



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:27 PM EDT

PDB ID : 3DH9 / pdb_00003dh9
Title : Crystal Structure of Drosophila Thioredoxin Reductase, wild-type
Authors : Eckenroth, B.E.; Hondal, R.J.; Everse, S.J.
Deposited on : 2008-06-17
Resolution : 2.25 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

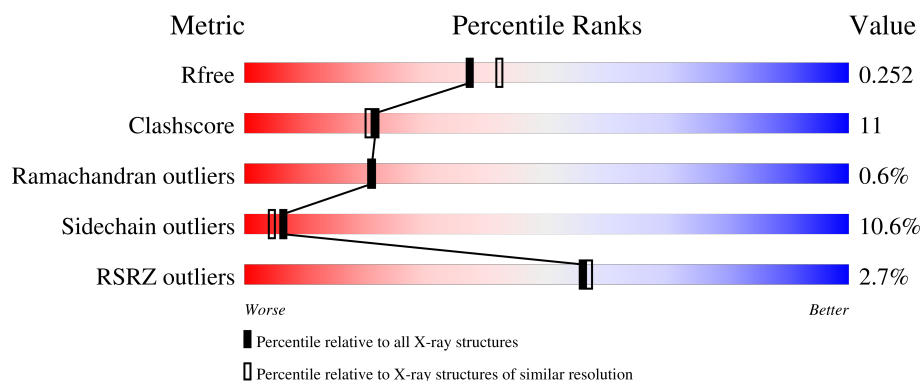
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	482	4% 75% 20% .
1	B	482	% 74% 20% ..

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8002 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.

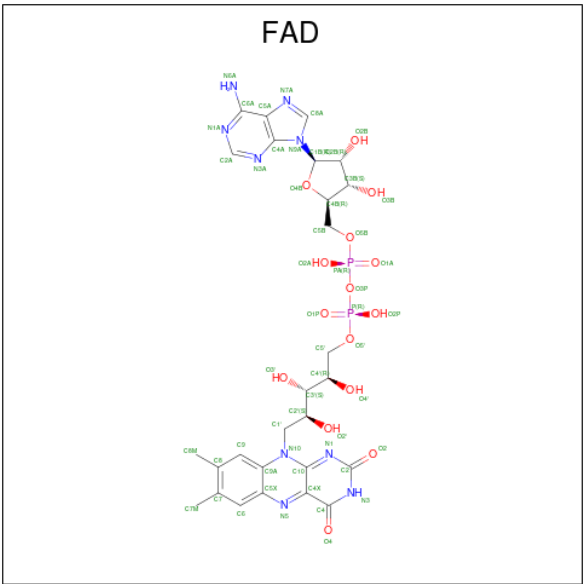
- Molecule 1 is a protein called Thioredoxin reductase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	0
			3692	2354	627	699	12			
1	B	482	Total	C	N	O	S	0	0	0
			3692	2354	627	699	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	GLN	-	expression tag	UNP P91938
A	90	ASP	GLU	engineered mutation	UNP P91938
A	274	SER	ALA	engineered mutation	UNP P91938
B	5	GLN	-	expression tag	UNP P91938
B	90	ASP	GLU	engineered mutation	UNP P91938
B	274	SER	ALA	engineered mutation	UNP P91938

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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		

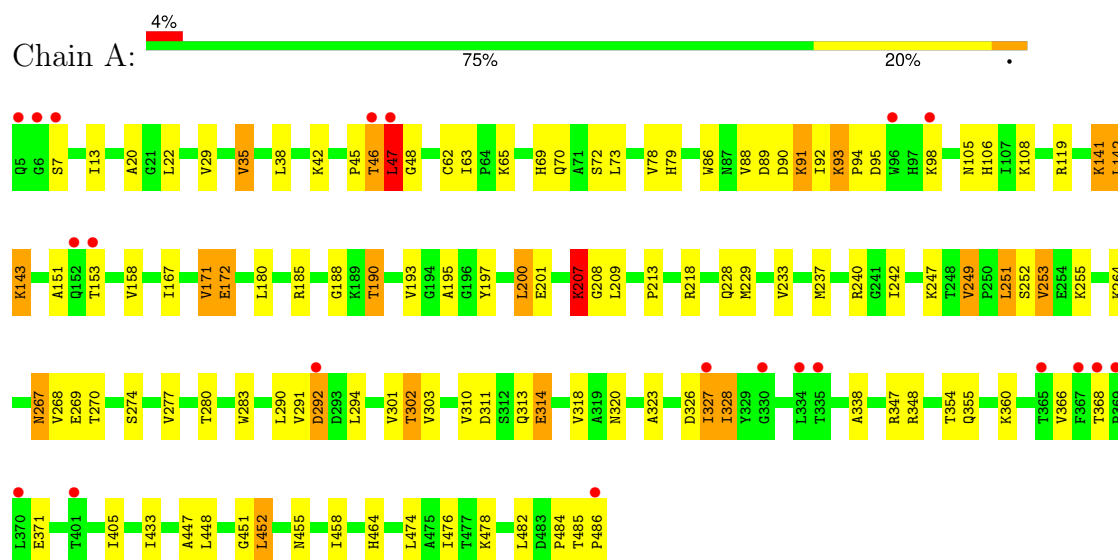
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	241	Total	O	0	0
			241	241		
3	B	271	Total	O	0	0
			271	271		

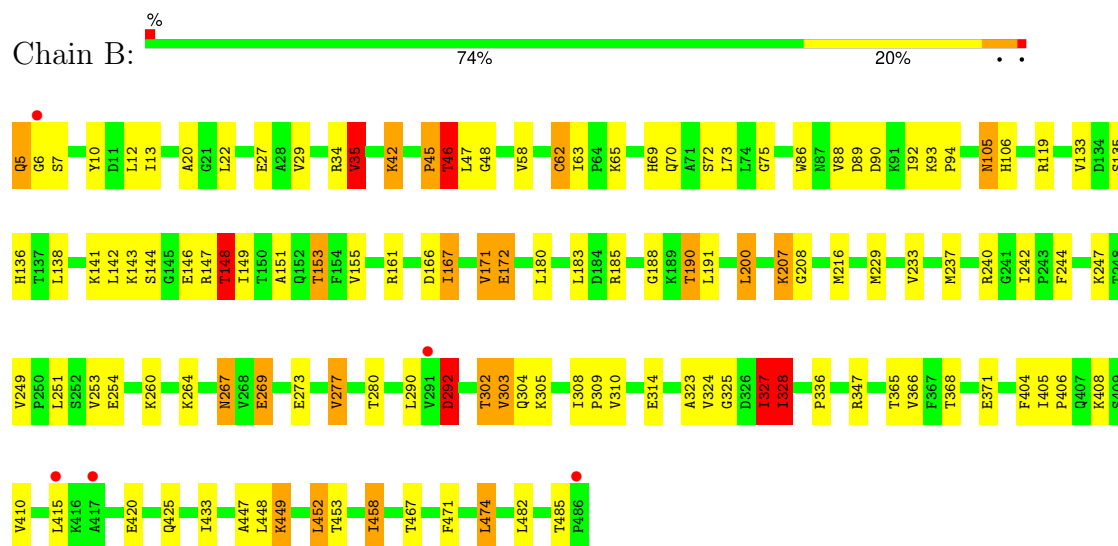
3 Residue-property plots [i](#)

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: Thioredoxin reductase 1



• Molecule 1: Thioredoxin reductase 1



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	150.97Å 150.97Å 267.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.17 – 2.25 31.17 – 2.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (31.17-2.25) 99.9 (31.17-2.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.92 (at 2.24Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.177 , 0.248 0.187 , 0.252	Depositor DCC
R_{free} test set	5611 reflections (10.07%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtrriage
Anisotropy	0.264	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8002	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 76.45 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0368e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.29	8/3767 (0.2%)	1.23	10/5114 (0.2%)
1	B	1.34	12/3767 (0.3%)	1.23	16/5114 (0.3%)
All	All	1.32	20/7534 (0.3%)	1.23	26/10228 (0.3%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	405	ILE	CA-CB	11.63	1.60	1.54
1	B	292	ASP	CB-CG	8.96	1.74	1.52
1	B	308	ILE	CA-CB	6.82	1.60	1.54
1	B	404	PHE	N-CA	6.61	1.54	1.46
1	B	171	VAL	CA-CB	6.45	1.63	1.54
1	B	365	THR	C-O	6.40	1.31	1.23
1	B	148	THR	N-CA	6.02	1.53	1.46
1	B	292	ASP	CA-C	5.68	1.60	1.52
1	A	242	ILE	N-CA	5.61	1.50	1.46
1	B	63	ILE	CA-CB	5.46	1.61	1.54
1	A	292	ASP	CB-CG	5.46	1.65	1.52
1	B	58	VAL	C-O	-5.42	1.18	1.24
1	B	46	THR	N-CA	5.39	1.53	1.46
1	A	171	VAL	CA-CB	5.19	1.61	1.54
1	A	249	VAL	CA-C	5.18	1.58	1.52
1	A	301	VAL	CA-CB	5.17	1.60	1.54
1	B	62	CYS	C-O	-5.11	1.18	1.24
1	A	47	LEU	N-CA	5.07	1.52	1.46
1	A	91	LYS	CE-NZ	5.07	1.64	1.49
1	B	105	ASN	CB-CG	5.05	1.64	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	410	VAL	N-CA-C	-7.64	105.40	112.43
1	B	133	VAL	N-CA-C	-7.10	104.93	111.67
1	B	45	PRO	N-CA-C	-7.01	100.91	111.57
1	B	35	VAL	N-CA-C	6.70	118.44	108.46
1	B	7	SER	N-CA-C	6.49	121.27	113.23
1	B	146	GLU	CA-C-N	-6.39	114.83	122.44
1	B	146	GLU	C-N-CA	-6.39	114.83	122.44
1	A	63	ILE	CA-C-N	-6.30	112.35	119.28
1	A	63	ILE	C-N-CA	-6.30	112.35	119.28
1	A	326	ASP	N-CA-C	6.21	119.70	111.75
1	B	328	ILE	N-CA-C	-6.16	101.61	109.80
1	B	404	PHE	N-CA-C	5.99	117.50	110.97
1	B	327	ILE	CG1-CB-CG2	5.98	128.63	110.70
1	B	63	ILE	CA-C-N	-5.87	112.83	119.28
1	B	63	ILE	C-N-CA	-5.87	112.83	119.28
1	B	405	ILE	CA-C-N	-5.71	114.38	121.00
1	B	405	ILE	C-N-CA	-5.71	114.38	121.00
1	B	467	THR	N-CA-C	-5.68	105.46	112.90
1	A	79	HIS	N-CA-C	5.59	117.38	111.28
1	A	93	LYS	CA-C-N	5.59	126.44	120.13
1	A	93	LYS	C-N-CA	5.59	126.44	120.13
1	A	253	VAL	CB-CA-C	5.23	117.96	110.33
1	B	148	THR	N-CA-CB	5.08	119.08	110.49
1	A	207	LYS	N-CA-C	-5.08	105.82	111.36
1	A	218	ARG	N-CA-C	5.06	116.48	111.07
1	A	314	GLU	N-CA-C	5.02	118.70	112.47

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	3692	0	3710	85	2
1	B	3692	0	3710	80	3
2	A	53	0	31	1	0
2	B	53	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	241	0	0	15	0
3	B	271	0	0	21	0
All	All	8002	0	7481	161	4

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 11.

All (161) 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:292:ASP:CB	1:B:292:ASP:CG	1.74	1.53
1:B:141:LYS:HB2	3:B:552:HOH:O	1.34	1.23
1:A:141:LYS:HD3	3:A:573:HOH:O	1.36	1.21
1:A:200:LEU:HG	1:A:237:MET:HE1	1.28	1.12
1:B:449:LYS:HD3	3:B:752:HOH:O	1.58	1.04
1:B:119:ARG:HD2	3:B:751:HOH:O	1.58	1.02
1:A:105:ASN:HB3	3:A:564:HOH:O	1.62	0.98
1:B:93:LYS:HD3	1:B:94:PRO:HD2	1.44	0.95
1:A:233:VAL:HG12	1:A:237:MET:HE2	1.55	0.89
1:A:185:ARG:HG2	3:A:516:HOH:O	1.72	0.87
1:A:302:THR:HG22	3:A:700:HOH:O	1.77	0.84
1:A:141:LYS:NZ	1:A:141:LYS:HB3	1.93	0.82
1:B:153:THR:CG2	3:B:591:HOH:O	2.29	0.80
1:A:86:TRP:CE3	1:B:92:ILE:HD12	2.18	0.79
1:B:233:VAL:HG12	1:B:237:MET:HE2	1.65	0.78
1:B:5:GLN:HG3	1:B:34:ARG:HH21	1.48	0.77
1:B:149:ILE:HB	3:B:754:HOH:O	1.85	0.77
1:A:455:ASN:HB3	3:A:552:HOH:O	1.90	0.71
1:B:190:THR:HB	1:B:280:THR:HB	1.73	0.71
1:B:69:HIS:HD2	3:B:509:HOH:O	1.74	0.70
1:A:29:VAL:CG2	1:A:35:VAL:HG13	2.21	0.70
1:A:190:THR:HB	1:A:280:THR:HB	1.72	0.70
1:B:10:TYR:HD1	3:B:754:HOH:O	1.75	0.69
1:B:166:ASP:O	1:B:167:ILE:HD12	1.91	0.69
1:A:29:VAL:CG2	1:A:35:VAL:CG1	2.71	0.68
1:A:233:VAL:HG12	1:A:237:MET:CE	2.24	0.67
1:B:45:PRO:O	1:B:46:THR:O	2.12	0.67
1:B:93:LYS:HD3	1:B:94:PRO:CD	2.22	0.67
1:A:119:ARG:HD2	3:A:710:HOH:O	1.96	0.66
1:B:188:GLY:O	1:B:190:THR:HG22	1.96	0.65
1:B:200:LEU:HG	1:B:237:MET:HE1	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:GLU:OE2	1:B:347:ARG:HD3	1.98	0.64
1:A:29:VAL:HG23	1:A:35:VAL:CG1	2.27	0.64
1:A:484:PRO:O	1:A:486:PRO:HD2	1.98	0.64
1:A:318:VAL:HG12	1:A:320:ASN:OD1	1.98	0.63
1:A:233:VAL:CG1	1:A:237:MET:HE2	2.28	0.63
1:A:92:ILE:HD12	1:B:86:TRP:CE3	2.35	0.62
1:A:323:ALA:O	1:A:328:ILE:HD11	2.00	0.61
1:B:267:ASN:HD22	1:B:269:GLU:H	1.46	0.61
1:A:29:VAL:HG23	1:A:35:VAL:HG11	1.83	0.60
1:B:5:GLN:CG	1:B:34:ARG:HH21	2.13	0.60
1:A:29:VAL:HG22	1:A:35:VAL:HG13	1.83	0.60
1:A:69:HIS:HD2	3:A:528:HOH:O	1.85	0.59
1:A:188:GLY:O	1:A:190:THR:HG22	2.03	0.58
1:B:136:HIS:HD2	1:B:151:ALA:O	1.87	0.58
1:B:147:ARG:HG2	1:B:149:ILE:HG23	1.86	0.58
1:A:29:VAL:HG22	1:A:35:VAL:CG1	2.34	0.57
1:A:323:ALA:HB1	1:A:327:ILE:HD13	1.85	0.57
1:B:93:LYS:CD	1:B:94:PRO:HD2	2.27	0.57
1:B:69:HIS:HE1	1:B:371:GLU:OE1	1.88	0.56
1:B:303:VAL:CG1	1:B:305:LYS:O	2.54	0.56
1:B:292:ASP:HB3	3:B:630:HOH:O	2.04	0.56
1:A:46:THR:O	1:A:48:GLY:N	2.38	0.56
1:A:70:GLN:HE21	1:A:70:GLN:HA	1.71	0.56
1:B:267:ASN:ND2	1:B:269:GLU:H	2.04	0.56
1:A:72:SER:OG	1:A:208:GLY:HA3	2.05	0.55
1:A:78:VAL:HG11	1:A:92:ILE:HD13	1.87	0.55
1:A:197:TYR:O	1:A:201:GLU:HG3	2.07	0.55
1:A:310:VAL:HG21	1:A:328:ILE:CD1	2.37	0.54
1:B:72:SER:OG	1:B:208:GLY:HA3	2.07	0.54
1:A:69:HIS:HE1	1:A:371:GLU:OE1	1.90	0.54
1:A:267:ASN:HD22	1:A:269:GLU:H	1.55	0.54
1:A:46:THR:O	1:A:47:LEU:HB2	2.06	0.54
1:B:327:ILE:HG13	3:B:501:HOH:O	2.06	0.54
1:B:207:LYS:HG3	1:B:242:ILE:HG12	1.90	0.54
1:A:20:ALA:HB2	1:A:338:ALA:HB1	1.90	0.53
1:B:65:LYS:HD2	1:B:65:LYS:C	2.34	0.52
1:B:303:VAL:CG1	1:B:304:GLN:N	2.72	0.52
1:A:247:LYS:O	1:A:268:VAL:HG12	2.08	0.52
1:B:323:ALA:HB1	1:B:327:ILE:HD13	1.92	0.52
1:A:185:ARG:HD2	3:A:706:HOH:O	2.10	0.52
1:A:141:LYS:CD	3:A:573:HOH:O	2.16	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:GLU:H	1:A:172:GLU:CD	2.18	0.52
1:A:267:ASN:ND2	1:A:269:GLU:H	2.07	0.51
1:B:46:THR:O	1:B:48:GLY:N	2.43	0.51
1:B:447:ALA:HB1	1:B:452:LEU:HG	1.92	0.51
1:A:185:ARG:HB3	3:A:706:HOH:O	2.11	0.50
1:B:105:ASN:HB3	3:B:598:HOH:O	2.10	0.50
1:B:260:LYS:HB3	1:B:277:VAL:HG23	1.93	0.50
1:A:251:LEU:HB3	1:A:264:LYS:HG3	1.94	0.50
1:A:207:LYS:HD2	1:A:240:ARG:O	2.12	0.50
1:A:89:ASP:OD2	1:A:90:ASP:N	2.45	0.49
1:A:366:VAL:HG12	1:A:368:THR:HG23	1.93	0.49
1:A:46:THR:HA	3:A:665:HOH:O	2.12	0.49
1:B:46:THR:O	1:B:47:LEU:HB2	2.13	0.49
1:A:45:PRO:O	1:A:46:THR:CB	2.58	0.49
1:B:292:ASP:CG	1:B:292:ASP:H	2.21	0.49
1:B:233:VAL:HG12	1:B:237:MET:CE	2.41	0.49
1:B:292:ASP:HB3	3:B:620:HOH:O	2.13	0.48
1:A:95:ASP:HB3	1:A:98:LYS:HD2	1.96	0.48
1:A:141:LYS:HB3	1:A:141:LYS:HZ2	1.76	0.48
1:B:191:LEU:HD11	1:B:216:MET:HE3	1.96	0.48
1:B:172:GLU:H	1:B:172:GLU:CD	2.22	0.47
1:B:147:ARG:O	1:B:148:THR:CB	2.62	0.47
1:A:447:ALA:HB1	1:A:452:LEU:HG	1.97	0.47
1:A:141:LYS:HB3	1:A:141:LYS:HZ1	1.79	0.47
1:A:119:ARG:CD	3:A:710:HOH:O	2.58	0.47
1:B:42:LYS:HE3	3:B:685:HOH:O	2.14	0.46
1:B:240:ARG:NE	3:B:729:HOH:O	2.13	0.46
1:A:311:ASP:C	1:A:311:ASP:OD1	2.59	0.46
1:A:94:PRO:HG3	1:A:209:LEU:O	2.15	0.46
1:A:267:ASN:HD22	1:A:267:ASN:C	2.22	0.46
1:B:183:LEU:HD13	1:B:185:ARG:HD3	1.97	0.46
1:A:327:ILE:HG13	3:A:529:HOH:O	2.16	0.46
1:B:420:GLU:HB3	1:B:425:GLN:HA	1.97	0.46
1:A:185:ARG:CG	3:A:516:HOH:O	2.45	0.46
1:B:106:HIS:HE1	3:B:619:HOH:O	1.98	0.46
1:A:310:VAL:HG21	1:A:328:ILE:HD11	1.98	0.46
1:B:13:ILE:HD11	3:B:754:HOH:O	2.14	0.45
1:B:302:THR:HG22	3:B:673:HOH:O	2.15	0.45
1:B:89:ASP:OD2	1:B:90:ASP:N	2.49	0.45
1:A:65:LYS:HD2	1:A:65:LYS:C	2.41	0.45
1:B:29:VAL:HG22	1:B:35:VAL:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:ALA:HB1	1:B:324:VAL:HG13	1.99	0.44
1:B:153:THR:HG22	3:B:591:HOH:O	2.07	0.44
1:B:247:LYS:CB	1:B:269:GLU:HG3	2.46	0.44
1:A:484:PRO:O	1:A:486:PRO:CD	2.66	0.44
1:B:70:GLN:HE21	1:B:70:GLN:HA	1.82	0.44
1:A:252:SER:OG	1:A:264:LYS:HG2	2.17	0.44
1:A:464:HIS:HB2	1:B:336:PRO:HG3	2.00	0.44
1:A:38:LEU:HD12	1:A:38:LEU:N	2.33	0.43
1:A:158:VAL:HG11	1:A:294:LEU:HD21	2.00	0.43
1:A:291:VAL:HA	1:A:294:LEU:HD12	1.99	0.43
1:B:161:ARG:HG2	1:B:290:LEU:HD11	1.99	0.43
1:B:12:LEU:HD11	1:B:155:VAL:HG23	2.00	0.43
1:A:13:ILE:HG13	1:A:151:ALA:HB2	2.00	0.43
1:A:106:HIS:HE1	3:B:680:HOH:O	2.02	0.43
1:A:229:MET:HE3	1:A:433:ILE:HG13	2.00	0.43
1:B:327:ILE:HD12	1:B:328:ILE:N	2.33	0.43
1:A:247:LYS:C	1:A:268:VAL:HG12	2.44	0.42
1:A:290:LEU:HD12	2:A:500:FAD:H8A	2.01	0.42
1:B:247:LYS:HB3	1:B:269:GLU:HG3	2.01	0.42
1:B:323:ALA:HB1	1:B:327:ILE:CD1	2.49	0.42
1:A:451:GLY:O	1:A:452:LEU:C	2.62	0.42
1:A:193:VAL:HG21	1:A:283:TRP:CZ3	2.55	0.42
1:B:406:PRO:HG2	1:B:408:LYS:HG3	2.00	0.42
1:A:448:LEU:HD12	3:A:707:HOH:O	2.19	0.42
1:B:327:ILE:HG13	1:B:327:ILE:H	1.62	0.42
1:A:228:GLN:OE1	1:A:478:LYS:NZ	2.43	0.42
1:B:310:VAL:CG2	1:B:328:ILE:HG12	2.50	0.42
1:B:304:GLN:HB2	1:B:309:PRO:HG3	2.01	0.42
1:B:138:LEU:O	1:B:148:THR:HA	2.19	0.42
1:B:366:VAL:HG12	1:B:368:THR:HG23	2.01	0.42
1:A:142:LEU:O	1:A:143:LYS:C	2.62	0.41
1:A:267:ASN:HD22	1:A:268:VAL:N	2.19	0.41
1:B:10:TYR:CD1	3:B:754:HOH:O	2.57	0.41
1:B:458:ILE:HD11	1:B:474:LEU:O	2.20	0.41
1:A:86:TRP:CZ2	1:B:75:GLY:HA3	2.56	0.41
1:A:190:THR:O	1:A:213:PRO:HA	2.20	0.41
1:A:476:ILE:HD13	1:A:484:PRO:HA	2.03	0.41
1:B:244:PHE:CD2	1:B:244:PHE:N	2.89	0.41
1:A:195:ALA:HA	1:A:200:LEU:HD13	2.02	0.41
1:A:348:ARG:HD3	1:A:355:GLN:O	2.21	0.41
1:B:325:GLY:O	1:B:328:ILE:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:VAL:HG21	1:A:328:ILE:HD13	2.03	0.41
1:B:229:MET:HE3	1:B:433:ILE:HG13	2.03	0.41
1:A:45:PRO:O	1:A:46:THR:HB	2.21	0.40
1:A:94:PRO:CB	3:B:763:HOH:O	2.68	0.40
1:B:452:LEU:HD22	1:B:453:THR:O	2.21	0.40
1:B:415:LEU:HD12	1:B:471:PHE:CD1	2.56	0.40
1:B:183:LEU:HD22	3:B:595:HOH:O	2.22	0.40

All (4) 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)
1:B:105:ASN:OD1	1:B:105:ASN:OD1[17_675]	1.40	0.80
1:A:105:ASN:OD1	1:A:105:ASN:OD1[12_765]	1.60	0.60
1:B:105:ASN:CG	1:B:105:ASN:OD1[17_675]	1.95	0.25
1:A:270:THR:O	1:B:135:SER:OG[18_765]	2.07	0.13

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	480/482 (100%)	458 (95%)	20 (4%)	2 (0%)	30	31
1	B	480/482 (100%)	461 (96%)	15 (3%)	4 (1%)	16	14
All	All	960/964 (100%)	919 (96%)	35 (4%)	6 (1%)	21	21

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	46	THR
1	A	7	SER
1	B	144	SER

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Mol	Chain	Res	Type
1	B	148	THR
1	A	46	THR
1	B	6	GLY

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	392/392 (100%)	349 (89%)	43 (11%)	6	4
1	B	392/392 (100%)	352 (90%)	40 (10%)	7	5
All	All	784/784 (100%)	701 (89%)	83 (11%)	6	4

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LEU
1	A	35	VAL
1	A	42	LYS
1	A	47	LEU
1	A	62	CYS
1	A	73	LEU
1	A	88	VAL
1	A	91	LYS
1	A	93	LYS
1	A	108	LYS
1	A	141	LYS
1	A	142	LEU
1	A	143	LYS
1	A	153	THR
1	A	167	ILE
1	A	171	VAL
1	A	172	GLU
1	A	180	LEU
1	A	190	THR
1	A	200	LEU

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Mol	Chain	Res	Type
1	A	207	LYS
1	A	249	VAL
1	A	251	LEU
1	A	253	VAL
1	A	255	LYS
1	A	267	ASN
1	A	274	SER
1	A	277	VAL
1	A	292	ASP
1	A	302	THR
1	A	303	VAL
1	A	313	GLN
1	A	314	GLU
1	A	327	ILE
1	A	328	ILE
1	A	347	ARG
1	A	354	THR
1	A	360	LYS
1	A	452	LEU
1	A	458	ILE
1	A	474	LEU
1	A	482	LEU
1	A	485	THR
1	B	5	GLN
1	B	22	LEU
1	B	35	VAL
1	B	42	LYS
1	B	46	THR
1	B	62	CYS
1	B	73	LEU
1	B	88	VAL
1	B	142	LEU
1	B	143	LYS
1	B	153	THR
1	B	167	ILE
1	B	171	VAL
1	B	172	GLU
1	B	180	LEU
1	B	190	THR
1	B	200	LEU
1	B	207	LYS
1	B	249	VAL

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Mol	Chain	Res	Type
1	B	251	LEU
1	B	253	VAL
1	B	254	GLU
1	B	264	LYS
1	B	267	ASN
1	B	269	GLU
1	B	273	GLU
1	B	277	VAL
1	B	292	ASP
1	B	302	THR
1	B	303	VAL
1	B	314	GLU
1	B	327	ILE
1	B	328	ILE
1	B	448	LEU
1	B	449	LYS
1	B	452	LEU
1	B	458	ILE
1	B	474	LEU
1	B	482	LEU
1	B	485	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	HIS
1	A	70	GLN
1	A	104	GLN
1	A	106	HIS
1	A	127	ASN
1	A	256	GLN
1	A	267	ASN
1	A	298	ASN
1	A	355	GLN
1	A	425	GLN
1	B	5	GLN
1	B	31	ASN
1	B	69	HIS
1	B	70	GLN
1	B	106	HIS
1	B	136	HIS
1	B	267	ASN

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Mol	Chain	Res	Type
1	B	298	ASN
1	B	407	GLN
1	B	422	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	B	500	-	58,58,58	1.30	7 (12%)	85,89,89	2.27	27 (31%)
2	FAD	A	500	-	58,58,58	1.11	3 (5%)	85,89,89	1.70	19 (22%)

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	B	500	-	-	3/34/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	500	-	-	3/34/50/50	0/6/6/6

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	FAD	C4X-N5	4.21	1.39	1.30
2	A	500	FAD	C4X-N5	4.06	1.39	1.30
2	A	500	FAD	C8A-N7A	2.72	1.36	1.31
2	B	500	FAD	C6-C7	2.60	1.43	1.39
2	B	500	FAD	C10-N1	2.58	1.38	1.33
2	B	500	FAD	C3B-C4B	-2.33	1.47	1.53
2	B	500	FAD	O5B-C5B	-2.28	1.36	1.44
2	B	500	FAD	C2A-N3A	2.13	1.37	1.33
2	B	500	FAD	PA-O3P	2.08	1.61	1.59
2	A	500	FAD	C5A-N7A	-2.02	1.35	1.39

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	FAD	N3A-C2A-N1A	-7.29	117.55	128.58
2	A	500	FAD	N3A-C2A-N1A	-6.31	119.03	128.58
2	B	500	FAD	N9A-C8A-N7A	-5.81	105.70	113.94
2	B	500	FAD	O3B-C3B-C4B	-5.67	94.79	111.08
2	B	500	FAD	O4B-C4B-C5B	5.51	127.00	109.33
2	B	500	FAD	O2A-PA-O5B	4.83	129.46	107.57
2	B	500	FAD	C5A-N7A-C8A	4.77	110.95	103.45
2	B	500	FAD	C9A-C5X-N5	-4.19	118.01	122.45
2	B	500	FAD	C2A-N3A-C4A	4.08	121.81	111.83
2	B	500	FAD	C4A-N9A-C8A	4.07	110.01	105.74
2	B	500	FAD	C5A-C4A-N3A	-4.04	121.15	126.72
2	A	500	FAD	C5A-C4A-N3A	-3.82	121.46	126.72
2	B	500	FAD	C4B-O4B-C1B	-3.73	101.22	109.47
2	A	500	FAD	N9A-C8A-N7A	-3.71	108.68	113.94
2	A	500	FAD	C2A-N1A-C6A	3.68	124.77	118.73
2	B	500	FAD	C5X-C9A-N10	3.47	121.11	117.97
2	A	500	FAD	C5A-N7A-C8A	3.46	108.89	103.45
2	A	500	FAD	C4X-C10-N10	3.44	121.41	116.48
2	B	500	FAD	N3A-C4A-N9A	3.26	132.70	127.17
2	A	500	FAD	C10-C4X-N5	-3.09	118.50	124.81
2	A	500	FAD	C4-N3-C2	-3.07	120.18	125.64
2	A	500	FAD	C4-C4X-N5	3.05	122.42	118.21
2	A	500	FAD	C2A-N3A-C4A	2.98	119.11	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	FAD	C4A-C5A-N7A	-2.96	107.20	110.58
2	A	500	FAD	C10-N1-C2	2.68	122.66	116.85
2	B	500	FAD	O4-C4-C4X	-2.66	119.50	126.53
2	B	500	FAD	O5B-PA-O1A	-2.66	98.39	108.94
2	B	500	FAD	O3P-PA-O1A	-2.65	102.72	110.70
2	A	500	FAD	O2A-PA-O3P	2.65	114.44	107.27
2	B	500	FAD	O2A-PA-O3P	2.53	114.10	107.27
2	A	500	FAD	N3A-C4A-N9A	2.49	131.40	127.17
2	A	500	FAD	C5'-C4'-C3'	-2.49	107.53	112.22
2	B	500	FAD	C2A-N1A-C6A	2.48	122.81	118.73
2	B	500	FAD	C4-N3-C2	-2.45	121.29	125.64
2	B	500	FAD	O5B-C5B-C4B	2.43	117.27	108.99
2	A	500	FAD	O2'-C2'-C3'	2.40	114.86	109.25
2	B	500	FAD	C4X-C10-N10	2.34	119.83	116.48
2	B	500	FAD	C4X-C4-N3	2.33	119.19	113.25
2	A	500	FAD	C4X-C4-N3	2.30	119.12	113.25
2	B	500	FAD	C9-C9A-N10	-2.28	118.78	121.85
2	A	500	FAD	C4A-C5A-N7A	-2.21	108.06	110.58
2	B	500	FAD	C4-C4X-N5	2.16	121.20	118.21
2	B	500	FAD	C10-C4X-N5	-2.09	120.53	124.81
2	A	500	FAD	C4X-C10-N1	-2.09	119.48	124.59
2	A	500	FAD	C4'-C3'-C2'	-2.07	110.13	113.57
2	B	500	FAD	O2-C2-N1	-2.05	118.39	121.80

There are no chirality outliers.

All (6) torsion outliers are listed below:

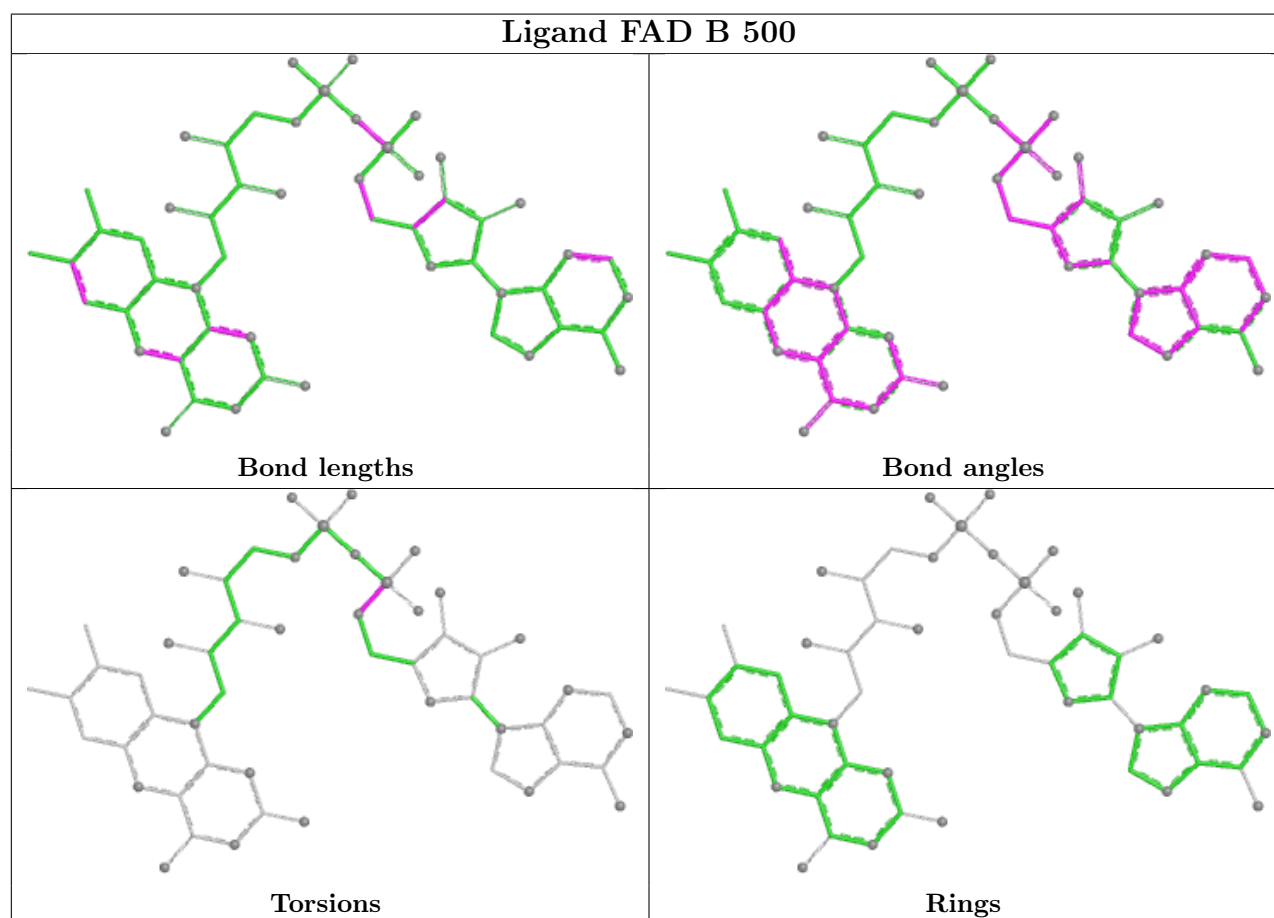
Mol	Chain	Res	Type	Atoms
2	B	500	FAD	C5B-O5B-PA-O1A
2	B	500	FAD	C5B-O5B-PA-O2A
2	B	500	FAD	C5B-O5B-PA-O3P
2	A	500	FAD	C3B-C4B-C5B-O5B
2	A	500	FAD	O4B-C4B-C5B-O5B
2	A	500	FAD	C2B-C1B-N9A-C8A

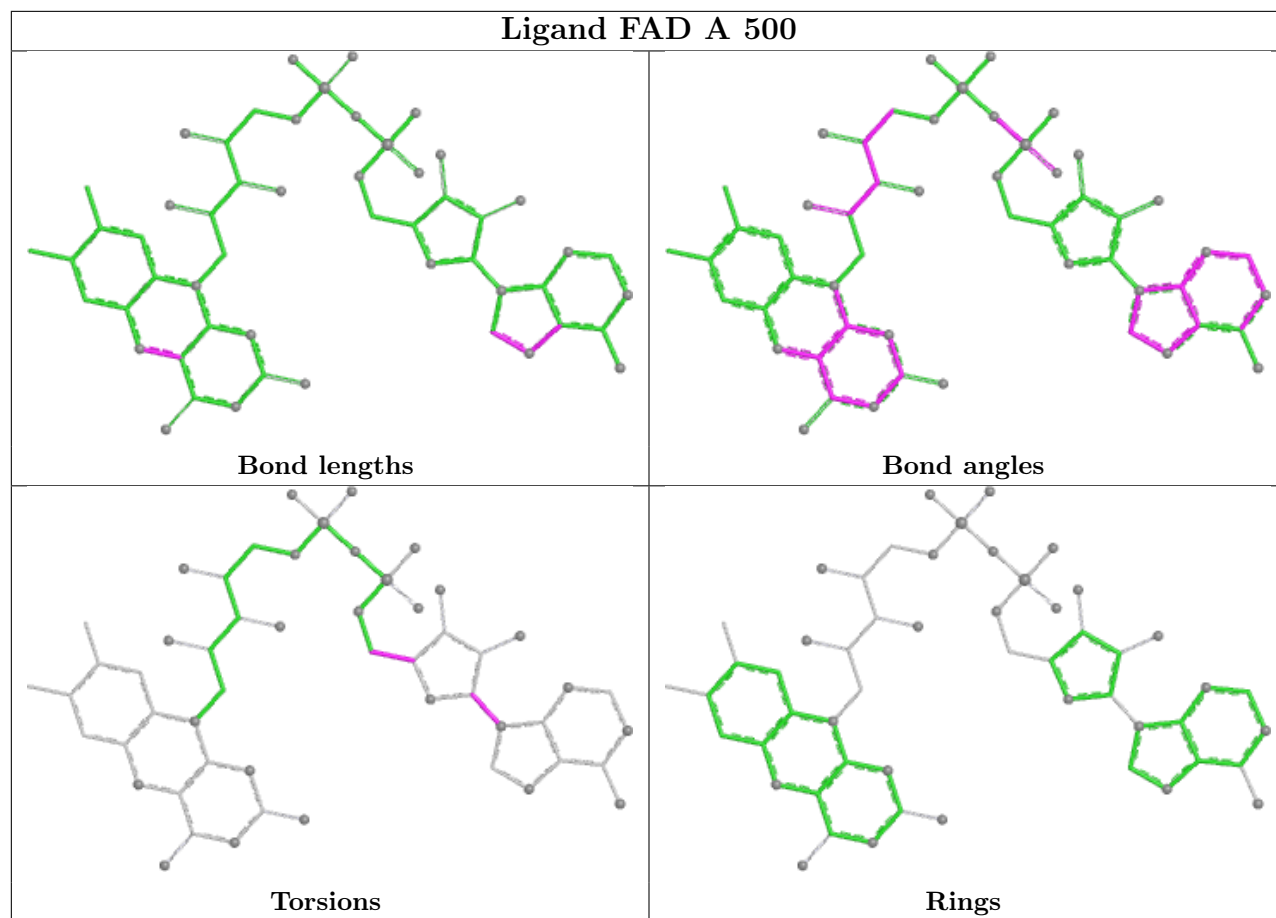
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	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

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	482/482 (100%)	0.20	21 (4%) 39 38	2, 14, 25, 46	0
1	B	482/482 (100%)	-0.08	5 (1%) 79 81	2, 13, 25, 49	0
All	All	964/964 (100%)	0.06	26 (2%) 56 57	2, 14, 25, 49	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	GLN	5.2
1	A	6	GLY	4.9
1	A	369	PRO	4.4
1	A	370	LEU	3.9
1	B	415	LEU	3.2
1	A	368	THR	3.1
1	A	292	ASP	2.8
1	A	365	THR	2.7
1	A	486	PRO	2.7
1	B	417	ALA	2.6
1	A	47	LEU	2.6
1	A	152	GLN	2.5
1	A	153	THR	2.4
1	A	334	LEU	2.4
1	A	46	THR	2.4
1	A	7	SER	2.4
1	A	367	PHE	2.4
1	A	330	GLY	2.3
1	A	401	THR	2.2
1	B	486	PRO	2.2
1	A	335	THR	2.2
1	B	6	GLY	2.1
1	A	98	LYS	2.1
1	A	327	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	96	TRP	2.1
1	B	291	VAL	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](#)

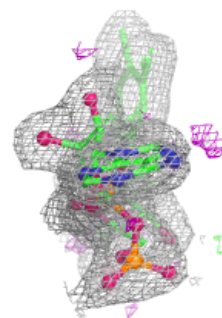
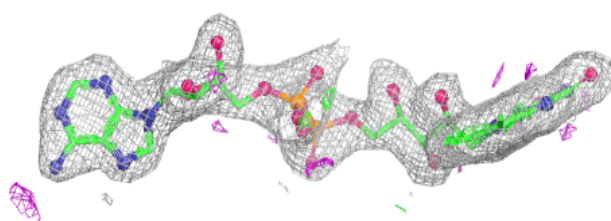
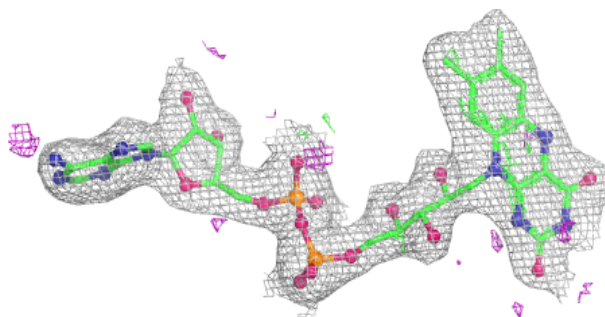
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	FAD	A	500	53/53	0.95	0.08	2,5,8,11	0
2	FAD	B	500	53/53	0.97	0.05	2,4,8,11	0

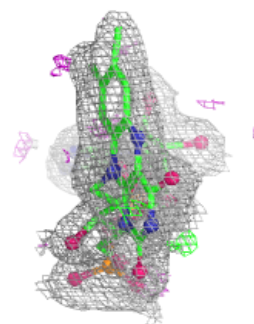
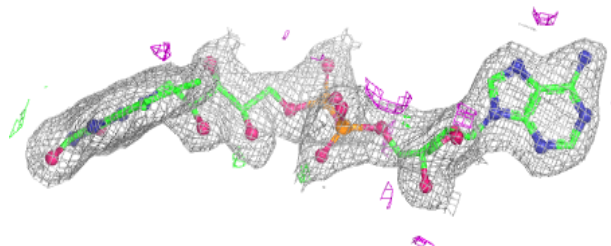
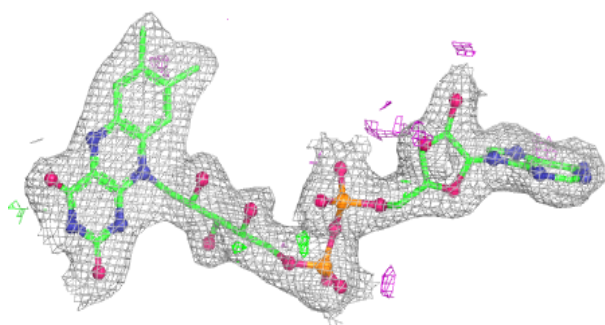
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD A 500:

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

**Electron density around FAD B 500:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.