



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 08:26 AM UTC

PDB ID : 4J57 / pdb_00004j57
Title : Structure of Plasmodium falciparum thioredoxin reductase-thioredoxin complex
Authors : Fritz-Wolf, K.; Jortzik, E.; Stumpf, M.; Preuss, J.; Iozef, R.; Rahlfs, S.; Becker, K.
Deposited on : 2013-02-08
Resolution : 2.50 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

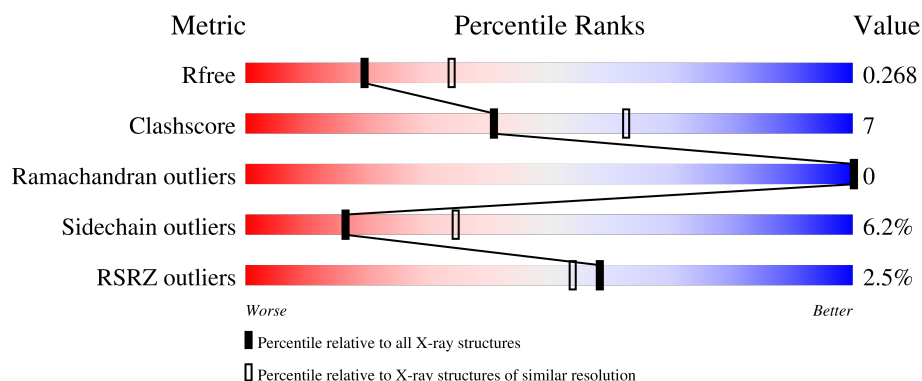
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	541	72% 16% • 11%
1	B	541	72% 16% • 11%
2	E	114	6% 69% 20% • 10%
2	F	114	12% 68% 22% • 10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9209 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	483	Total	C	N	O	S	0	0	0
			3723	2375	619	707	22			
1	B	483	Total	C	N	O	S	0	0	0
			3723	2375	619	707	22			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	540	SER	CYS	engineered mutation	UNP P61076
B	540	SER	CYS	engineered mutation	UNP P61076

- Molecule 2 is a protein called Thioredoxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	103	Total	C	N	O	S	0	0	0
			813	521	124	164	4			
2	F	103	Total	C	N	O	S	0	0	0
			813	521	124	164	4			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-9	ARG	-	expression tag	UNP Q7KQL8
E	-8	GLY	-	expression tag	UNP Q7KQL8
E	-7	SER	-	expression tag	UNP Q7KQL8
E	-6	HIS	-	expression tag	UNP Q7KQL8
E	-5	HIS	-	expression tag	UNP Q7KQL8
E	-4	HIS	-	expression tag	UNP Q7KQL8
E	-3	HIS	-	expression tag	UNP Q7KQL8
E	-2	HIS	-	expression tag	UNP Q7KQL8
E	-1	HIS	-	expression tag	UNP Q7KQL8
E	0	GLY	-	expression tag	UNP Q7KQL8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1	SER	-	expression tag	UNP Q7KQL8
E	33	SER	CYS	engineered mutation	UNP Q7KQL8
F	-9	ARG	-	expression tag	UNP Q7KQL8
F	-8	GLY	-	expression tag	UNP Q7KQL8
F	-7	SER	-	expression tag	UNP Q7KQL8
F	-6	HIS	-	expression tag	UNP Q7KQL8
F	-5	HIS	-	expression tag	UNP Q7KQL8
F	-4	HIS	-	expression tag	UNP Q7KQL8
F	-3	HIS	-	expression tag	UNP Q7KQL8
F	-2	HIS	-	expression tag	UNP Q7KQL8
F	-1	HIS	-	expression tag	UNP Q7KQL8
F	0	GLY	-	expression tag	UNP Q7KQL8
F	1	SER	-	expression tag	UNP Q7KQL8
F	33	SER	CYS	engineered mutation	UNP Q7KQL8

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

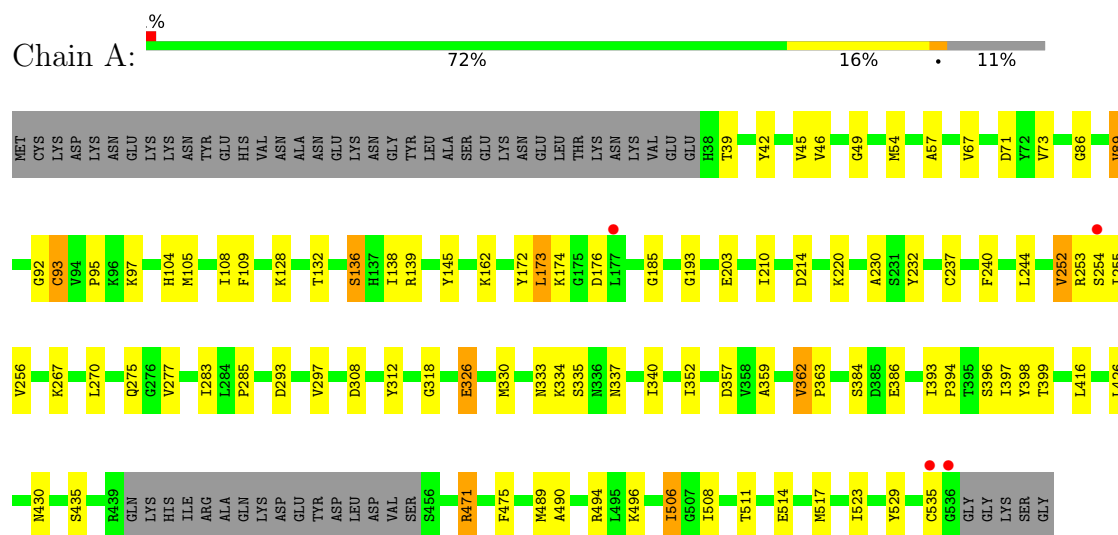
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	14	Total	O	0	0
			14	14		
5	B	11	Total	O	0	0
			11	11		

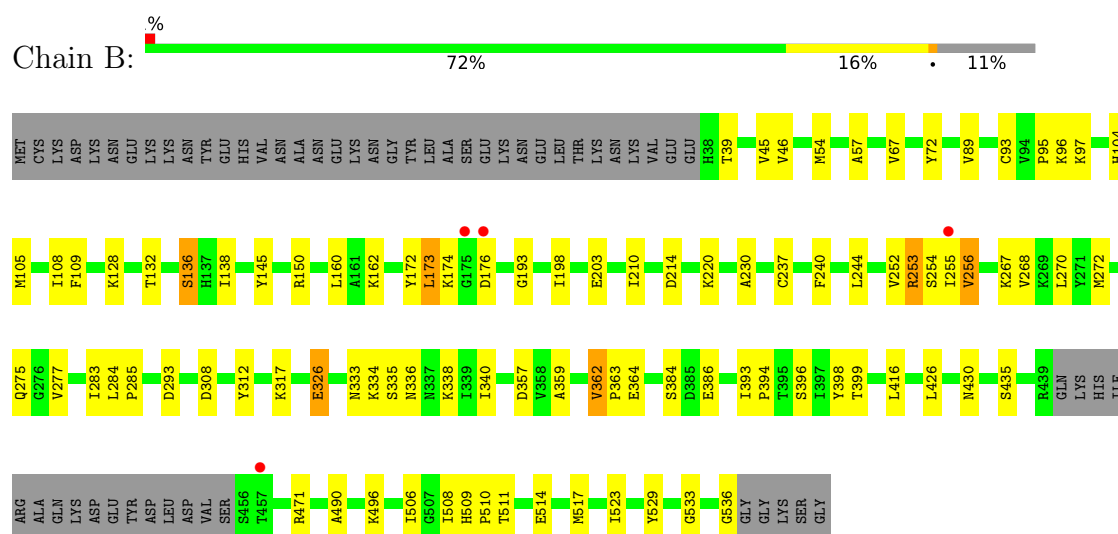
3 Residue-property plots

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: Thioredoxin reductase 2

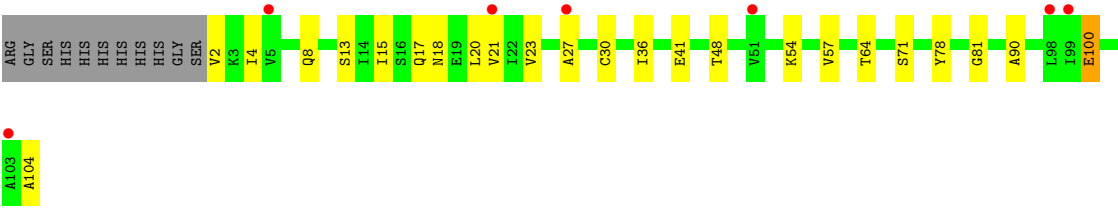


• Molecule 1: Thioredoxin reductase 2

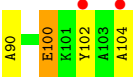
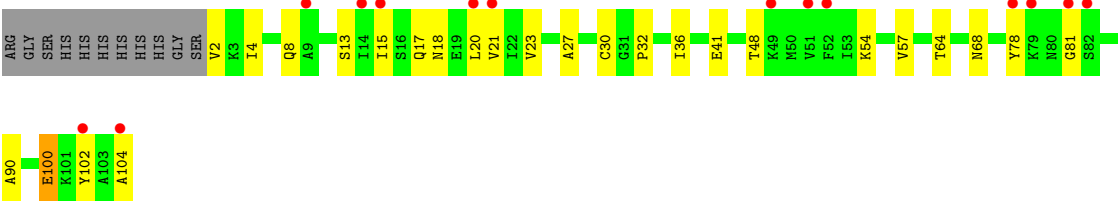


• Molecule 2: Thioredoxin





● Molecule 2: Thioredoxin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.80Å 100.60Å 142.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.50) 99.7 (20.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.23	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.50Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.216 , 0.268 0.218 , 0.268	Depositor DCC
R_{free} test set	2777 reflections (5.99%)	wwPDB-VP
Wilson B-factor (Å ²)	44.6	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 26.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9209	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.53 % 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 2.7005e-04. 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	0.58	0/3794	0.86	1/5119 (0.0%)
1	B	0.59	0/3794	0.86	0/5119
2	E	0.45	0/827	0.79	0/1117
2	F	0.44	0/827	0.78	0/1117
All	All	0.57	0/9242	0.85	1/12472 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	VAL	N-CA-C	5.06	114.03	106.85

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	3723	0	3740	51	0
1	B	3723	0	3740	51	0
2	E	813	0	807	11	0
2	F	813	0	807	13	0
3	A	53	0	31	3	0
3	B	53	0	31	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	6	0	8	0	0
5	A	14	0	0	0	0
5	B	11	0	0	2	0
All	All	9209	0	9164	120	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 7.

All (120) 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:150:ARG:HH22	2:F:68:ASN:HA	1.12	1.08
1:B:150:ARG:NH2	2:F:68:ASN:HA	1.96	0.73
2:E:15:ILE:HG22	2:E:81:GLY:HA2	1.75	0.67
1:B:253:ARG:HB2	1:B:284:LEU:HG	1.76	0.67
2:F:15:ILE:HG22	2:F:81:GLY:HA2	1.78	0.65
1:B:333:ASN:HB2	1:B:340:ILE:HD11	1.81	0.63
1:A:333:ASN:HB2	1:A:340:ILE:HD11	1.81	0.62
2:F:21:VAL:HG13	2:F:78:TYR:HB2	1.83	0.60
1:B:334:LYS:HG3	1:B:335:SER:HA	1.84	0.60
1:B:230:ALA:HB2	1:B:252:VAL:HG13	1.84	0.60
2:E:4:ILE:HG12	2:E:54:LYS:HB2	1.84	0.59
1:A:230:ALA:HB1	1:A:256:VAL:HA	1.82	0.59
2:E:21:VAL:HG13	2:E:78:TYR:HB2	1.85	0.59
1:B:173:LEU:HD23	1:B:174:LYS:HG2	1.84	0.59
2:F:4:ILE:HG12	2:F:54:LYS:HB2	1.86	0.58
1:B:162:LYS:HZ2	1:B:172:TYR:HE2	1.49	0.58
1:B:252:VAL:HG12	1:B:254:SER:H	1.67	0.58
1:A:334:LYS:HG3	1:A:335:SER:HA	1.87	0.56
1:A:162:LYS:HZ2	1:A:172:TYR:HE2	1.52	0.56
1:A:363:PRO:HG2	1:A:393:ILE:HD12	1.86	0.56
1:A:173:LEU:HD23	1:A:174:LYS:HG2	1.87	0.55
1:A:426:LEU:HD11	1:A:529:TYR:CZ	2.42	0.55
2:E:13:SER:O	2:E:17:GLN:HG2	2.07	0.54
1:B:426:LEU:HD11	1:B:529:TYR:CZ	2.43	0.54
2:F:100:GLU:HG3	2:F:104:ALA:HB3	1.90	0.54
1:B:471:ARG:CZ	1:B:496:LYS:HD3	2.38	0.54
1:A:471:ARG:CZ	1:A:496:LYS:HD3	2.38	0.53
1:B:363:PRO:HG2	1:B:393:ILE:HD12	1.88	0.53
1:A:128:LYS:O	1:A:132:THR:HG23	2.09	0.53
1:A:384:SER:OG	1:A:386:GLU:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:PRO:HB3	1:B:138:ILE:HD11	1.91	0.53
2:E:100:GLU:HG3	2:E:104:ALA:HB3	1.90	0.53
1:B:128:LYS:O	1:B:132:THR:HG23	2.10	0.52
1:A:359:ALA:O	1:A:362:VAL:HG13	2.09	0.52
1:A:132:THR:O	1:A:136:SER:HB3	2.09	0.52
2:F:13:SER:O	2:F:17:GLN:HG2	2.09	0.51
1:A:230:ALA:HB2	1:A:252:VAL:HG22	1.92	0.51
1:A:494:ARG:HD2	5:B:711:HOH:O	2.09	0.51
1:B:359:ALA:O	1:B:362:VAL:HG13	2.11	0.50
1:A:511:THR:O	1:A:514:GLU:HG2	2.12	0.50
2:F:57:VAL:HA	2:F:64:THR:HG21	1.93	0.49
1:B:384:SER:OG	1:B:386:GLU:HG3	2.13	0.49
1:B:334:LYS:CG	1:B:335:SER:HA	2.42	0.49
1:B:54:MET:HE1	1:B:145:TYR:CD1	2.48	0.49
1:A:95:PRO:HB3	1:A:138:ILE:HD11	1.95	0.49
1:B:511:THR:O	1:B:514:GLU:HG2	2.13	0.48
2:E:57:VAL:HA	2:E:64:THR:HG21	1.94	0.48
1:A:220:LYS:NZ	1:A:308:ASP:O	2.45	0.48
1:B:132:THR:O	1:B:136:SER:HB3	2.13	0.48
1:A:54:MET:HE1	1:A:145:TYR:CD1	2.49	0.48
1:B:72:TYR:H	3:B:600:FAD:C2A	2.27	0.48
2:E:36:ILE:HD12	2:E:90:ALA:HA	1.96	0.48
1:A:89:VAL:HG21	1:A:145:TYR:CE1	2.49	0.47
1:A:508:ILE:HD11	1:B:394:PRO:HB2	1.97	0.47
1:B:97:LYS:HE3	1:B:398:TYR:CE1	2.48	0.47
1:A:104:HIS:O	1:A:108:ILE:HG13	2.13	0.47
1:A:97:LYS:HE3	1:A:398:TYR:CE1	2.49	0.47
1:B:326:GLU:H	1:B:326:GLU:CD	2.21	0.47
1:B:172:TYR:HB3	1:B:176:ASP:O	2.15	0.46
1:A:93:CYS:HB3	3:A:601:FAD:C4	2.46	0.46
2:F:36:ILE:HD12	2:F:90:ALA:HA	1.97	0.46
1:B:220:LYS:NZ	1:B:308:ASP:O	2.48	0.46
1:A:334:LYS:HD2	1:A:334:LYS:HA	1.74	0.46
1:B:210:ILE:HB	1:B:214:ASP:HB2	1.98	0.46
1:A:253:ARG:C	1:A:254:SER:HG	2.24	0.46
1:A:172:TYR:HB3	1:A:176:ASP:O	2.15	0.46
1:A:210:ILE:HB	1:A:214:ASP:HB2	1.99	0.45
1:B:105:MET:HG2	1:B:109:PHE:CZ	2.51	0.45
1:A:193:GLY:HA2	1:A:357:ASP:HB2	1.97	0.45
1:B:89:VAL:HG21	1:B:145:TYR:CE1	2.51	0.45
1:B:230:ALA:HB1	1:B:256:VAL:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:LYS:HD2	1:B:96:LYS:C	2.41	0.45
1:B:193:GLY:HA2	1:B:357:ASP:HB2	1.98	0.45
1:B:533:GLY:HA2	1:B:536:GLY:C	2.42	0.45
1:B:54:MET:HE1	1:B:145:TYR:HD1	1.82	0.45
1:A:326:GLU:H	1:A:326:GLU:CD	2.24	0.44
1:A:334:LYS:CG	1:A:335:SER:HA	2.45	0.44
1:B:523:ILE:HD13	1:B:523:ILE:HA	1.88	0.44
1:A:105:MET:HG2	1:A:109:PHE:CZ	2.52	0.44
1:A:237:CYS:HA	1:A:240:PHE:CE2	2.52	0.44
1:B:509:HIS:HA	1:B:510:PRO:HA	1.82	0.44
1:A:475:PHE:CZ	1:A:489:MET:HG3	2.53	0.44
1:A:92:GLY:HA2	3:A:601:FAD:C7	2.48	0.44
1:A:139:ARG:HD2	1:A:139:ARG:HA	1.85	0.43
1:A:318:GLY:HA3	1:A:337:ASN:O	2.18	0.43
1:A:42:TYR:O	1:A:185:GLY:HA2	2.18	0.43
2:E:20:LEU:HD23	2:E:20:LEU:HA	1.86	0.43
1:A:394:PRO:HB2	1:B:508:ILE:HD11	2.00	0.43
1:A:285:PRO:HG2	1:A:312:TYR:OH	2.18	0.43
1:A:232:TYR:HB2	1:A:397:ILE:HG23	2.00	0.42
1:A:430:ASN:HB3	1:A:435:SER:HB3	2.00	0.42
1:B:536:GLY:HA2	2:E:71:SER:HA	2.01	0.42
1:B:237:CYS:HA	1:B:240:PHE:CE2	2.55	0.42
1:B:57:ALA:HB1	1:B:67:VAL:HG11	2.01	0.42
1:B:72:TYR:CD2	1:B:160:LEU:HD13	2.55	0.42
1:A:523:ILE:HD13	1:A:523:ILE:HA	1.91	0.42
1:A:57:ALA:HB1	1:A:67:VAL:HG11	2.01	0.42
1:A:535:CYS:SG	2:F:32:PRO:HD2	2.60	0.42
1:B:394:PRO:HB3	1:B:490:ALA:HB2	2.02	0.42
1:A:54:MET:HE1	1:A:145:TYR:HD1	1.84	0.41
1:B:268:VAL:O	1:B:272:MET:HG3	2.20	0.41
1:B:334:LYS:HA	1:B:334:LYS:HD2	1.71	0.41
1:A:330:MET:HE1	1:A:352:ILE:HG21	2.02	0.41
1:A:506:ILE:HD13	5:B:710:HOH:O	2.19	0.41
1:B:285:PRO:HG2	1:B:312:TYR:OH	2.19	0.41
2:E:23:VAL:HG11	2:E:78:TYR:HE2	1.85	0.41
1:B:160:LEU:HD12	1:B:160:LEU:HA	1.92	0.41
2:F:23:VAL:HG11	2:F:78:TYR:HE2	1.85	0.41
2:F:27:ALA:HB3	2:F:30:CYS:HB2	2.03	0.41
1:B:430:ASN:HB3	1:B:435:SER:HB3	2.01	0.41
1:A:394:PRO:HB3	1:A:490:ALA:HB2	2.03	0.41
2:F:20:LEU:HD11	2:F:102:TYR:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:HIS:O	1:B:108:ILE:HG13	2.20	0.40
1:A:86:GLY:HA2	3:A:601:FAD:O3B	2.21	0.40
1:A:49:GLY:HA3	1:A:71:ASP:HB2	2.03	0.40
1:B:317:LYS:HZ3	1:B:335:SER:HB2	1.86	0.40
1:B:364:GLU:O	3:B:600:FAD:H1'2	2.21	0.40
1:A:285:PRO:HB3	1:A:297:VAL:HG13	2.03	0.40
1:B:336:ASN:HB3	1:B:338:LYS:CG	2.51	0.40
2:E:27:ALA:HB3	2:E:30:CYS:HB2	2.04	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	479/541 (88%)	456 (95%)	23 (5%)	0	100	100
1	B	479/541 (88%)	458 (96%)	21 (4%)	0	100	100
2	E	101/114 (89%)	91 (90%)	10 (10%)	0	100	100
2	F	101/114 (89%)	91 (90%)	10 (10%)	0	100	100
All	All	1160/1310 (88%)	1096 (94%)	64 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	406/457 (89%)	381 (94%)	25 (6%)	16	34
1	B	406/457 (89%)	381 (94%)	25 (6%)	16	34
2	E	93/102 (91%)	87 (94%)	6 (6%)	15	32
2	F	93/102 (91%)	87 (94%)	6 (6%)	15	32
All	All	998/1118 (89%)	936 (94%)	62 (6%)	16	34

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	THR
1	A	45	VAL
1	A	46	VAL
1	A	89	VAL
1	A	93	CYS
1	A	136	SER
1	A	173	LEU
1	A	203	GLU
1	A	244	LEU
1	A	252	VAL
1	A	255	ILE
1	A	267	LYS
1	A	270	LEU
1	A	275	GLN
1	A	277	VAL
1	A	283	ILE
1	A	293	ASP
1	A	326	GLU
1	A	362	VAL
1	A	396	SER
1	A	399	THR
1	A	416	LEU
1	A	471	ARG
1	A	506	ILE
1	A	517	MET
1	B	39	THR
1	B	45	VAL
1	B	46	VAL
1	B	93	CYS
1	B	136	SER
1	B	173	LEU
1	B	198	ILE
1	B	203	GLU

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Mol	Chain	Res	Type
1	B	244	LEU
1	B	253	ARG
1	B	255	ILE
1	B	256	VAL
1	B	267	LYS
1	B	270	LEU
1	B	275	GLN
1	B	277	VAL
1	B	283	ILE
1	B	293	ASP
1	B	326	GLU
1	B	362	VAL
1	B	396	SER
1	B	399	THR
1	B	416	LEU
1	B	506	ILE
1	B	517	MET
2	E	2	VAL
2	E	8	GLN
2	E	18	ASN
2	E	41	GLU
2	E	48	THR
2	E	100	GLU
2	F	2	VAL
2	F	8	GLN
2	F	18	ASN
2	F	41	GLU
2	F	48	THR
2	F	100	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	HIS
1	A	242	ASN
1	A	331	ASN
1	A	333	ASN
1	B	63	HIS
1	B	158	ASN
1	B	242	ASN
1	B	331	ASN
1	B	333	ASN

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Mol	Chain	Res	Type
2	E	8	GLN
2	E	18	ASN
2	F	8	GLN
2	F	18	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	FAD	A	601	-	58,58,58	2.07	12 (20%)	85,89,89	1.87	21 (24%)
4	GOL	A	602	-	5,5,5	0.40	0	5,5,5	0.52	0
3	FAD	B	600	-	58,58,58	2.10	11 (18%)	85,89,89	1.91	21 (24%)

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	FAD	A	601	-	-	4/34/50/50	0/6/6/6
4	GOL	A	602	-	-	2/4/4/4	-
3	FAD	B	600	-	-	9/34/50/50	0/6/6/6

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	600	FAD	O2-C2	8.11	1.40	1.24
3	A	601	FAD	O4-C4	8.06	1.38	1.23
3	B	600	FAD	O4-C4	8.06	1.38	1.23
3	A	601	FAD	O2-C2	7.70	1.39	1.24
3	B	600	FAD	C2B-C3B	-5.59	1.38	1.53
3	A	601	FAD	C2B-C3B	-5.30	1.39	1.53
3	B	600	FAD	C6A-N6A	3.75	1.43	1.34
3	A	601	FAD	O4B-C4B	-2.76	1.38	1.45
3	B	600	FAD	O4B-C4B	-2.75	1.38	1.45
3	A	601	FAD	C6A-N6A	2.75	1.41	1.34
3	A	601	FAD	C3B-C4B	-2.55	1.46	1.53
3	A	601	FAD	C5X-N5	-2.53	1.34	1.39
3	A	601	FAD	C2-N3	-2.53	1.33	1.39
3	A	601	FAD	C4-N3	-2.42	1.34	1.38
3	B	600	FAD	C2-N3	-2.41	1.33	1.39
3	B	600	FAD	O4'-C4'	-2.34	1.38	1.43
3	A	601	FAD	C9A-N10	-2.25	1.37	1.41
3	B	600	FAD	C5X-N5	-2.21	1.35	1.39
3	B	600	FAD	C4-N3	-2.19	1.34	1.38
3	A	601	FAD	O3'-C3'	-2.17	1.37	1.43
3	A	601	FAD	O4'-C4'	-2.14	1.38	1.43
3	B	600	FAD	C3B-C4B	-2.03	1.47	1.53
3	B	600	FAD	O3'-C3'	-2.03	1.37	1.43

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	FAD	C5A-C4A-N3A	-5.61	118.99	126.72
3	B	600	FAD	C5A-C4A-N3A	-5.53	119.11	126.72
3	B	600	FAD	N3A-C4A-N9A	4.94	135.57	127.17
3	A	601	FAD	N3A-C2A-N1A	-4.53	121.72	128.58
3	A	601	FAD	N3A-C4A-N9A	4.53	134.86	127.17
3	B	600	FAD	N9A-C8A-N7A	-4.31	107.82	113.94
3	B	600	FAD	C4A-N9A-C8A	4.17	110.11	105.74
3	B	600	FAD	N3A-C2A-N1A	-4.11	122.36	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	FAD	C2A-N3A-C4A	3.93	121.43	111.83
3	B	600	FAD	C5A-N7A-C8A	3.92	109.61	103.45
3	A	601	FAD	N9A-C8A-N7A	-3.74	108.64	113.94
3	A	601	FAD	C4-N3-C2	-3.62	119.21	125.64
3	B	600	FAD	C2A-N3A-C4A	3.47	120.31	111.83
3	B	600	FAD	C4-N3-C2	-3.44	119.53	125.64
3	A	601	FAD	C4A-N9A-C1B	-3.42	118.64	126.63
3	A	601	FAD	C2B-C1B-N9A	3.39	121.72	113.30
3	B	600	FAD	C4X-C10-N1	-3.26	116.60	124.59
3	A	601	FAD	C4A-N9A-C8A	3.25	109.15	105.74
3	A	601	FAD	C5A-N7A-C8A	3.23	108.52	103.45
3	B	600	FAD	C2B-C1B-N9A	3.20	121.26	113.30
3	B	600	FAD	O5'-C5'-C4'	3.10	117.64	109.36
3	A	601	FAD	C4X-C4-N3	3.10	121.14	113.25
3	A	601	FAD	C2B-C3B-C4B	3.06	108.53	102.61
3	B	600	FAD	C4A-C5A-N7A	-3.03	107.12	110.58
3	B	600	FAD	C4X-C4-N3	3.02	120.94	113.25
3	B	600	FAD	O4-C4-C4X	-3.01	118.58	126.53
3	B	600	FAD	C4X-C10-N10	2.79	120.48	116.48
3	B	600	FAD	C10-N1-C2	2.77	122.85	116.85
3	A	601	FAD	O4-C4-C4X	-2.76	119.23	126.53
3	A	601	FAD	C4X-C10-N1	-2.74	117.87	124.59
3	B	600	FAD	C4A-N9A-C1B	-2.72	120.26	126.63
3	B	600	FAD	C1'-C2'-C3'	2.72	117.04	109.66
3	A	601	FAD	C4A-C5A-N7A	-2.66	107.55	110.58
3	B	600	FAD	O4B-C1B-C2B	-2.61	101.03	106.62
3	A	601	FAD	C5X-C9A-N10	2.49	120.22	117.97
3	A	601	FAD	C4X-C10-N10	2.33	119.81	116.48
3	A	601	FAD	C9A-C5X-N5	-2.26	120.05	122.45
3	A	601	FAD	C1B-N9A-C8A	2.25	132.09	127.09
3	A	601	FAD	C10-N1-C2	2.18	121.58	116.85
3	B	600	FAD	C9-C9A-C5X	-2.10	116.31	120.03
3	B	600	FAD	C1'-N10-C9A	2.03	124.57	120.63
3	A	601	FAD	C3B-C2B-C1B	2.01	105.26	101.46

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	FAD	PA-O3P-P-O5'
3	B	600	FAD	C5B-O5B-PA-O1A
3	B	600	FAD	C3'-C4'-C5'-O5'

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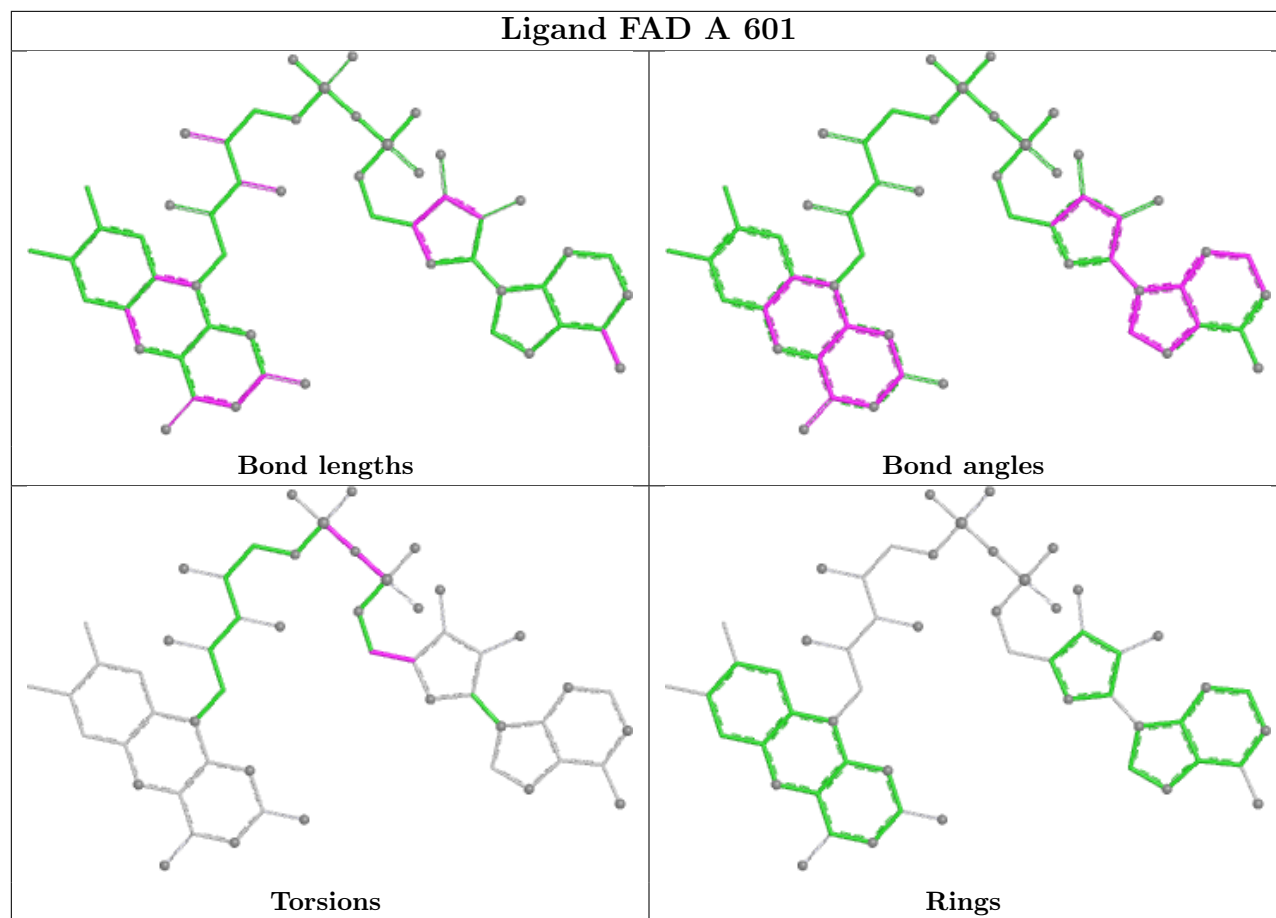
Mol	Chain	Res	Type	Atoms
3	B	600	FAD	O4'-C4'-C5'-O5'
3	B	600	FAD	C5'-O5'-P-O1P
3	B	600	FAD	C5'-O5'-P-O2P
3	B	600	FAD	C5'-O5'-P-O3P
4	A	602	GOL	O1-C1-C2-C3
4	A	602	GOL	O1-C1-C2-O2
3	A	601	FAD	C3B-C4B-C5B-O5B
3	A	601	FAD	O4B-C4B-C5B-O5B
3	B	600	FAD	PA-O3P-P-O5'
3	A	601	FAD	P-O3P-PA-O1A
3	B	600	FAD	O3'-C3'-C4'-C5'
3	B	600	FAD	O3'-C3'-C4'-O4'

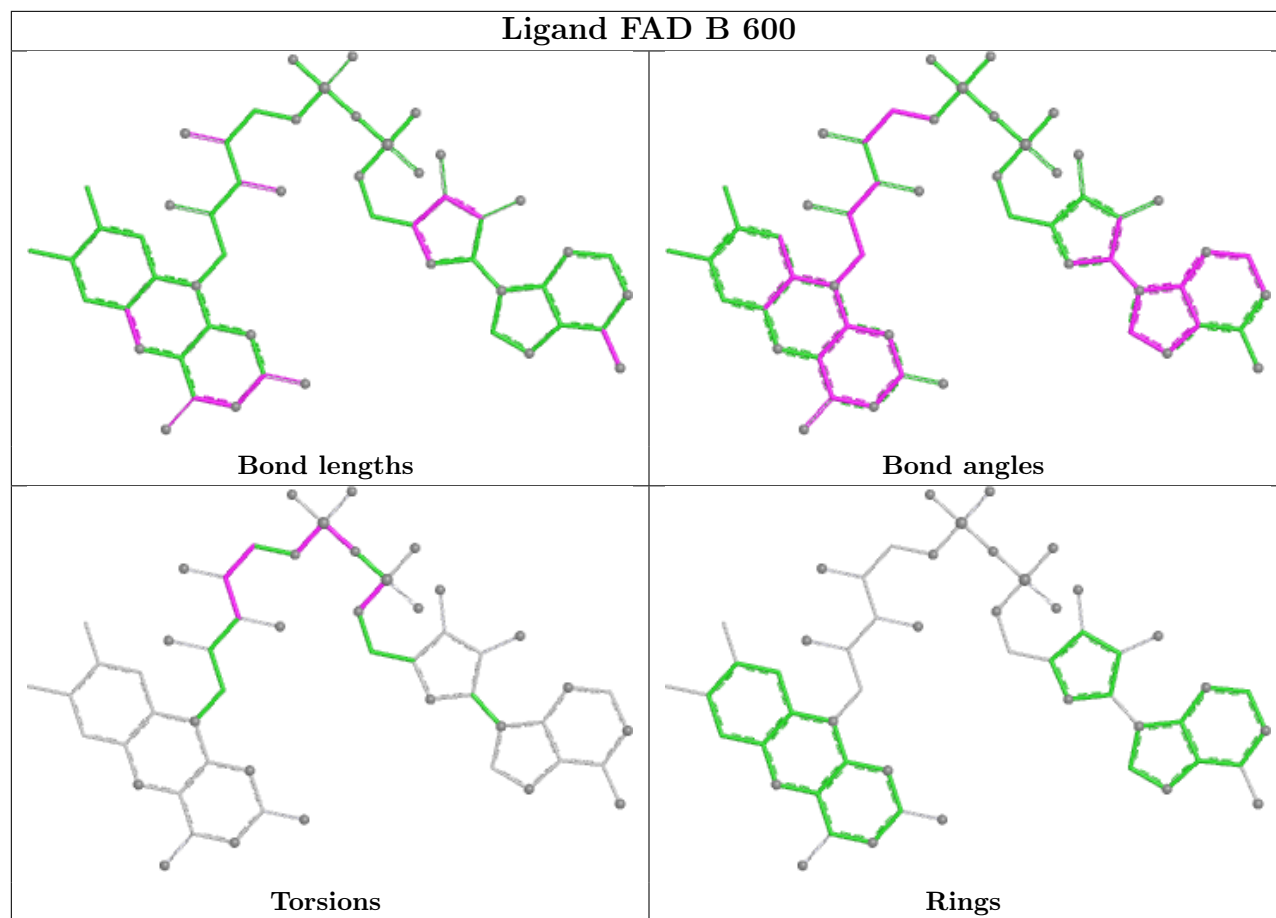
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	FAD	3	0
3	B	600	FAD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	483/541 (89%)	-0.28	4 (0%) 82 80	23, 38, 62, 89	0
1	B	483/541 (89%)	-0.35	4 (0%) 82 80	21, 37, 58, 89	0
2	E	103/114 (90%)	0.84	7 (6%) 23 20	53, 83, 100, 105	0
2	F	103/114 (90%)	1.01	14 (13%) 7 5	57, 93, 115, 124	0
All	All	1172/1310 (89%)	-0.09	29 (2%) 58 54	21, 40, 97, 124	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	27	ALA	3.3
2	F	78	TYR	3.1
2	E	98	LEU	3.1
1	A	254	SER	2.9
2	F	9	ALA	2.8
2	F	82	SER	2.7
2	F	81	GLY	2.6
1	B	175	GLY	2.5
1	A	535	CYS	2.5
2	F	21	VAL	2.5
1	A	536	GLY	2.4
2	F	14	ILE	2.4
1	A	177	LEU	2.3
1	B	255	ILE	2.3
2	E	51	VAL	2.3
2	E	99	ILE	2.3
2	F	51	VAL	2.3
2	F	104	ALA	2.2
2	E	5	VAL	2.2
2	E	21	VAL	2.2
1	B	457	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	20	LEU	2.2
2	F	15	ILE	2.2
1	B	176	ASP	2.2
2	F	79	LYS	2.2
2	E	103	ALA	2.1
2	F	102	TYR	2.1
2	F	49	LYS	2.1
2	F	52	PHE	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](#)

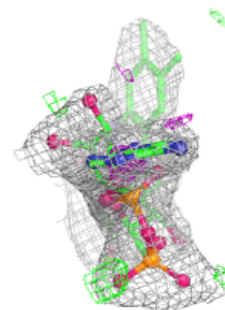
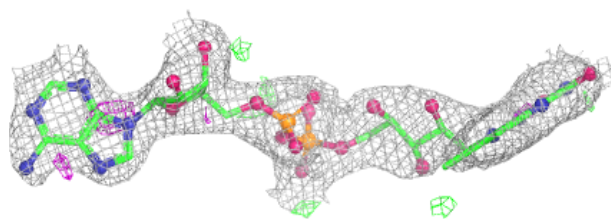
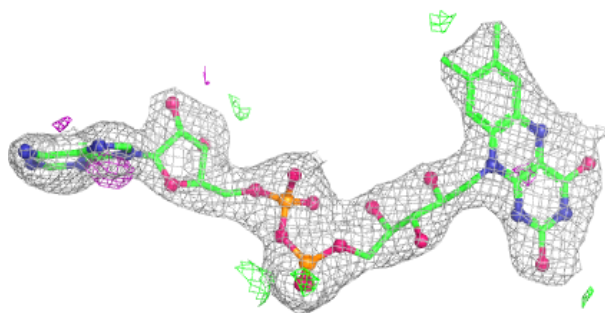
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	GOL	A	602	6/6	0.78	0.13	52,58,63,64	0
3	FAD	B	600	53/53	0.95	0.07	29,37,43,43	0
3	FAD	A	601	53/53	0.96	0.06	29,37,41,43	0

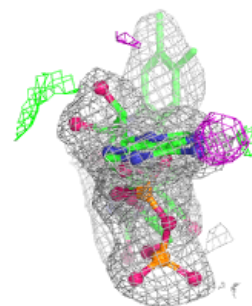
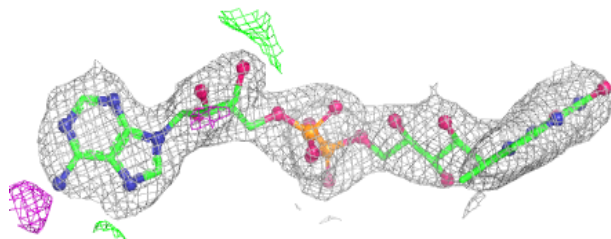
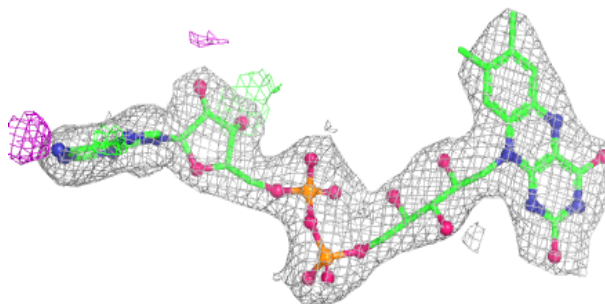
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD B 600:

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

**Electron density around FAD A 601:**

$2mF_o-DF_c$ (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.