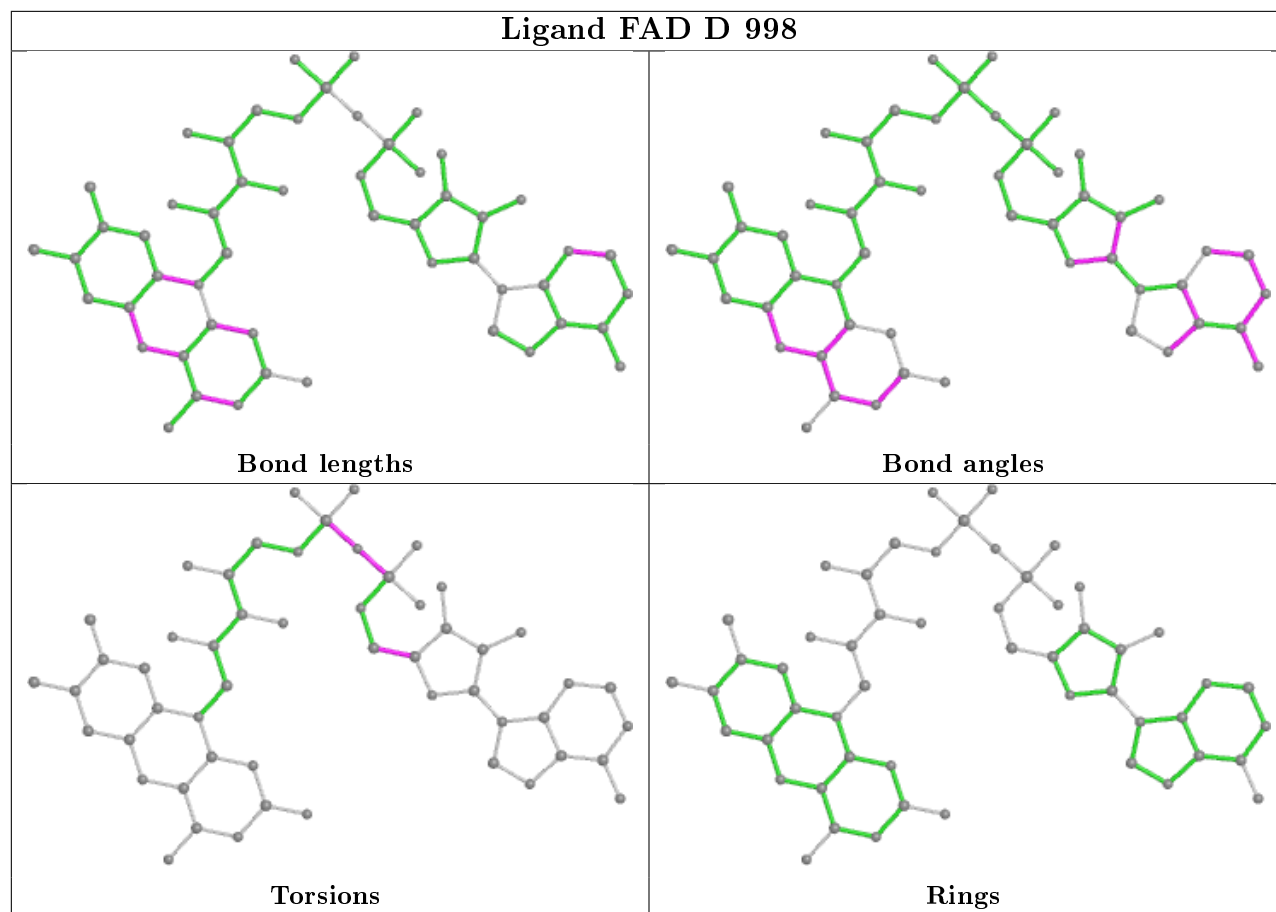
There are no ring outliers.

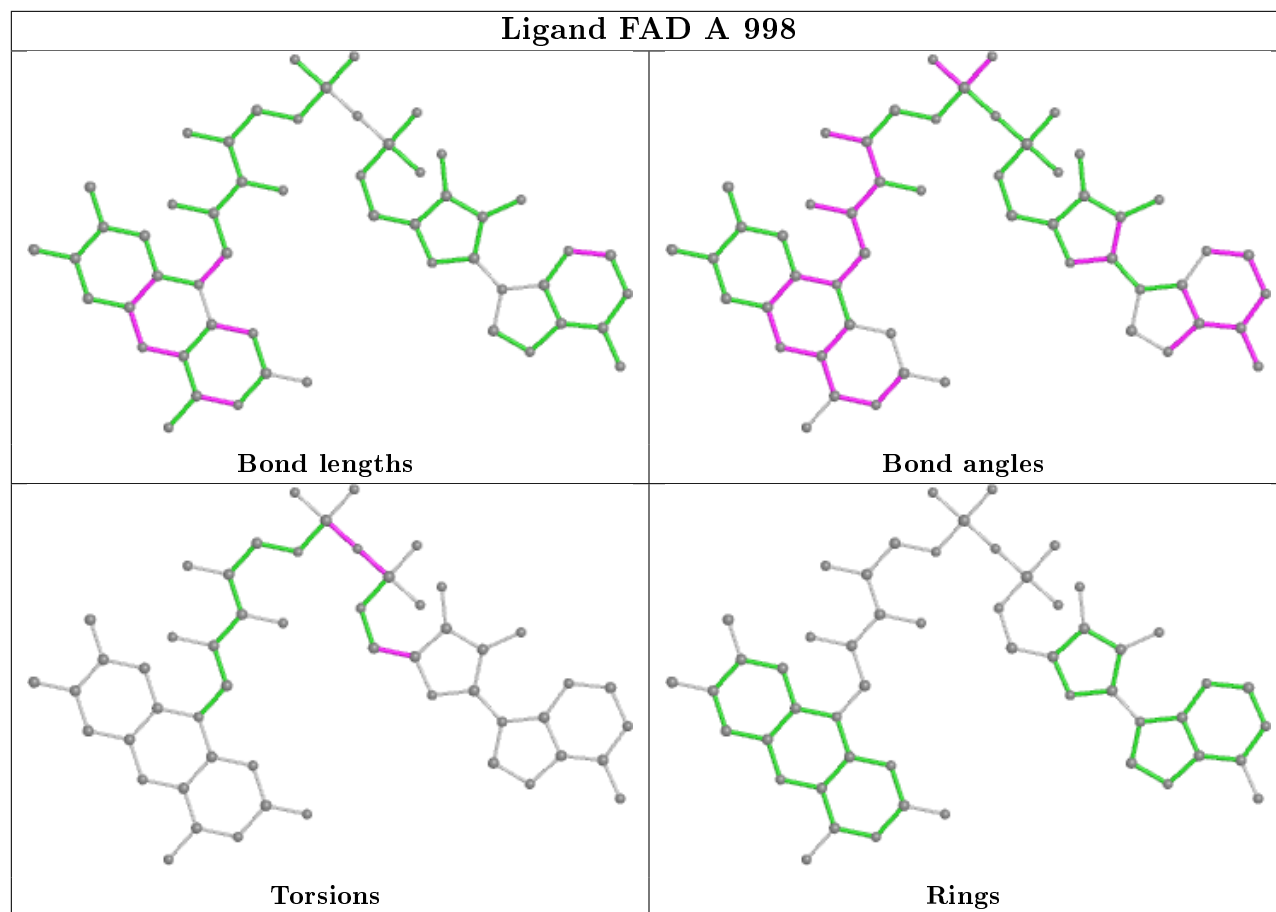
1 monomer is involved in 1 short contact:

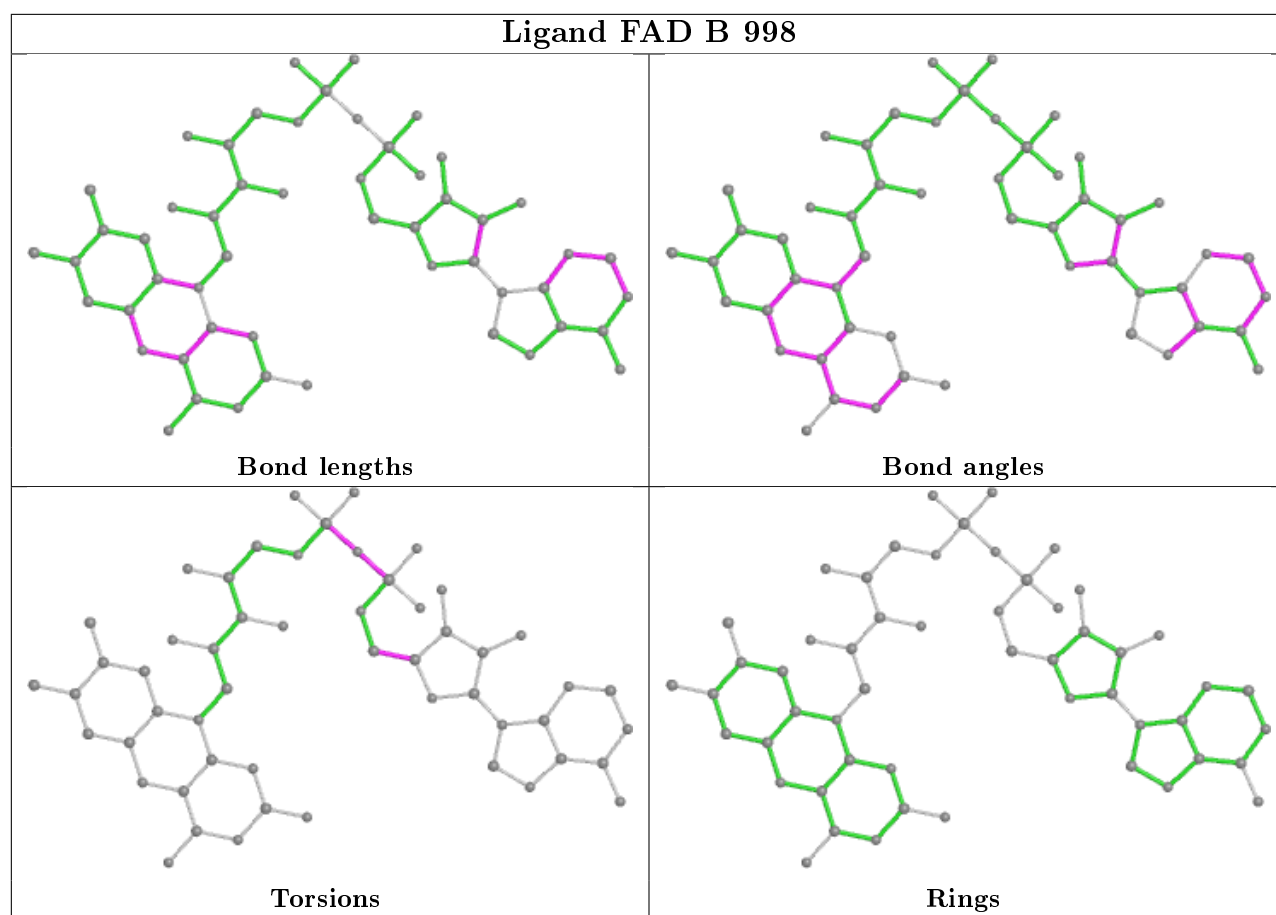
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	998	FAD	1	0

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.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	490/495 (98%)	-0.42	4 (0%) 86 88	12, 21, 40, 58	0
1	B	487/495 (98%)	-0.22	1 (0%) 95 95	14, 27, 50, 59	0
1	C	484/495 (97%)	-0.19	2 (0%) 92 93	15, 29, 55, 68	0
1	D	489/495 (98%)	-0.41	4 (0%) 86 88	12, 25, 39, 61	0
All	All	1950/1980 (98%)	-0.31	11 (0%) 89 91	12, 25, 49, 68	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	352	ASN	3.7
1	A	305	PRO	3.3
1	C	30	ARG	3.2
1	A	306	LYS	2.9
1	D	305	PRO	2.5
1	B	352	ASN	2.5
1	D	437	ILE	2.4
1	A	488	PRO	2.3
1	A	437	ILE	2.1
1	D	480	LYS	2.1
1	D	306	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands

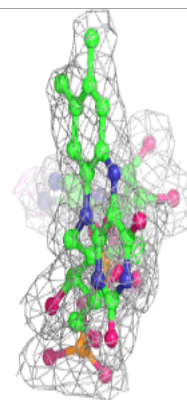
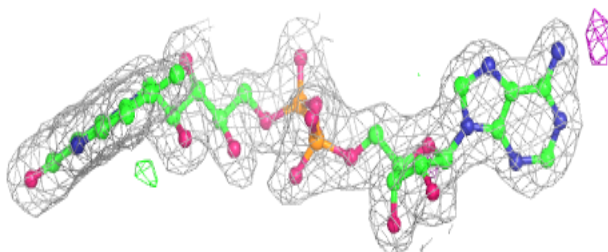
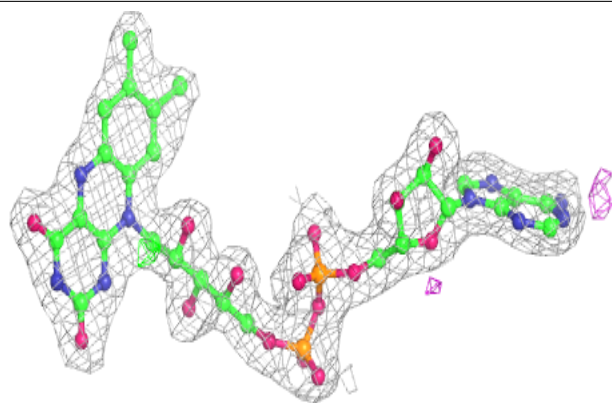
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NA	C	1488	1/1	0.88	0.15	53,53,53,53	0
4	NA	B	1491	1/1	0.89	0.08	46,46,46,46	0
4	NA	D	1488	1/1	0.95	0.16	36,36,36,36	0
3	CL	B	1490	1/1	0.97	0.07	50,50,50,50	0
2	FAD	B	998	53/53	0.98	0.10	14,22,29,32	0
4	NA	D	1489	1/1	0.98	0.05	21,21,21,21	0
2	FAD	C	998	53/53	0.98	0.09	15,23,33,35	0
2	FAD	D	998	53/53	0.98	0.09	11,17,20,23	0
4	NA	A	1491	1/1	0.99	0.09	31,31,31,31	0
3	CL	A	1490	1/1	0.99	0.06	22,22,22,22	0
3	CL	D	1487	1/1	0.99	0.07	32,32,32,32	0
2	FAD	A	998	53/53	0.99	0.10	10,14,18,22	0
3	CL	B	1489	1/1	0.99	0.04	26,26,26,26	0
3	CL	C	1487	1/1	1.00	0.06	28,28,28,28	0
3	CL	A	1489	1/1	1.00	0.04	28,28,28,28	0

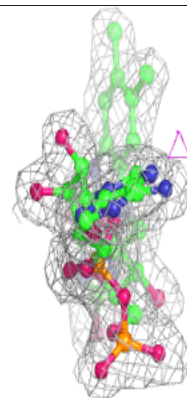
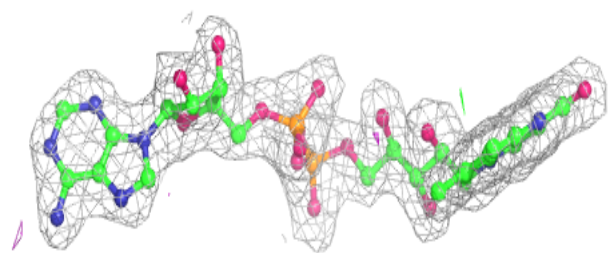
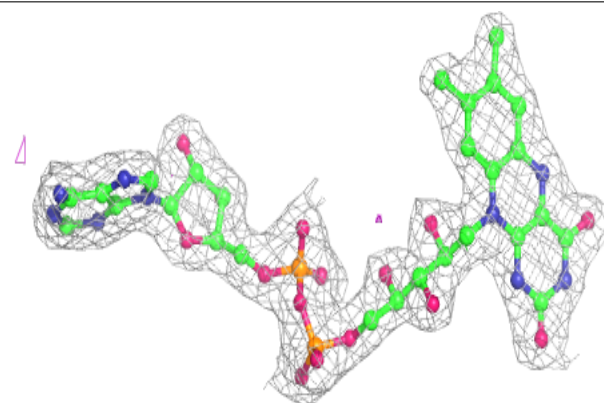
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD B 998:

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

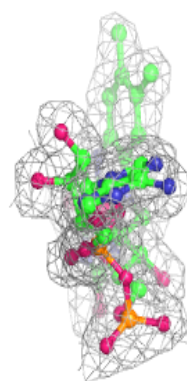
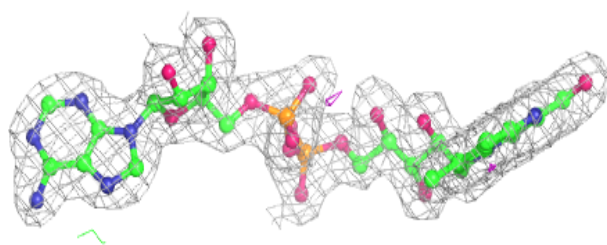
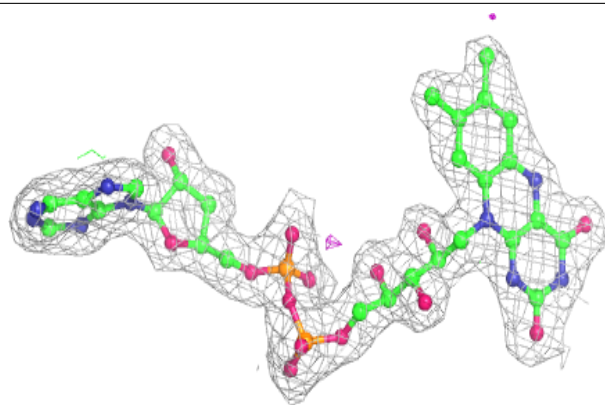
**Electron density around FAD C 998:**

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

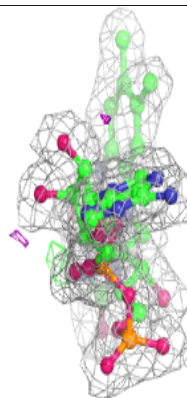
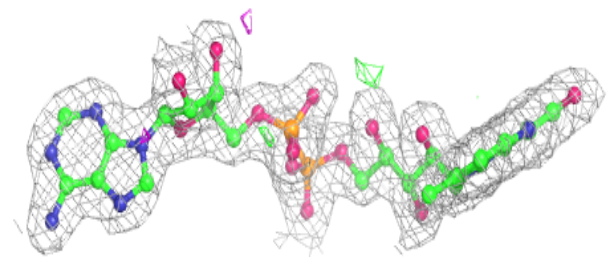
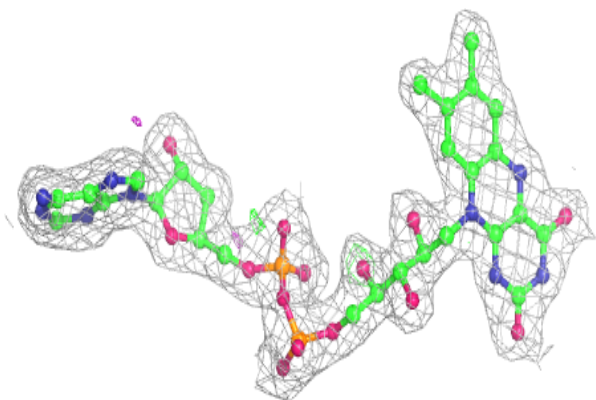


Electron density around FAD D 998:

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

**Electron density around FAD A 998:**

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



6.5 Other polymers

There are no such residues in this entry.