



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:23 AM UTC

PDB ID : 6I7N / pdb_00006i7n
Title : Trypanothione Reductase from Leishmania infantum in complex with TRL156
Authors : Carriles, A.A.; Hermoso, J.A.
Deposited on : 2018-11-16
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

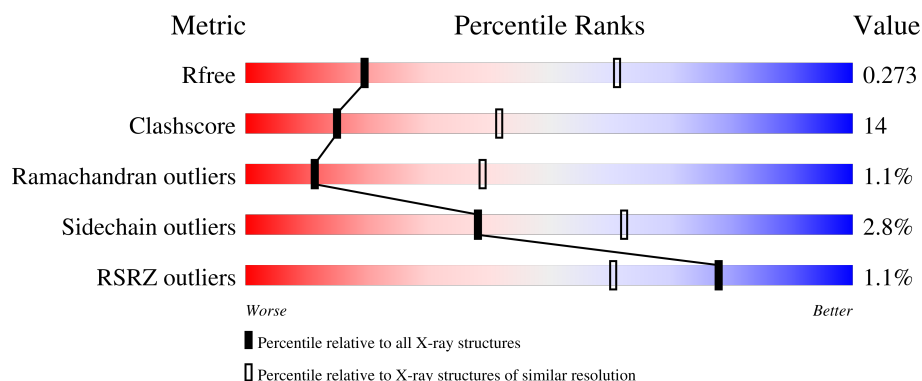
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	492	% 73% 25% .
1	B	492	% 75% 22% ..

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 7766 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.

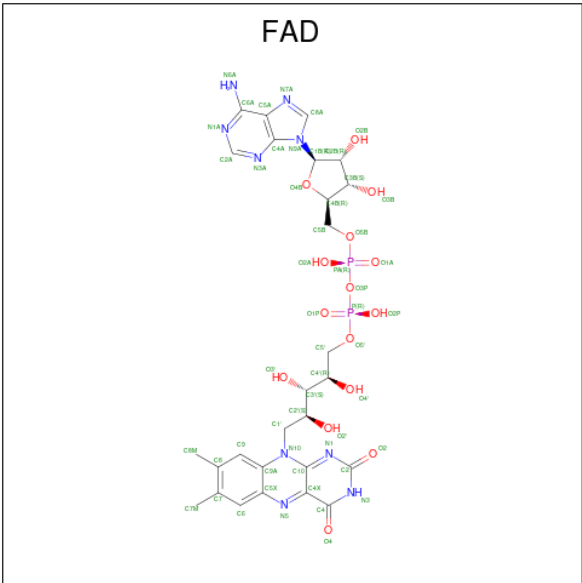
- Molecule 1 is a protein called Trypanothione reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	0	0	0
			3707	2330	636	714	27			
1	B	488	Total	C	N	O	S	0	0	0
			3694	2322	634	711	27			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	PRO	-	expression tag	UNP A4HSF7
B	0	PRO	-	expression tag	UNP A4HSF7

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



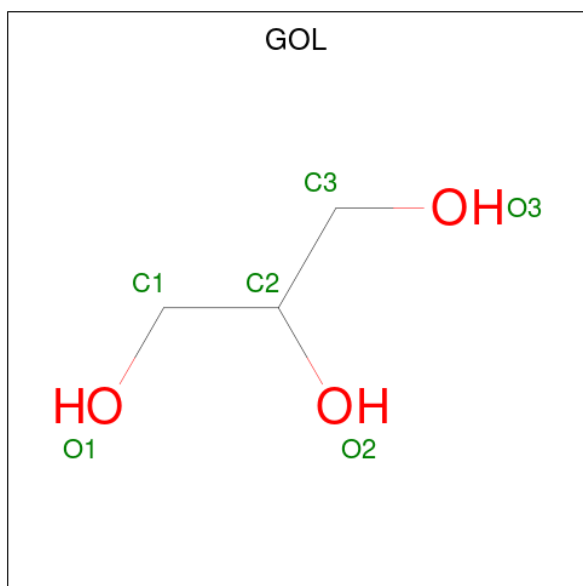
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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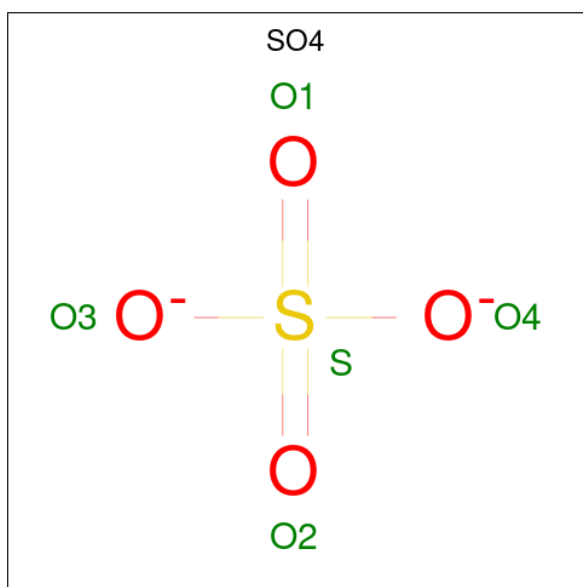
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



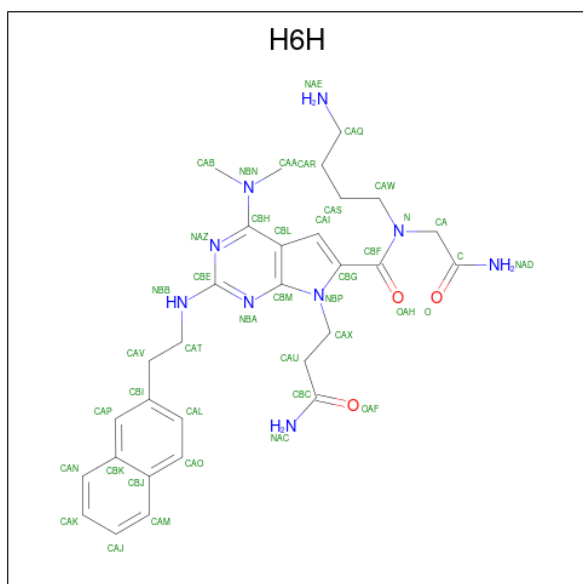
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 5 is {N}-(4-azanylbutyl)- {N}-(2-azanyl-2-oxidanylidene-ethyl)-7-(3-azanyl-3-oxidanylidene-propyl)-4-(dimethylamino)-2-(2-naphthalen-2-ylethylamino)pyrrolo[2,3-d]pyrimidine-6-carboxamide (CCD ID: H6H) (formula: C₃₀H₃₉N₉O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			42	30	9	3		

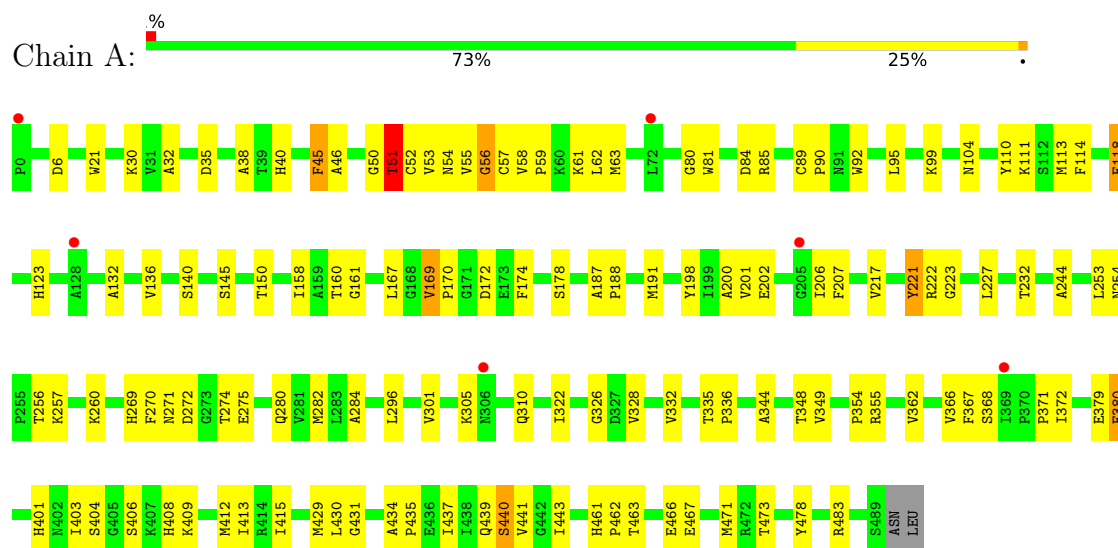
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	87	Total	O	0	0
			87	87		
6	B	108	Total	O	0	0
			108	108		

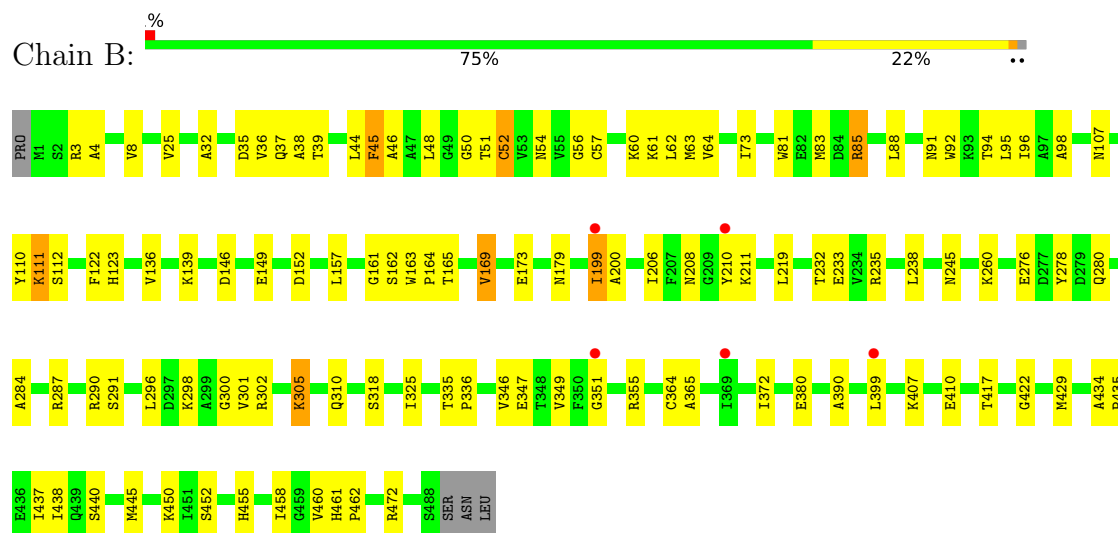
3 Residue-property plots

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: Trypanothione reductase



• Molecule 1: Trypanothione reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.18Å 106.39Å 186.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.68 – 3.30 46.68 – 3.30	Depositor EDS
% Data completeness (in resolution range)	80.7 (46.68-3.30) 80.7 (46.68-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.237 , 0.273 0.239 , 0.273	Depositor DCC
R_{free} test set	1111 reflections (3.84%)	wwPDB-VP
Wilson B-factor (Å ²)	80.3	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 56.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7766	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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: SO4, FAD, H6H, GOL

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	1.01	0/3781	1.30	10/5119 (0.2%)
1	B	1.00	0/3767	1.35	3/5100 (0.1%)
All	All	1.01	0/7548	1.32	13/10219 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	169	VAL	CB-CA-C	5.89	116.25	109.89
1	A	473	THR	CB-CA-C	-5.73	103.32	109.85
1	A	56	GLY	CA-C-N	5.62	130.12	121.19
1	A	56	GLY	C-N-CA	5.62	130.12	121.19
1	A	380	GLU	CA-C-N	5.52	127.67	120.28
1	A	380	GLU	C-N-CA	5.52	127.67	120.28
1	A	51	THR	N-CA-C	-5.46	106.93	113.21
1	A	178	SER	CA-C-N	5.38	128.27	120.79
1	A	178	SER	C-N-CA	5.38	128.27	120.79
1	B	111	LYS	N-CA-C	-5.32	105.40	111.14
1	A	221	TYR	CA-C-N	5.08	127.54	120.63
1	A	221	TYR	C-N-CA	5.08	127.54	120.63
1	B	165	THR	CB-CA-C	5.00	118.06	109.51

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3707	0	3656	116	0
1	B	3694	0	3644	98	0
2	A	53	0	31	10	0
2	B	53	0	31	9	0
3	A	6	0	8	1	0
3	B	6	0	8	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	B	42	0	0	3	0
6	A	87	0	0	3	0
6	B	108	0	0	8	0
All	All	7766	0	7378	204	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (204) 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:46:ALA:HB1	2:B:501:FAD:O3B	1.39	1.16
1:B:347:GLU:OE2	1:B:355:ARG:NH1	1.94	0.99
1:B:52:CYS:HA	1:B:56:GLY:HA3	1.45	0.94
1:A:51:THR:N	2:A:501:FAD:O1A	2.01	0.92
1:B:347:GLU:CD	1:B:355:ARG:NH1	2.28	0.91
1:B:347:GLU:HA	1:B:351:GLY:HA3	1.56	0.88
1:A:61:LYS:HE2	1:A:367:PHE:CE2	2.10	0.87
1:A:335:THR:HG22	1:A:336:PRO:HD3	1.55	0.87
1:B:52:CYS:O	1:B:52:CYS:SG	2.31	0.87
1:B:260:LYS:HE3	6:B:639:HOH:O	1.74	0.86
1:B:346:VAL:O	1:B:351:GLY:N	2.10	0.83
1:A:335:THR:CG2	1:A:336:PRO:HD3	2.08	0.83
1:A:191:MET:HG2	1:A:207:PHE:CD2	2.13	0.82
1:A:46:ALA:HB1	2:A:501:FAD:O3B	1.78	0.82
1:B:347:GLU:OE1	1:B:355:ARG:NH1	2.13	0.81
1:B:110:TYR:OH	5:B:502:H6H:CA	2.29	0.80
1:A:200:ALA:HB2	1:A:284:ALA:HB3	1.62	0.79
1:B:52:CYS:HB2	2:B:501:FAD:O2'	1.83	0.78
1:B:38:ALA:HB3	6:B:652:HOH:O	1.81	0.78
1:A:462:PRO:HG2	1:B:61:LYS:HD3	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:ASP:OD1	2:B:501:FAD:O2B	2.02	0.76
1:B:51:THR:HG22	1:B:51:THR:O	1.86	0.76
1:A:305:LYS:HD2	1:A:310:GLN:HE22	1.53	0.73
1:B:3:ARG:HG3	1:B:4:ALA:H	1.54	0.72
1:A:89:CYS:O	1:A:89:CYS:SG	2.48	0.71
1:A:401:HIS:HA	1:A:404:SER:HB3	1.74	0.70
1:B:199:ILE:HG22	1:B:284:ALA:HB1	1.73	0.69
1:A:478:TYR:CE1	1:A:483:ARG:HB3	2.28	0.69
1:B:364:CYS:SG	1:B:365:ALA:N	2.68	0.67
1:B:57:CYS:HB3	2:B:501:FAD:N5	2.11	0.66
1:B:347:GLU:CA	1:B:351:GLY:HA3	2.25	0.65
5:B:502:H6H:NAD	5:B:502:H6H:OAH	2.30	0.64
1:A:52:CYS:O	1:A:57:CYS:SG	2.56	0.64
1:B:37:GLN:HG3	1:B:44:LEU:HD12	1.79	0.64
1:B:57:CYS:HB3	2:B:501:FAD:C4X	2.29	0.63
1:A:429:MET:HE1	1:A:437:ILE:HB	1.81	0.62
1:A:140:SER:HB3	1:A:145:SER:OG	1.99	0.62
1:A:167:LEU:HG	1:A:169:VAL:HG23	1.82	0.61
1:A:113:MET:HG3	1:A:114:PHE:N	2.15	0.61
1:B:302:ARG:NH2	1:B:318:SER:HB2	2.17	0.60
1:A:169:VAL:HG12	1:A:170:PRO:HD2	1.82	0.60
1:A:62:LEU:HD21	1:B:399:LEU:HB3	1.82	0.60
1:A:63:MET:HG2	1:A:95:LEU:HD21	1.82	0.60
1:A:52:CYS:SG	2:A:501:FAD:O2'	2.57	0.60
1:A:174:PHE:CD1	1:A:260:LYS:HD3	2.36	0.60
1:B:35:ASP:CG	2:B:501:FAD:O2B	2.45	0.60
1:A:332:VAL:O	6:A:601:HOH:O	2.16	0.59
1:A:21:TRP:CE3	1:A:113:MET:HE3	2.37	0.59
1:A:61:LYS:HD2	1:B:462:PRO:HG2	1.84	0.59
1:A:463:THR:O	1:A:466:GLU:HG2	2.03	0.59
1:A:403:ILE:HG23	1:B:98:ALA:HB1	1.83	0.59
1:B:200:ALA:HB2	1:B:284:ALA:HB3	1.85	0.59
1:A:191:MET:SD	1:A:207:PHE:CE2	2.96	0.58
1:A:221:TYR:O	1:A:253:LEU:O	2.21	0.58
1:A:221:TYR:CD1	1:A:222:ARG:N	2.71	0.58
1:A:282:MET:HE3	1:A:284:ALA:HB2	1.86	0.57
1:B:8:VAL:HG22	1:B:32:ALA:HB3	1.85	0.57
1:A:61:LYS:CD	1:B:462:PRO:HG2	2.35	0.57
1:B:302:ARG:NH2	1:B:318:SER:CB	2.67	0.57
1:A:461:HIS:CD2	1:B:335:THR:HG21	2.39	0.57
1:A:403:ILE:HD12	1:B:62:LEU:HD22	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:ILE:HD12	1:A:467:GLU:HB3	1.86	0.57
1:B:38:ALA:CB	6:B:652:HOH:O	2.48	0.56
1:A:6:ASP:OD1	3:A:502:GOL:H11	2.05	0.56
1:A:21:TRP:CE3	1:A:113:MET:CE	2.88	0.56
1:A:372:ILE:HG13	1:A:430:LEU:HD12	1.86	0.56
1:B:46:ALA:HB1	2:B:501:FAD:C3B	2.34	0.56
1:B:434:ALA:HB3	1:B:435:PRO:HD3	1.87	0.56
1:B:3:ARG:HG3	1:B:4:ALA:N	2.19	0.56
1:A:191:MET:CG	1:A:207:PHE:CD2	2.89	0.56
1:A:52:CYS:HA	1:A:56:GLY:HA3	1.88	0.56
1:A:160:THR:HA	2:A:501:FAD:H52A	1.88	0.55
1:A:63:MET:HB3	1:A:206:ILE:HD12	1.88	0.55
1:B:162:SER:O	6:B:601:HOH:O	2.18	0.55
1:B:91:ASN:ND2	6:B:604:HOH:O	2.35	0.55
1:A:136:VAL:HG22	1:A:150:THR:HG23	1.89	0.54
1:B:51:THR:O	1:B:51:THR:CG2	2.54	0.54
1:A:202:GLU:HG2	1:A:367:PHE:C	2.32	0.54
1:B:57:CYS:HA	1:B:60:LYS:HE3	1.90	0.54
1:B:57:CYS:HA	1:B:60:LYS:HB3	1.89	0.54
1:A:45:PHE:HB3	1:A:55:VAL:HG11	1.88	0.54
1:A:440:SER:HA	1:A:443:ILE:HD12	1.90	0.54
1:A:188:PRO:CG	1:A:207:PHE:CD1	2.91	0.54
1:B:452:SER:HA	1:B:455:HIS:CE1	2.42	0.54
1:B:302:ARG:HH21	1:B:318:SER:HB2	1.74	0.53
1:B:335:THR:HB	1:B:336:PRO:HD3	1.90	0.53
1:A:188:PRO:HG3	1:A:207:PHE:CD1	2.44	0.52
1:B:157:LEU:HD21	1:B:325:ILE:HD11	1.92	0.52
1:B:163:TRP:CD2	1:B:164:PRO:HD2	2.44	0.52
1:A:40:HIS:HB3	1:A:54:ASN:OD1	2.10	0.52
1:A:110:TYR:O	1:A:113:MET:HG2	2.10	0.52
1:A:21:TRP:HE3	1:A:113:MET:CE	2.23	0.52
1:B:36:VAL:HG23	1:B:37:GLN:HB2	1.92	0.52
1:B:60:LYS:O	1:B:64:VAL:HG23	2.09	0.52
1:A:305:LYS:CD	1:A:310:GLN:HE22	2.23	0.51
1:A:372:ILE:HG13	1:A:430:LEU:CD1	2.40	0.51
1:B:92:TRP:CZ2	1:B:96:ILE:HD11	2.46	0.51
1:A:296:LEU:HB3	1:A:301:VAL:HB	1.92	0.51
1:B:429:MET:HE1	1:B:437:ILE:HB	1.91	0.51
1:A:58:VAL:HB	1:A:59:PRO:CD	2.41	0.51
1:A:221:TYR:CG	1:A:222:ARG:N	2.78	0.51
1:A:174:PHE:CE1	1:A:260:LYS:HG2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:LEU:HD11	1:A:272:ASP:OD1	2.11	0.50
1:A:478:TYR:CZ	1:A:483:ARG:HB3	2.46	0.50
1:B:422:GLY:O	1:B:450:LYS:HB3	2.11	0.50
1:B:472:ARG:HG2	6:B:617:HOH:O	2.11	0.50
1:B:73:ILE:HG23	1:B:83:MET:HE1	1.93	0.50
1:A:61:LYS:HE3	1:B:462:PRO:O	2.11	0.50
1:B:390:ALA:HB3	1:B:417:THR:OG1	2.11	0.50
1:A:80:GLY:HA2	1:B:94:THR:OG1	2.12	0.50
1:A:257:LYS:HD3	1:A:269:HIS:CD2	2.47	0.50
1:A:406:SER:O	1:A:409:LYS:HG3	2.12	0.50
1:B:48:LEU:HD13	1:B:122:PHE:CE1	2.47	0.50
1:A:344:ALA:HB2	1:A:355:ARG:NH2	2.26	0.49
1:A:198:TYR:HB2	1:A:366:VAL:HG22	1.93	0.49
1:A:50:GLY:CA	2:A:501:FAD:O1A	2.60	0.49
1:A:52:CYS:CB	2:A:501:FAD:O2'	2.61	0.49
1:A:167:LEU:HD12	1:A:167:LEU:O	2.13	0.48
1:B:46:ALA:HB1	2:B:501:FAD:HO3A	1.68	0.48
1:A:371:PRO:HG2	1:A:431:GLY:O	2.13	0.48
1:B:63:MET:HG2	1:B:95:LEU:HD21	1.95	0.48
1:B:139:LYS:HD2	1:B:146:ASP:HB2	1.94	0.48
1:A:254:ASN:N	1:A:271:ASN:OD1	2.45	0.48
1:B:111:LYS:O	1:B:112:SER:C	2.57	0.48
1:B:139:LYS:CD	1:B:146:ASP:HB2	2.44	0.48
1:A:158:ILE:HG22	1:A:328:VAL:HG11	1.96	0.47
1:A:191:MET:SD	1:A:207:PHE:CD2	3.08	0.47
5:B:502:H6H:NAZ	5:B:502:H6H:CAV	2.77	0.47
1:A:160:THR:HG22	2:A:501:FAD:C5A	2.44	0.47
1:B:95:LEU:HD22	1:B:210:TYR:CZ	2.49	0.47
1:A:326:GLY:O	6:A:601:HOH:O	2.20	0.47
1:A:132:ALA:HA	1:A:322:ILE:HD11	1.95	0.47
1:A:167:LEU:HB3	1:A:172:ASP:OD1	2.15	0.47
1:A:58:VAL:HB	1:A:59:PRO:HD3	1.96	0.47
1:B:52:CYS:CA	1:B:56:GLY:HA3	2.32	0.47
1:B:305:LYS:HG2	6:B:664:HOH:O	2.15	0.47
1:A:35:ASP:OD1	2:A:501:FAD:O2B	2.24	0.47
1:A:272:ASP:OD2	1:A:274:THR:OG1	2.34	0.46
1:B:208:ASN:HD21	1:B:245:ASN:HD22	1.63	0.46
1:B:73:ILE:HG21	1:B:88:LEU:CD2	2.46	0.45
1:A:335:THR:HG23	1:A:336:PRO:HD3	1.98	0.45
1:A:379:GLU:HG3	1:A:380:GLU:CD	2.42	0.45
1:A:257:LYS:HB3	1:A:269:HIS:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:ARG:NH1	6:B:601:HOH:O	2.48	0.45
1:A:81:TRP:O	1:A:85:ARG:NH2	2.50	0.44
1:A:362:VAL:HG22	1:B:458:ILE:HD12	1.99	0.44
1:B:95:LEU:HD22	1:B:210:TYR:CE2	2.52	0.44
1:A:335:THR:CG2	1:A:336:PRO:CD	2.89	0.44
1:A:57:CYS:O	1:A:58:VAL:C	2.61	0.44
1:A:348:THR:HA	1:A:354:PRO:HA	1.99	0.43
1:B:435:PRO:HA	1:B:438:ILE:HG22	2.00	0.43
1:A:434:ALA:HB3	1:A:435:PRO:HD3	2.00	0.43
1:A:372:ILE:CG1	1:A:430:LEU:HD13	2.49	0.43
1:A:90:PRO:HB3	1:B:81:TRP:CZ3	2.54	0.43
1:A:92:TRP:HB2	1:A:187:ALA:HB2	2.00	0.43
1:B:63:MET:HE2	1:B:206:ILE:HD13	2.00	0.43
1:A:415:ILE:HD12	1:A:471:MET:HE2	2.00	0.43
1:B:276:GLU:OE2	1:B:278:TYR:OH	2.35	0.43
1:B:296:LEU:O	1:B:300:GLY:N	2.49	0.43
1:A:169:VAL:CG1	1:A:256:THR:O	2.66	0.43
1:B:157:LEU:HD21	1:B:325:ILE:CD1	2.49	0.43
1:A:401:HIS:CE1	1:A:409:LYS:HE3	2.54	0.43
1:B:161:GLY:HA3	2:B:501:FAD:O2A	2.19	0.43
1:A:50:GLY:C	1:A:52:CYS:H	2.27	0.42
1:A:191:MET:HB3	1:A:217:VAL:HG12	2.01	0.42
1:A:232:THR:OG1	1:A:380:GLU:OE2	2.17	0.42
1:A:253:LEU:HD23	1:A:270:PHE:CE1	2.54	0.42
1:B:445:MET:HE2	1:B:445:MET:HB3	1.93	0.42
1:A:198:TYR:HA	1:A:227:LEU:HD21	2.00	0.42
1:B:233:GLU:HA	1:B:233:GLU:OE1	2.18	0.42
1:A:201:VAL:HG12	1:A:368:SER:HB3	2.00	0.42
1:A:222:ARG:HA	1:A:254:ASN:HD21	1.83	0.42
1:A:461:HIS:HA	1:A:462:PRO:HA	1.80	0.42
1:A:253:LEU:CD2	1:A:270:PHE:CE1	3.02	0.42
1:B:208:ASN:OD1	1:B:211:LYS:NZ	2.53	0.42
1:A:269:HIS:ND1	1:A:275:GLU:OE2	2.38	0.42
1:B:164:PRO:HA	1:B:287:ARG:HG2	2.02	0.42
1:B:291:SER:O	1:B:296:LEU:CD1	2.67	0.42
1:A:160:THR:CA	2:A:501:FAD:H52A	2.49	0.42
1:A:439:GLN:OE1	1:B:460:VAL:N	2.49	0.42
1:B:50:GLY:O	1:B:54:ASN:ND2	2.53	0.42
1:B:45:PHE:CG	1:B:179:ASN:HB3	2.55	0.41
1:A:202:GLU:HG2	1:A:367:PHE:O	2.19	0.41
1:A:335:THR:HA	2:A:501:FAD:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:HIS:ND1	1:B:149:GLU:OE1	2.43	0.41
1:B:45:PHE:CD1	1:B:179:ASN:HB3	2.55	0.41
1:B:238:LEU:HD22	1:B:372:ILE:HD11	2.01	0.41
1:A:372:ILE:CG1	1:A:430:LEU:CD1	2.99	0.41
1:B:83:MET:HE3	1:B:85:ARG:HE	1.85	0.41
1:B:302:ARG:NH2	1:B:318:SER:HB3	2.35	0.41
1:B:302:ARG:CZ	1:B:318:SER:HB3	2.51	0.41
1:A:412:MET:O	1:A:429:MET:HA	2.21	0.41
1:A:32:ALA:HB1	1:A:123:HIS:CD2	2.56	0.41
1:A:161:GLY:HA2	6:A:605:HOH:O	2.21	0.41
1:A:437:ILE:O	1:A:441:VAL:HG23	2.21	0.41
1:B:3:ARG:HD2	1:B:152:ASP:OD1	2.21	0.41
1:B:461:HIS:HA	1:B:462:PRO:HA	1.79	0.41
1:A:221:TYR:CE2	1:A:223:GLY:N	2.84	0.41
1:B:232:THR:HA	1:B:235:ARG:HD3	2.03	0.40
1:B:39:THR:HA	1:B:107:ASN:CG	2.46	0.40
1:B:296:LEU:HB3	1:B:301:VAL:CG2	2.51	0.40
1:A:169:VAL:HG12	1:A:256:THR:O	2.22	0.40
1:A:244:ALA:HB1	1:A:408:HIS:NE2	2.37	0.40
1:B:73:ILE:HG21	1:B:88:LEU:HD21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	488/492 (99%)	432 (88%)	50 (10%)	6 (1%)	10	37
1	B	486/492 (99%)	430 (88%)	51 (10%)	5 (1%)	12	40
All	All	974/984 (99%)	862 (88%)	101 (10%)	11 (1%)	11	39

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	305	LYS
1	A	45	PHE
1	A	84	ASP
1	B	45	PHE
1	A	104	ASN
1	A	118	GLU
1	B	85	ARG
1	A	38	ALA
1	B	349	VAL
1	A	349	VAL
1	B	199	ILE

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	399/401 (100%)	390 (98%)	9 (2%)	44	66
1	B	397/401 (99%)	384 (97%)	13 (3%)	33	59
All	All	796/802 (99%)	774 (97%)	22 (3%)	38	62

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LYS
1	A	51	THR
1	A	53	VAL
1	A	99	LYS
1	A	111	LYS
1	A	118	GLU
1	A	169	VAL
1	A	280	GLN
1	A	440	SER
1	B	25	VAL
1	B	52	CYS
1	B	136	VAL
1	B	169	VAL

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Mol	Chain	Res	Type
1	B	173	GLU
1	B	219	LEU
1	B	280	GLN
1	B	298	LYS
1	B	310	GLN
1	B	380	GLU
1	B	407	LYS
1	B	410	GLU
1	B	440	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	GLN
1	A	254	ASN
1	A	310	GLN
1	A	401	HIS
1	A	402	ASN
1	A	418	ASN
1	B	22	ASN
1	B	37	GLN
1	B	104	ASN
1	B	179	ASN
1	B	245	ASN
1	B	306	ASN
1	B	310	GLN
1	B	455	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	GOL	A	502	-	5,5,5	0.12	0	5,5,5	0.35	0
4	SO4	B	504	-	4,4,4	0.32	0	6,6,6	0.08	0
2	FAD	A	501	-	58,58,58	0.62	0	85,89,89	0.67	1 (1%)
4	SO4	A	503	-	4,4,4	0.34	0	6,6,6	0.07	0
3	GOL	B	503	-	5,5,5	0.11	0	5,5,5	0.31	0
5	H6H	B	502	-	45,45,45	1.81	6 (13%)	58,62,62	1.74	12 (20%)
2	FAD	B	501	-	58,58,58	0.64	0	85,89,89	0.73	1 (1%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	502	-	-	4/4/4/4	-
2	FAD	B	501	-	-	4/34/50/50	0/6/6/6
2	FAD	A	501	-	-	17/34/50/50	0/6/6/6
3	GOL	B	503	-	-	4/4/4/4	-
5	H6H	B	502	-	-	12/32/32/32	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	502	H6H	CBF-N	8.62	1.49	1.34
5	B	502	H6H	CBG-NBP	3.47	1.43	1.39
5	B	502	H6H	CBE-NBB	3.27	1.39	1.34
5	B	502	H6H	CBM-NBA	2.66	1.37	1.34
5	B	502	H6H	CA-N	2.31	1.49	1.45
5	B	502	H6H	CAL-CBI	2.09	1.43	1.38

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	502	H6H	CBF-CBG-NBP	4.91	128.09	121.57
5	B	502	H6H	CA-N-CAW	4.40	125.09	117.46
5	B	502	H6H	CBG-CBF-N	-4.37	111.92	118.45
5	B	502	H6H	C-CA-N	-4.07	105.79	113.05
5	B	502	H6H	CAU-CAX-NBP	3.70	116.27	112.27
5	B	502	H6H	CBL-CBM-NBA	-3.16	124.55	126.56
5	B	502	H6H	CAI-CBG-CBF	-2.93	122.29	128.79
5	B	502	H6H	O-C-CA	2.91	125.89	120.77
5	B	502	H6H	OAF-CBC-NAC	-2.60	115.58	122.53
5	B	502	H6H	CAX-CAU-CBC	-2.53	107.81	112.27
5	B	502	H6H	O-C-NAD	-2.38	116.17	122.53
2	A	501	FAD	C4-N3-C2	-2.20	121.73	125.64
2	B	501	FAD	C4-N3-C2	-2.12	121.88	125.64
5	B	502	H6H	CBE-NAZ-CBH	2.09	120.69	113.99

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	FAD	C5B-O5B-PA-O1A
2	A	501	FAD	C3B-C4B-C5B-O5B
2	A	501	FAD	C1'-C2'-C3'-C4'
2	A	501	FAD	C2'-C3'-C4'-O4'
2	A	501	FAD	O3'-C3'-C4'-O4'
2	A	501	FAD	C3'-C4'-C5'-O5'
2	A	501	FAD	O4'-C4'-C5'-O5'
2	B	501	FAD	O4B-C4B-C5B-O5B
3	B	503	GOL	O1-C1-C2-C3
3	B	503	GOL	C1-C2-C3-O3
5	B	502	H6H	CAV-CAT-NBB-CBE
5	B	502	H6H	CAU-CAX-NBP-CBM
5	B	502	H6H	CAU-CAX-NBP-CBG
5	B	502	H6H	O-C-CA-N
5	B	502	H6H	NAD-C-CA-N
5	B	502	H6H	CAS-CAW-N-CA
2	B	501	FAD	C3B-C4B-C5B-O5B
2	A	501	FAD	O3'-C3'-C4'-C5'
2	A	501	FAD	C2'-C3'-C4'-C5'
5	B	502	H6H	CAS-CAW-N-CBF
2	A	501	FAD	O4B-C4B-C5B-O5B
5	B	502	H6H	CBC-CAU-CAX-NBP

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Mol	Chain	Res	Type	Atoms
3	A	502	GOL	C1-C2-C3-O3
3	B	503	GOL	O1-C1-C2-O2
3	B	503	GOL	O2-C2-C3-O3
2	A	501	FAD	O2'-C2'-C3'-C4'
3	A	502	GOL	O1-C1-C2-C3
2	A	501	FAD	O2'-C2'-C3'-O3'
2	A	501	FAD	C4B-C5B-O5B-PA
2	B	501	FAD	PA-O3P-P-O5'
5	B	502	H6H	CAT-CAV-CBI-CAL
5	B	502	H6H	CAT-CAV-CBI-CAP
5	B	502	H6H	CAQ-CAR-CAS-CAW
2	A	501	FAD	N10-C1'-C2'-O2'
2	A	501	FAD	PA-O3P-P-O1P
3	A	502	GOL	O2-C2-C3-O3
2	A	501	FAD	PA-O3P-P-O2P
2	A	501	FAD	C1'-C2'-C3'-O3'
2	B	501	FAD	PA-O3P-P-O1P
3	A	502	GOL	O1-C1-C2-O2
5	B	502	H6H	N-CBF-CBG-CAI

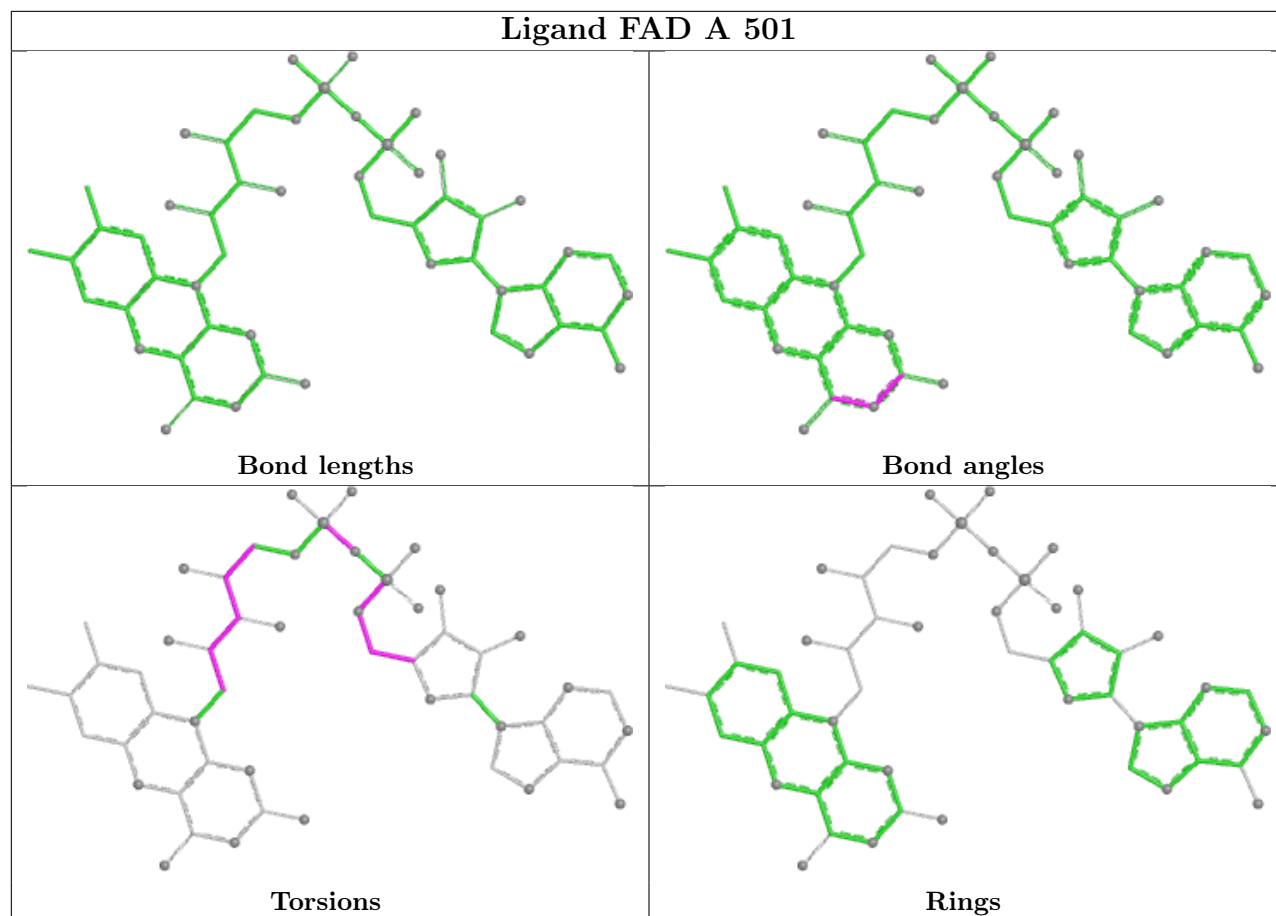
There are no ring outliers.

4 monomers are involved in 23 short contacts:

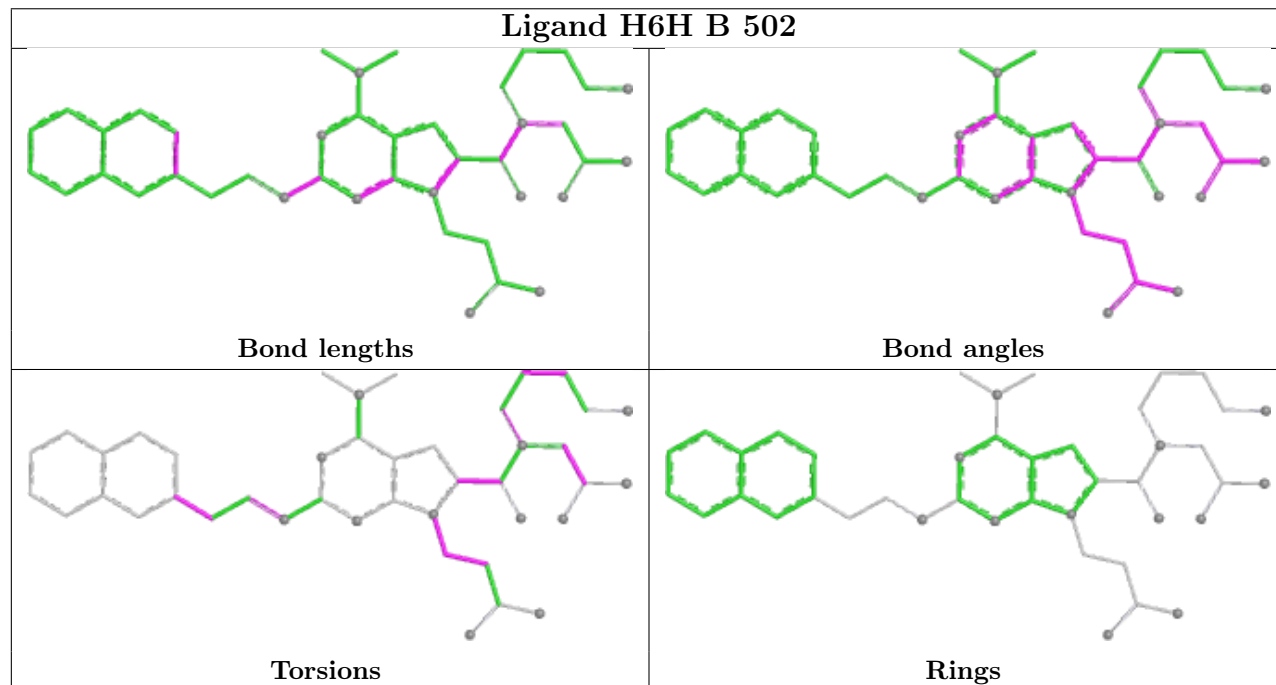
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	GOL	1	0
2	A	501	FAD	10	0
5	B	502	H6H	3	0
2	B	501	FAD	9	0

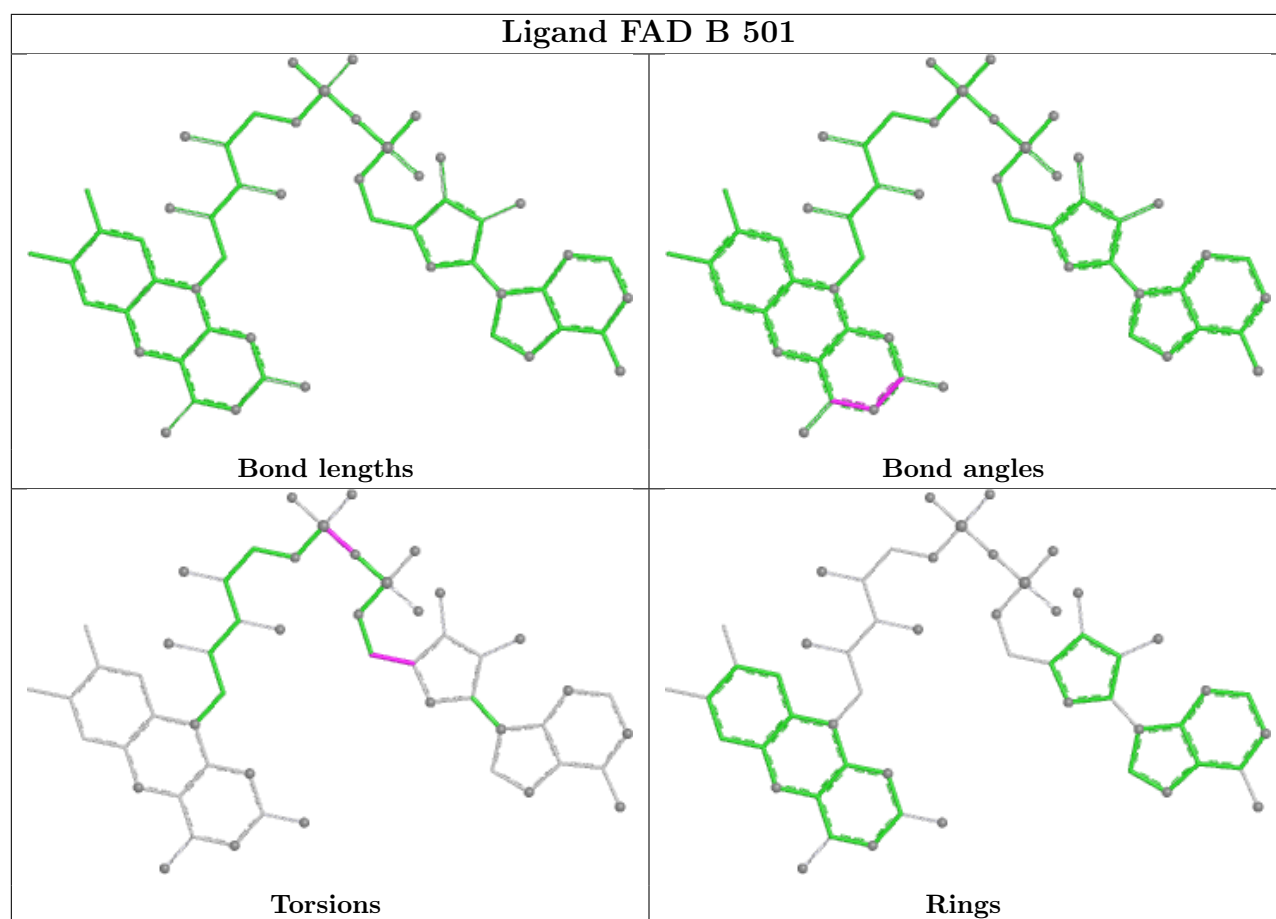
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 FAD A 501



Ligand H6H B 502





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	490/492 (99%)	-0.21	6 (1%) 76 58	69, 91, 120, 164	0
1	B	488/492 (99%)	-0.12	5 (1%) 79 63	63, 89, 119, 190	0
All	All	978/984 (99%)	-0.16	11 (1%) 78 60	63, 90, 120, 190	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	0	PRO	3.1
1	B	351	GLY	3.0
1	A	369	ILE	2.7
1	B	199	ILE	2.4
1	B	369	ILE	2.4
1	B	210	TYR	2.4
1	A	306	ASN	2.3
1	B	399	LEU	2.3
1	A	205	GLY	2.2
1	A	128	ALA	2.0
1	A	72	LEU	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 ⓘ

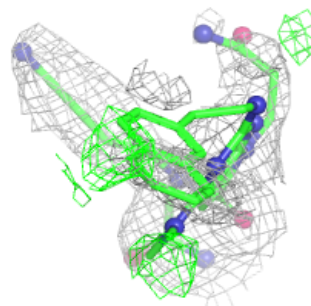
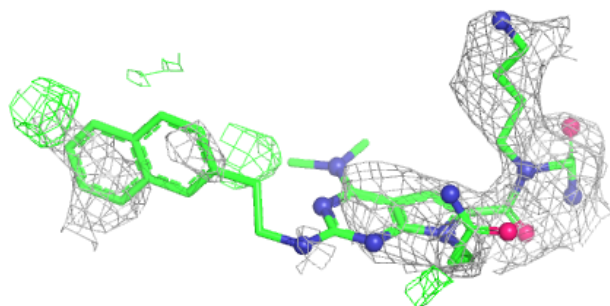
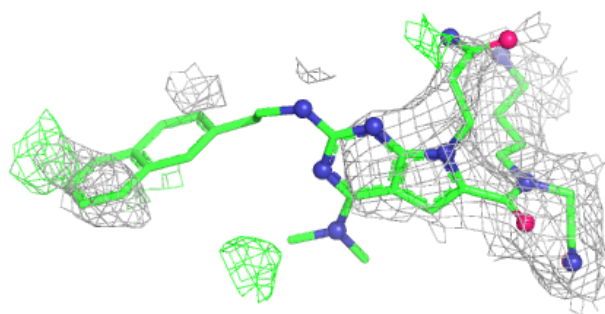
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	B	503	6/6	0.62	0.10	100,105,109,111	0
4	SO4	A	503	5/5	0.78	0.08	176,181,188,189	0
5	H6H	B	502	42/42	0.79	0.19	114,143,154,159	0
3	GOL	A	502	6/6	0.82	0.11	94,99,112,113	0
4	SO4	B	504	5/5	0.83	0.09	162,163,164,167	0
2	FAD	B	501	53/53	0.95	0.09	65,79,97,110	0
2	FAD	A	501	53/53	0.95	0.09	70,85,104,114	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.

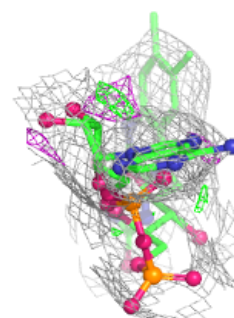
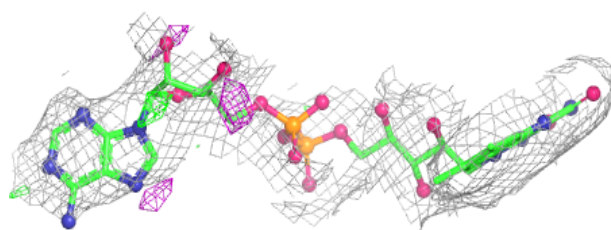
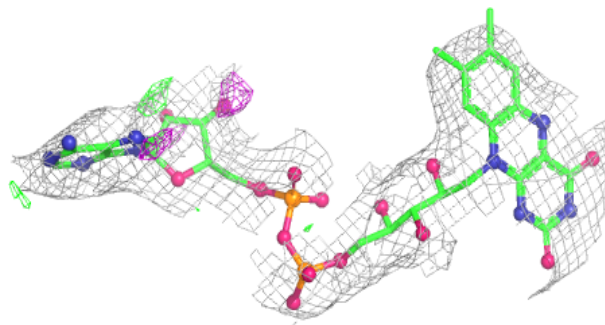
Electron density around H6H B 502:

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

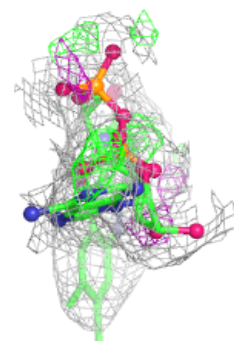
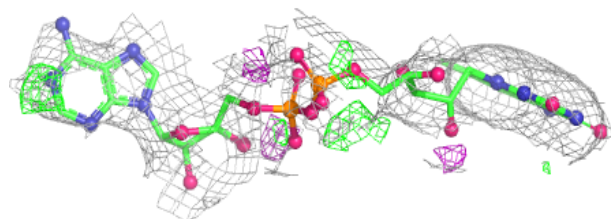
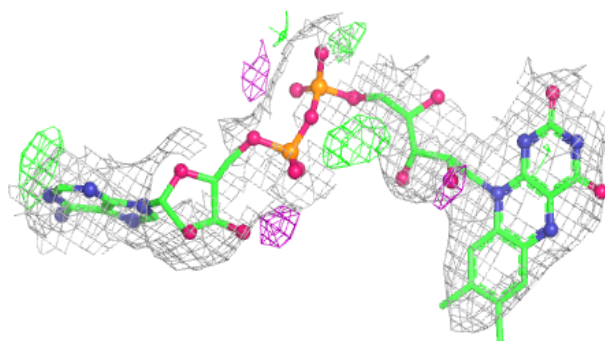


Electron density around FAD B 501:

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

**Electron density around FAD A 501:**

$2mF_o - DF_c$ (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.