



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2026 – 11:51 PM UTC

PDB ID : 5J60 / pdb_00005j60
Title : Structure of a thioredoxin reductase from *Gloeobacter violaceus*
Authors : Buey, R.M.; de Pereda, J.M.; Balsera, M.
Deposited on : 2016-04-04
Resolution : 1.90 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

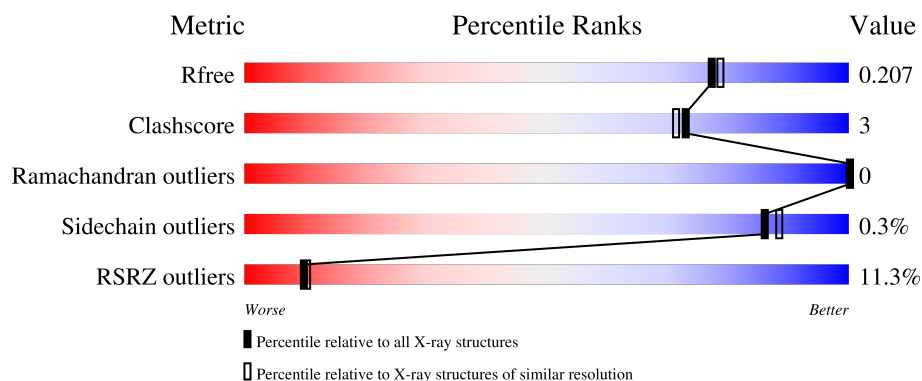
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	320	6% 94% 5%
1	B	320	5% 94% 5%
1	C	320	19% 84% 8% 8%
1	D	320	14% 88% 5% 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18562 atoms, of which 8740 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.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	316	Total	C	H	N	O	S	0	0	0
			4577	1484	2247	398	436	12			
1	B	316	Total	C	H	N	O	S	0	0	0
			4587	1489	2252	397	437	12			
1	C	296	Total	C	H	N	O	S	0	0	0
			4208	1370	2062	371	393	12			
1	D	297	Total	C	H	N	O	S	0	0	0
			4159	1368	2021	365	393	12			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q7NMP6
A	-1	SER	-	expression tag	UNP Q7NMP6
A	0	HIS	-	expression tag	UNP Q7NMP6
B	-2	GLY	-	expression tag	UNP Q7NMP6
B	-1	SER	-	expression tag	UNP Q7NMP6
B	0	HIS	-	expression tag	UNP Q7NMP6
C	-2	GLY	-	expression tag	UNP Q7NMP6
C	-1	SER	-	expression tag	UNP Q7NMP6
C	0	HIS	-	expression tag	UNP Q7NMP6
D	-2	GLY	-	expression tag	UNP Q7NMP6
D	-1	SER	-	expression tag	UNP Q7NMP6
D	0	HIS	-	expression tag	UNP Q7NMP6

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			83	27	30	9	15	2		
2	B	1	Total	C	H	N	O	P	0	0
			83	27	30	9	15	2		
2	C	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		
2	D	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			31	8	18	5		
4	B	1	Total	C	H	O	0	0
			31	8	18	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	198	Total	O	0	0
			198	198		
5	B	206	Total	O	0	0
			206	206		
5	C	107	Total	O	0	0
			107	107		
5	D	122	Total	O	0	0
			122	122		

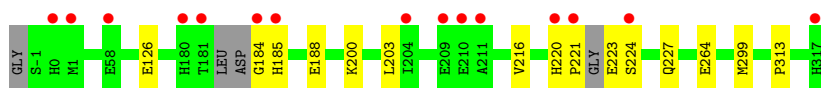
3 Residue-property plots [i](#)

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.

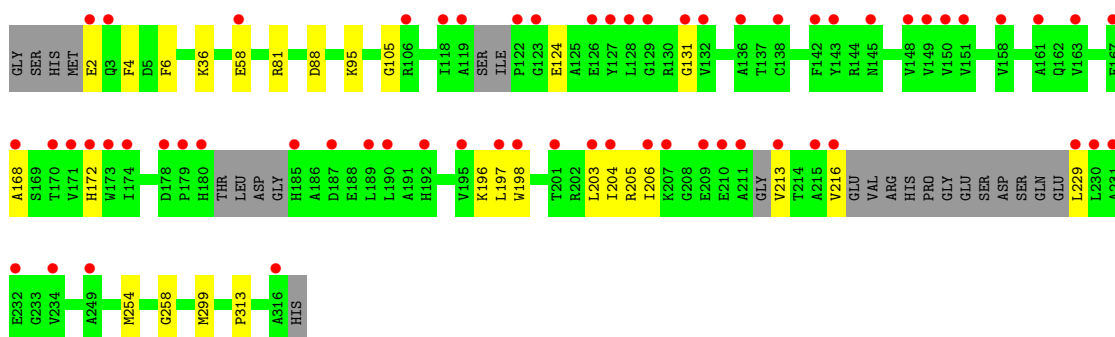
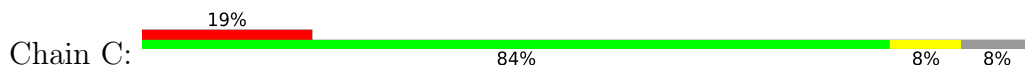
- Molecule 1: Thioredoxin reductase



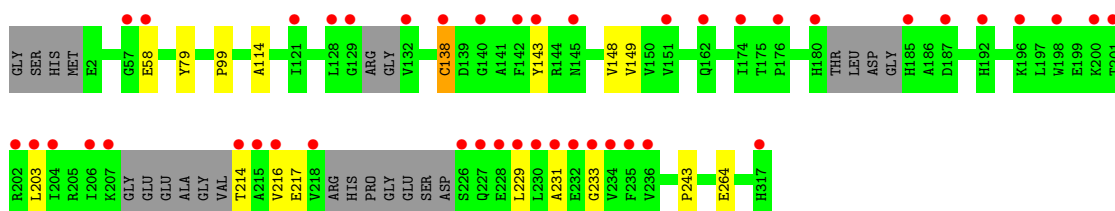
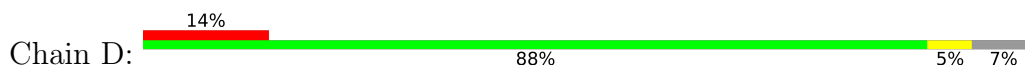
- Molecule 1: Thioredoxin reductase



- Molecule 1: Thioredoxin reductase



- Molecule 1: Thioredoxin reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.28Å 122.04Å 139.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.22 – 1.90 49.22 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.22-1.90) 100.0 (49.22-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 1.90Å)	Xtriage
Refinement program	PHENIX (dev_2341: ???)	Depositor
R, R_{free}	0.177 , 0.202 0.183 , 0.207	Depositor DCC
R_{free} test set	5599 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	18562	wwPDB-VP
Average B, all atoms (Å ²)	51.0	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 21.87 % 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 6.4061e-03. 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: CA, PG4, 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	0.37	0/2380	0.54	1/3243 (0.0%)
1	B	0.38	0/2386	0.52	0/3251
1	C	0.33	0/2190	0.53	0/2983
1	D	0.34	0/2183	0.52	1/2979 (0.0%)
All	All	0.36	0/9139	0.53	2/12456 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	310	ALA	N-CA-C	5.47	118.00	109.52
1	D	138	CYS	N-CA-C	5.34	117.18	111.36

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	2330	2247	2244	12	0
1	B	2335	2252	2251	10	0
1	C	2146	2062	2062	22	0
1	D	2138	2021	2016	15	0
2	A	53	30	31	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	53	30	31	0	0
2	C	53	31	31	0	0
2	D	53	31	31	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	13	18	17	1	0
4	B	13	18	17	1	0
5	A	198	0	0	6	0
5	B	206	0	0	1	1
5	C	107	0	0	3	0
5	D	122	0	0	0	0
All	All	9822	8740	8731	58	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (58) 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:C:168:ALA:O	5:C:601:HOH:O	1.76	1.03
4:A:403:PG4:O5	1:D:264:GLU:OE2	1.84	0.96
1:A:251:GLN:NE2	5:A:501:HOH:O	2.08	0.84
1:D:99:PRO:HG3	1:D:138:CYS:SG	2.21	0.81
1:D:203:LEU:HD13	1:D:216:VAL:HG13	1.70	0.73
1:A:245:THR:HG21	1:A:254:MET:HE1	1.71	0.71
1:A:205:ARG:HD2	5:A:650:HOH:O	1.92	0.68
1:B:220:HIS:NE2	1:B:227:GLN:OE1	2.27	0.67
1:D:216:VAL:N	1:D:229:LEU:O	2.25	0.67
1:C:6:PHE:O	1:C:105:GLY:HA2	1.99	0.62
1:B:184:GLY:HA2	1:B:185:HIS:C	2.25	0.62
1:D:214:THR:HA	1:D:231:ALA:O	2.02	0.59
1:D:216:VAL:O	1:D:229:LEU:N	2.29	0.58
1:C:124:GLU:HA	1:C:206:ILE:HD12	1.86	0.58
1:A:254:MET:CE	5:A:506:HOH:O	2.52	0.58
1:C:36:LYS:NZ	5:C:605:HOH:O	2.37	0.56
1:D:149:VAL:HG23	1:D:231:ALA:CB	2.37	0.54
1:D:143:TYR:CD2	1:D:148:VAL:HG12	2.44	0.53
1:C:58:GLU:HA	5:C:638:HOH:O	2.08	0.52
1:A:302:ASP:CG	1:A:308:ARG:HH22	2.15	0.52
1:C:196:LYS:HZ3	1:C:198:TRP:CB	2.23	0.51
1:C:196:LYS:NZ	1:C:198:TRP:CB	2.74	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:MET:HE3	5:A:506:HOH:O	2.11	0.51
1:C:254:MET:CE	1:C:258:GLY:O	2.59	0.49
1:D:143:TYR:CE2	1:D:233:GLY:HA3	2.47	0.49
1:A:302:ASP:OD2	1:A:308:ARG:NH2	2.27	0.49
1:C:131:GLY:HA3	1:C:213:VAL:HG23	1.94	0.48
1:B:220:HIS:HB2	1:B:221:PRO:HD2	1.94	0.48
1:C:172:HIS:CE1	1:C:229:LEU:HD21	2.49	0.46
1:D:203:LEU:HD13	1:D:216:VAL:CG1	2.42	0.45
1:C:2:GLU:O	1:C:4:PHE:CE1	2.70	0.45
1:C:203:LEU:HD12	1:C:203:LEU:C	2.43	0.44
1:C:299:MET:HE3	1:C:313:PRO:HA	1.99	0.44
1:D:143:TYR:HB3	1:D:148:VAL:CG1	2.48	0.44
1:B:223:GLU:O	1:B:224:SER:CB	2.66	0.43
1:C:203:LEU:HD12	1:C:204:ILE:N	2.33	0.43
1:D:114:ALA:HA	1:D:243:PRO:HA	2.00	0.43
1:C:203:LEU:HD11	1:C:205:ARG:O	2.19	0.43
1:A:203:LEU:HD11	1:A:216:VAL:HB	2.00	0.43
1:B:299:MET:HE3	1:B:313:PRO:HA	2.01	0.42
1:C:36:LYS:O	1:C:81:ARG:HD2	2.18	0.42
1:A:299:MET:HE3	1:A:313:PRO:HA	2.00	0.42
1:C:131:GLY:HA3	1:C:213:VAL:CG2	2.49	0.42
1:A:309:LYS:HB2	5:A:505:HOH:O	2.20	0.42
1:A:50:ALA:HA	5:A:503:HOH:O	2.19	0.42
1:C:88:ASP:HB3	1:C:95:LYS:HB2	2.02	0.42
1:B:126:GLU:HB2	5:B:612:HOH:O	2.19	0.42
1:B:203:LEU:CD1	1:B:216:VAL:HB	2.50	0.41
1:B:188:GLU:HG2	1:D:79:TYR:HB3	2.02	0.41
1:D:203:LEU:CD1	1:D:216:VAL:HG13	2.46	0.41
1:A:245:THR:CG2	1:A:254:MET:HE1	2.46	0.41
1:B:264:GLU:HA	4:B:501:PG4:H31	2.02	0.41
1:C:197:LEU:HD12	1:C:198:TRP:N	2.36	0.41
1:C:172:HIS:NE2	1:C:229:LEU:HD21	2.36	0.41
1:C:203:LEU:HD11	1:C:216:VAL:HB	2.02	0.40
1:B:200:LYS:O	1:B:221:PRO:HD3	2.21	0.40
1:D:216:VAL:HG12	1:D:217:GLU:N	2.36	0.40
1:C:206:ILE:HA	1:C:216:VAL:HG12	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:683:HOH:O	5:B:702:HOH:O[3_555]	2.10	0.10

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	310/320 (97%)	301 (97%)	9 (3%)	0	100	100
1	B	310/320 (97%)	300 (97%)	10 (3%)	0	100	100
1	C	286/320 (89%)	276 (96%)	10 (4%)	0	100	100
1	D	287/320 (90%)	279 (97%)	8 (3%)	0	100	100
All	All	1193/1280 (93%)	1156 (97%)	37 (3%)	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	228/252 (90%)	226 (99%)	2 (1%)	70	73
1	B	229/252 (91%)	229 (100%)	0	100	100
1	C	205/252 (81%)	205 (100%)	0	100	100
1	D	199/252 (79%)	198 (100%)	1 (0%)	81	84
All	All	861/1008 (85%)	858 (100%)	3 (0%)	86	88

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	ARG
1	A	145	ASN
1	D	58	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	251	GLN
1	C	306	ASN
1	D	180	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](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FAD	B	500	-	58,58,58	1.53	10 (17%)	85,89,89	1.39	11 (12%)
4	PG4	A	403	3	12,12,12	0.52	0	11,11,11	0.31	0
4	PG4	B	501	3	12,12,12	0.49	0	11,11,11	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	C	500	-	58,58,58	1.71	15 (25%)	85,89,89	1.39	10 (11%)
2	FAD	D	401	-	58,58,58	1.80	13 (22%)	85,89,89	1.34	9 (10%)
2	FAD	A	401	-	58,58,58	1.53	6 (10%)	85,89,89	1.24	9 (10%)

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	-	-	1/34/50/50	0/6/6/6
4	PG4	A	403	3	-	5/10/10/10	-
4	PG4	B	501	3	-	3/10/10/10	-
2	FAD	C	500	-	-	2/34/50/50	0/6/6/6
2	FAD	D	401	-	-	3/34/50/50	0/6/6/6
2	FAD	A	401	-	-	1/34/50/50	0/6/6/6

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	FAD	C1'-C2'	-7.43	1.42	1.52
2	A	401	FAD	C1'-C2'	-6.10	1.44	1.52
2	B	500	FAD	C1'-C2'	-5.87	1.44	1.52
2	C	500	FAD	C1'-C2'	-5.42	1.45	1.52
2	D	401	FAD	PA-O3P	3.60	1.63	1.59
2	C	500	FAD	P-O3P	-3.56	1.55	1.59
2	C	500	FAD	PA-O3P	3.55	1.63	1.59
2	A	401	FAD	C8A-N9A	3.39	1.43	1.37
2	C	500	FAD	C4-N3	3.30	1.45	1.38
2	C	500	FAD	PA-O1A	3.21	1.61	1.50
2	A	401	FAD	O2-C2	-2.96	1.18	1.24
2	C	500	FAD	O2-C2	-2.93	1.18	1.24
2	D	401	FAD	P-O1P	2.90	1.60	1.50
2	C	500	FAD	C6-C5X	2.90	1.44	1.40
2	D	401	FAD	C6-C5X	2.88	1.44	1.40
2	B	500	FAD	C6-C5X	2.65	1.44	1.40
2	C	500	FAD	C5A-C4A	2.64	1.43	1.39
2	D	401	FAD	C8A-N9A	2.60	1.42	1.37
2	D	401	FAD	PA-O1A	2.57	1.59	1.50
2	A	401	FAD	C3B-C4B	2.50	1.59	1.53
2	C	500	FAD	P-O1P	2.47	1.59	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	FAD	O4'-C4'	-2.46	1.38	1.43
2	D	401	FAD	O2-C2	-2.43	1.19	1.24
2	C	500	FAD	C2-N1	2.42	1.42	1.36
2	D	401	FAD	C3B-C4B	2.39	1.59	1.53
2	D	401	FAD	C5'-C4'	-2.38	1.48	1.51
2	C	500	FAD	C8A-N9A	2.38	1.41	1.37
2	B	500	FAD	C2-N3	2.28	1.44	1.39
2	B	500	FAD	O2-C2	-2.28	1.19	1.24
2	D	401	FAD	O5'-C5'	-2.23	1.36	1.44
2	D	401	FAD	C2-N1	2.23	1.41	1.36
2	B	500	FAD	O4-C4	-2.23	1.19	1.23
2	B	500	FAD	C1B-N9A	-2.22	1.40	1.46
2	C	500	FAD	O4-C4	-2.22	1.19	1.23
2	B	500	FAD	C2B-C3B	2.21	1.59	1.53
2	D	401	FAD	O4-C4	-2.20	1.19	1.23
2	C	500	FAD	C3B-C4B	2.16	1.58	1.53
2	C	500	FAD	PA-O2A	-2.16	1.45	1.55
2	D	401	FAD	C4-N3	2.16	1.42	1.38
2	B	500	FAD	C4'-C3'	-2.10	1.49	1.53
2	B	500	FAD	P-O1P	2.09	1.58	1.50
2	A	401	FAD	C2-N1	2.05	1.41	1.36
2	A	401	FAD	O4-C4	-2.01	1.19	1.23
2	C	500	FAD	C7M-C7	2.01	1.54	1.51

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	FAD	O3P-P-O1P	-5.24	94.93	110.70
2	D	401	FAD	O3P-P-O1P	-5.18	95.12	110.70
2	C	500	FAD	O3P-P-O1P	-4.87	96.06	110.70
2	C	500	FAD	O3P-PA-O1A	-4.43	97.37	110.70
2	D	401	FAD	O3P-PA-O1A	-3.88	99.02	110.70
2	C	500	FAD	C9A-C9-C8	3.73	126.72	119.22
2	A	401	FAD	O3P-P-O1P	-3.68	99.65	110.70
2	A	401	FAD	C9A-C9-C8	3.52	126.30	119.22
2	B	500	FAD	O3P-PA-O1A	-3.52	100.12	110.70
2	B	500	FAD	C9A-C9-C8	3.46	126.18	119.22
2	D	401	FAD	C9A-C9-C8	3.35	125.95	119.22
2	B	500	FAD	C9-C9A-N10	3.19	126.14	121.85
2	A	401	FAD	O3P-PA-O1A	-2.97	101.78	110.70
2	C	500	FAD	O2A-PA-O3P	2.92	115.16	107.27
2	C	500	FAD	O2P-P-O3P	2.89	115.08	107.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	FAD	C9-C9A-N10	2.86	125.69	121.85
2	D	401	FAD	C9-C9A-N10	2.74	125.53	121.85
2	D	401	FAD	C10-N1-C2	2.70	122.70	116.85
2	C	500	FAD	C9-C9A-N10	2.62	125.38	121.85
2	B	500	FAD	N3-C2-N1	-2.60	113.97	119.50
2	B	500	FAD	C10-N1-C2	2.57	122.41	116.85
2	B	500	FAD	O2P-P-O3P	2.57	114.21	107.27
2	C	500	FAD	C10-N1-C2	2.47	122.19	116.85
2	B	500	FAD	C4'-C3'-C2'	-2.46	109.47	113.57
2	D	401	FAD	O2P-P-O3P	2.45	113.90	107.27
2	B	500	FAD	C5X-C6-C7	2.39	125.26	120.83
2	D	401	FAD	N3-C2-N1	-2.38	114.45	119.50
2	A	401	FAD	O2A-PA-O1A	2.21	122.74	112.44
2	A	401	FAD	O2A-PA-O3P	2.18	113.16	107.27
2	A	401	FAD	C5X-C6-C7	2.17	124.84	120.83
2	C	500	FAD	C4'-C3'-C2'	-2.14	110.00	113.57
2	C	500	FAD	O4'-C4'-C3'	-2.14	104.25	109.25
2	C	500	FAD	C5X-C6-C7	2.13	124.78	120.83
2	B	500	FAD	C6-C5X-N5	2.07	121.88	118.44
2	A	401	FAD	C4'-C3'-C2'	-2.06	110.14	113.57
2	A	401	FAD	O4'-C4'-C3'	-2.03	104.49	109.25
2	B	500	FAD	C9-C9A-C5X	-2.02	116.45	120.03
2	D	401	FAD	C4'-C3'-C2'	-2.01	110.22	113.57
2	D	401	FAD	O2A-PA-O3P	2.01	112.71	107.27

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	FAD	PA-O3P-P-O5'
2	B	500	FAD	PA-O3P-P-O5'
4	A	403	PG4	O1-C1-C2-O2
4	A	403	PG4	O3-C5-C6-O4
2	C	500	FAD	PA-O3P-P-O5'
2	D	401	FAD	PA-O3P-P-O5'
4	B	501	PG4	O1-C1-C2-O2
4	A	403	PG4	C6-C5-O3-C4
2	C	500	FAD	P-O3P-PA-O1A
4	B	501	PG4	C1-C2-O2-C3
4	B	501	PG4	C3-C4-O3-C5
2	D	401	FAD	O4B-C4B-C5B-O5B
4	A	403	PG4	C5-C6-O4-C7

Continued on next page...

Continued from previous page...

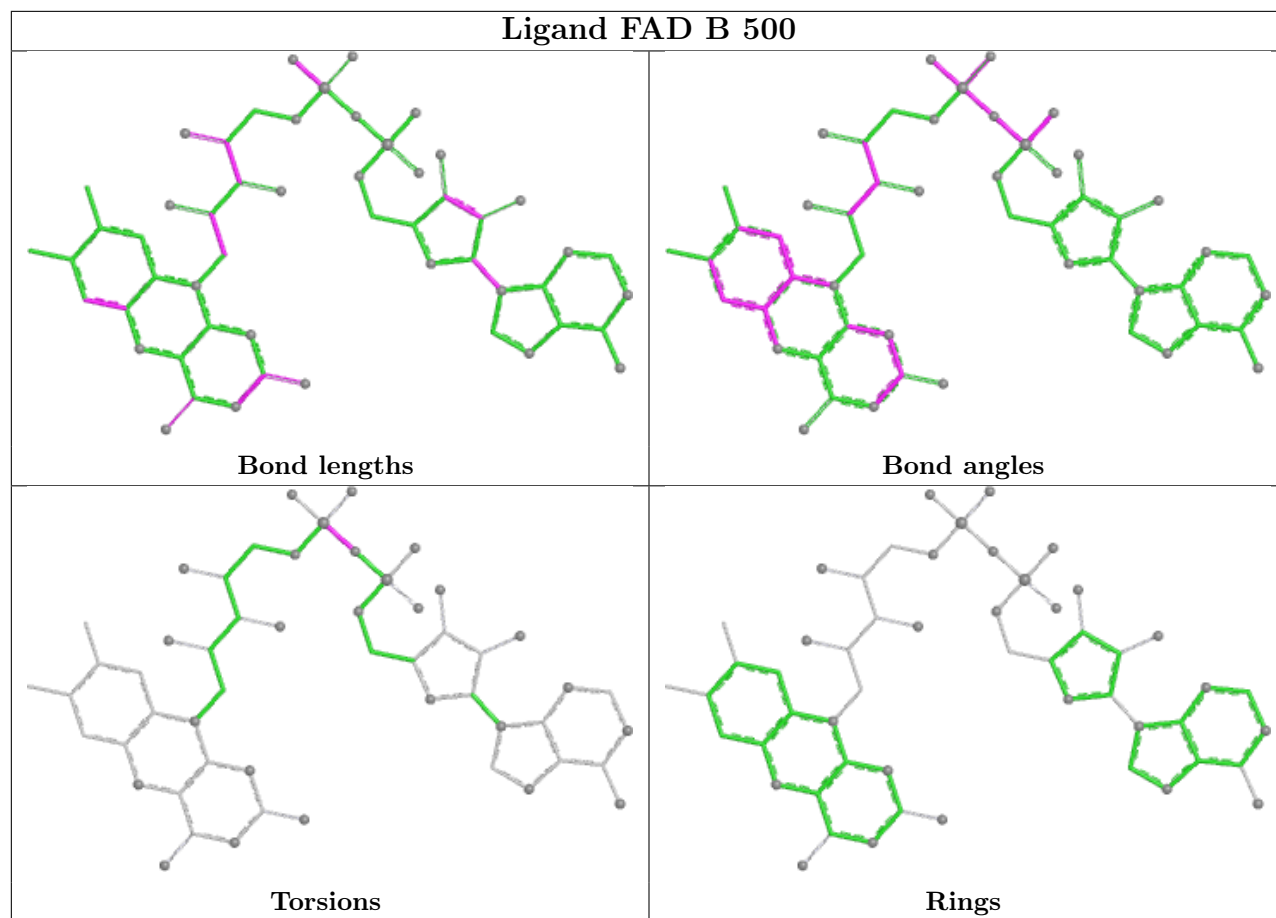
Mol	Chain	Res	Type	Atoms
4	A	403	PG4	O4-C7-C8-O5
2	D	401	FAD	P-O3P-PA-O2A

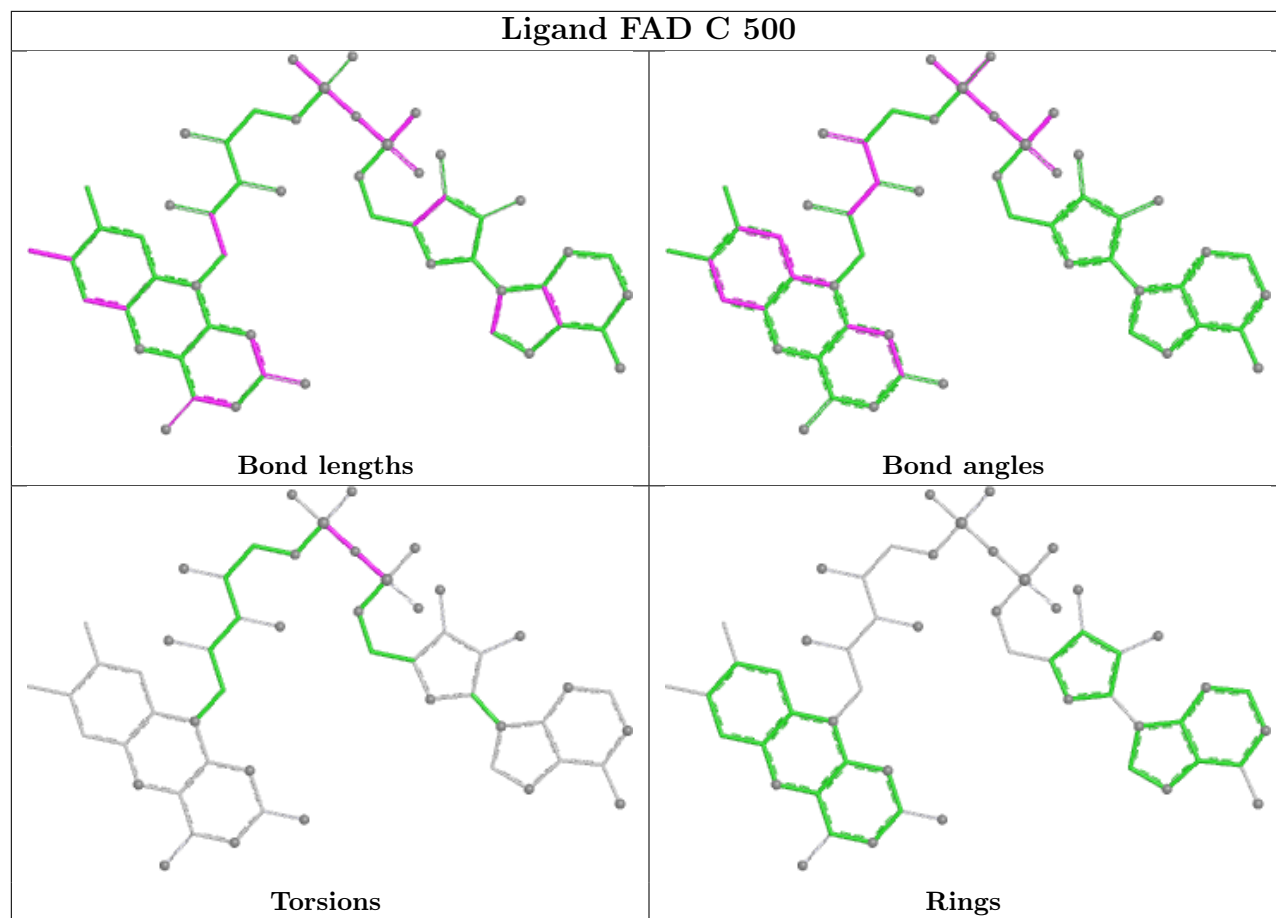
There are no ring outliers.

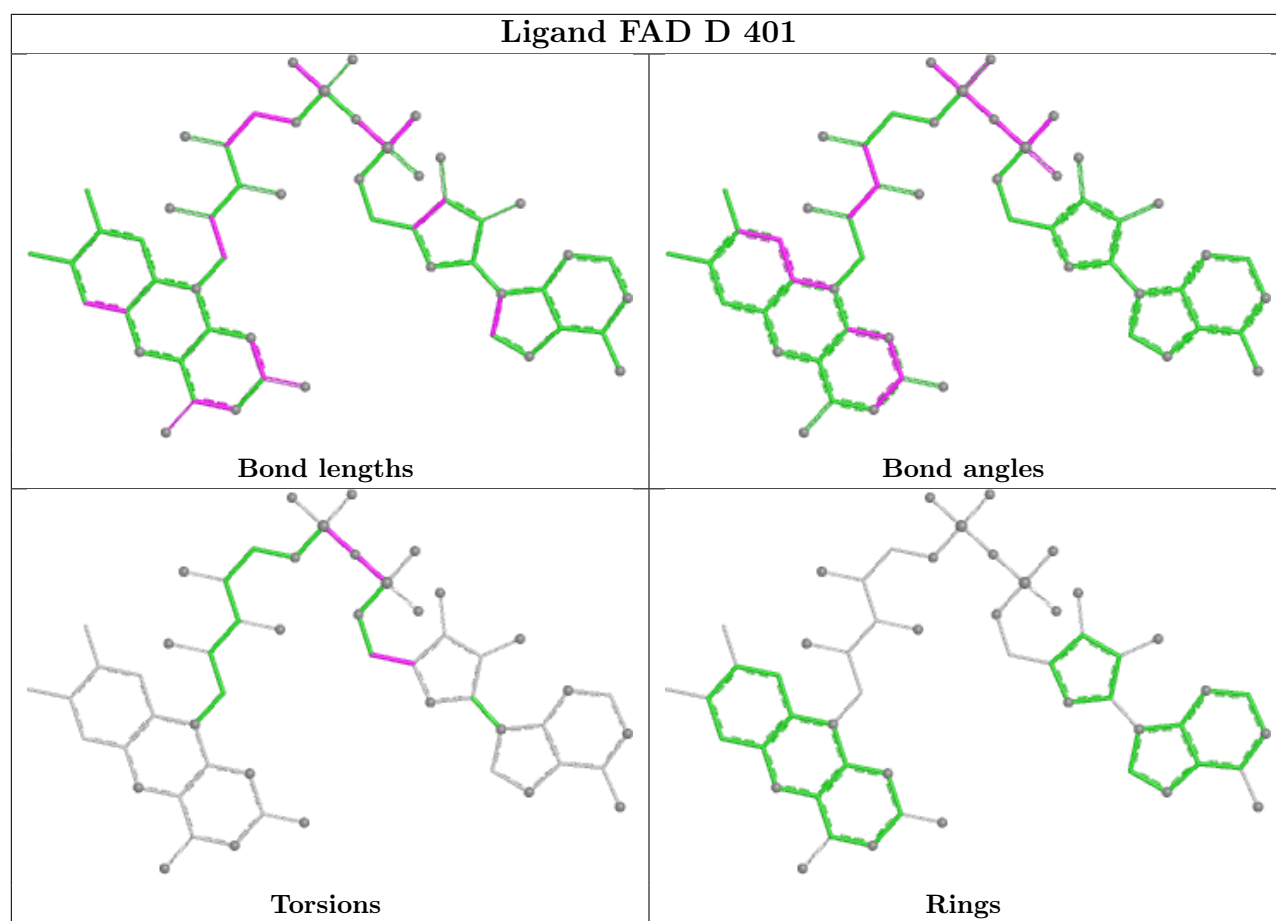
2 monomers are involved in 2 short contacts:

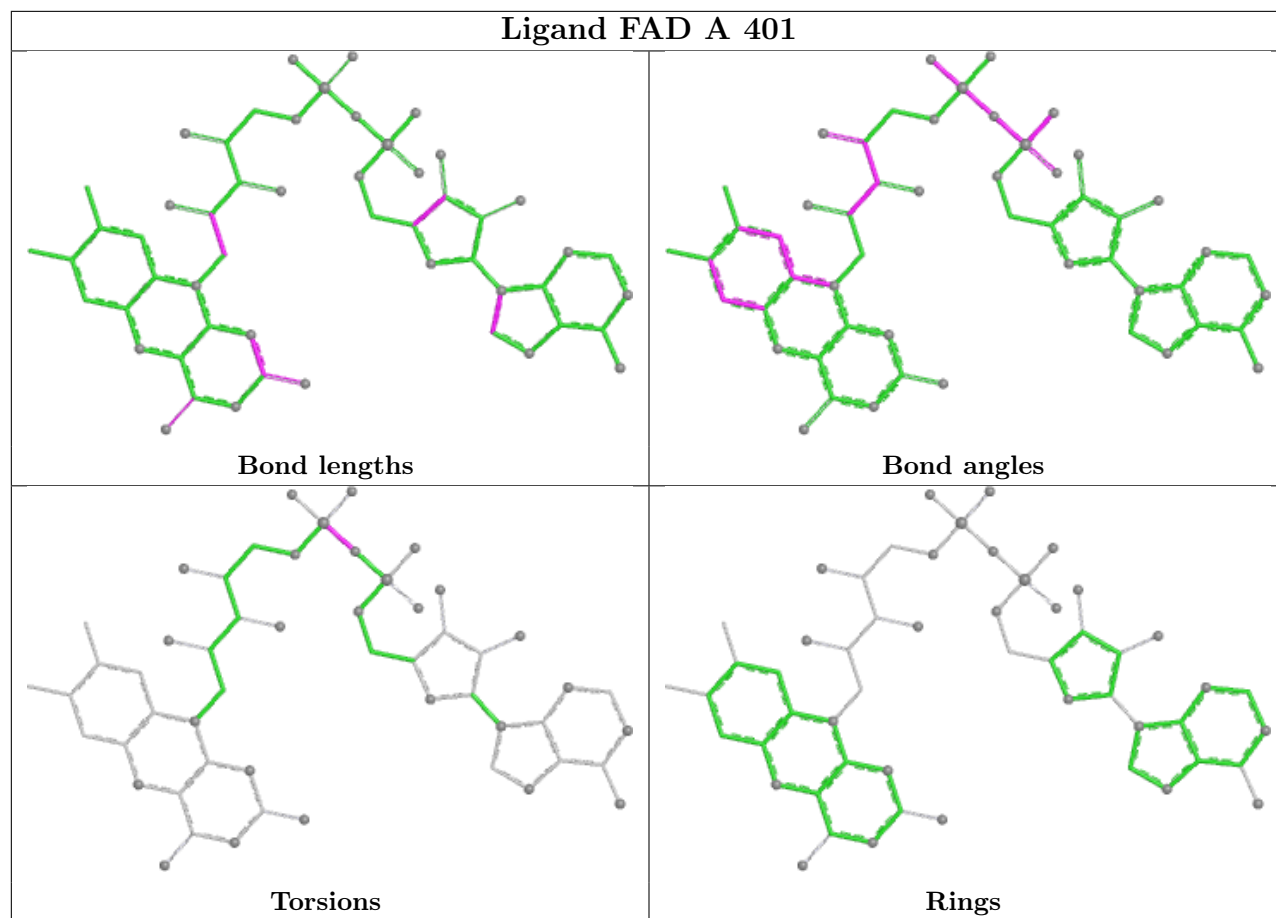
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	403	PG4	1	0
4	B	501	PG4	1	0

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	316/320 (98%)	-0.08	18 (5%)	29 31	23, 39, 76, 128	0
1	B	316/320 (98%)	-0.08	15 (4%)	36 39	24, 41, 73, 126	0
1	C	296/320 (92%)	0.81	62 (20%)	2 2	26, 56, 113, 134	0
1	D	297/320 (92%)	0.67	44 (14%)	5 6	26, 52, 106, 164	0
All	All	1225/1280 (95%)	0.32	139 (11%)	10 10	23, 45, 105, 164	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	231	ALA	7.8
1	D	215	ALA	7.3
1	C	229	LEU	6.5
1	D	132	VAL	6.4
1	C	122	PRO	6.0
1	C	230	LEU	5.8
1	D	216	VAL	5.6
1	D	218	VAL	5.4
1	D	230	LEU	5.3
1	C	174	ILE	5.2
1	C	119	ALA	5.0
1	A	184	GLY	5.0
1	D	142	PHE	4.9
1	C	206	ILE	4.8
1	A	181	THR	4.8
1	D	201	THR	4.7
1	B	181	THR	4.6
1	C	203	LEU	4.5
1	D	234	VAL	4.5
1	D	233	GLY	4.2
1	C	211	ALA	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	227	GLN	4.2
1	D	204	ILE	4.1
1	D	232	GLU	3.9
1	A	220	HIS	3.8
1	B	220	HIS	3.8
1	B	209	GLU	3.8
1	C	185	HIS	3.8
1	B	1	MET	3.7
1	C	3	GLN	3.7
1	D	226	SER	3.7
1	D	145	ASN	3.7
1	C	316	ALA	3.7
1	D	138	CYS	3.7
1	C	204	ILE	3.7
1	D	121	ILE	3.7
1	D	185	HIS	3.6
1	C	163	VAL	3.6
1	C	180	HIS	3.6
1	D	143	TYR	3.6
1	C	161	ALA	3.6
1	D	207	LYS	3.6
1	C	131	GLY	3.5
1	A	317	HIS	3.5
1	D	57	GLY	3.5
1	D	229	LEU	3.5
1	C	213	VAL	3.4
1	A	57	GLY	3.4
1	C	148	VAL	3.4
1	C	171	VAL	3.4
1	C	178	ASP	3.3
1	C	128	LEU	3.3
1	C	179	PRO	3.3
1	A	225	ASP	3.3
1	C	129	GLY	3.3
1	C	172	HIS	3.2
1	D	151	VAL	3.2
1	C	142	PHE	3.2
1	C	123	GLY	3.2
1	D	129	GLY	3.2
1	C	173	TRP	3.2
1	C	118	ILE	3.2
1	A	1	MET	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	203	LEU	3.2
1	C	167	PHE	3.2
1	A	224	SER	3.1
1	A	180	HIS	3.1
1	C	132	VAL	3.1
1	C	216	VAL	3.1
1	D	236	VAL	3.1
1	D	214	THR	3.1
1	A	-2	GLY	3.1
1	C	198	TRP	3.1
1	D	180	HIS	3.0
1	C	168	ALA	3.0
1	C	127	TYR	3.0
1	A	58	GLU	3.0
1	C	58	GLU	3.0
1	B	184	GLY	3.0
1	C	187	ASP	3.0
1	C	149	VAL	3.0
1	C	145	ASN	3.0
1	D	198	TRP	2.9
1	C	106	ARG	2.9
1	C	189	LEU	2.9
1	B	180	HIS	2.9
1	D	140	GLY	2.9
1	B	221	PRO	2.8
1	B	317	HIS	2.8
1	C	170	THR	2.8
1	C	158	VAL	2.8
1	C	2	GLU	2.8
1	D	228	GLU	2.8
1	B	211	ALA	2.7
1	D	202	ARG	2.7
1	B	185	HIS	2.7
1	D	58	GLU	2.6
1	C	190	LEU	2.6
1	B	210	GLU	2.6
1	D	174	ILE	2.6
1	C	151	VAL	2.6
1	C	231	ALA	2.6
1	C	201	THR	2.5
1	D	200	LYS	2.5
1	A	0	HIS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	234	VAL	2.4
1	B	224	SER	2.4
1	C	150	VAL	2.4
1	B	0	HIS	2.4
1	C	126	GLU	2.4
1	C	249	ALA	2.3
1	C	209	GLU	2.3
1	C	136	ALA	2.3
1	C	195	VAL	2.3
1	D	317	HIS	2.3
1	A	309	LYS	2.3
1	D	128	LEU	2.3
1	B	204	ILE	2.2
1	C	207	LYS	2.2
1	A	-1	SER	2.2
1	D	176	PRO	2.2
1	B	58	GLU	2.1
1	C	232	GLU	2.1
1	D	235	PHE	2.1
1	D	162	GLN	2.1
1	C	138	CYS	2.1
1	C	215	ALA	2.1
1	C	143	TYR	2.1
1	C	210	GLU	2.1
1	A	185	HIS	2.0
1	C	197	LEU	2.0
1	A	308	ARG	2.0
1	A	316	ALA	2.0
1	D	187	ASP	2.0
1	D	196	LYS	2.0
1	A	47	HIS	2.0
1	C	192	HIS	2.0
1	D	192	HIS	2.0
1	D	206	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

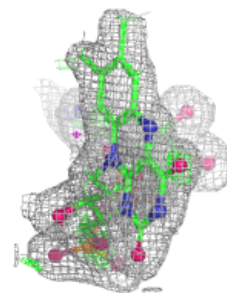
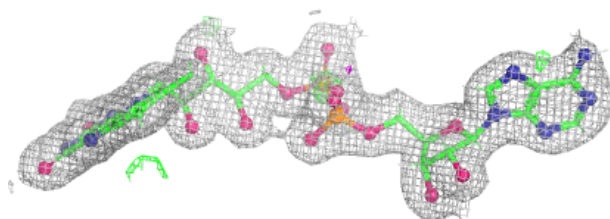
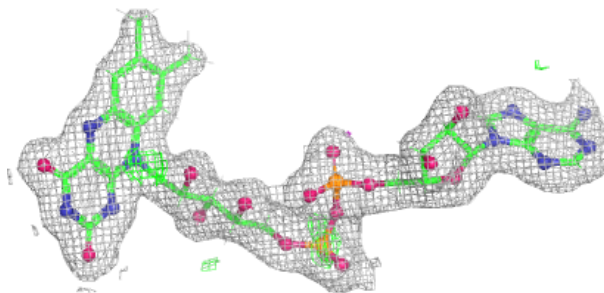
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PG4	A	403	13/13	0.88	0.11	43,54,62,66	0
4	PG4	B	501	13/13	0.88	0.11	41,52,62,71	0
2	FAD	C	500	53/53	0.98	0.06	22,34,47,50	0
2	FAD	D	401	53/53	0.98	0.06	21,33,47,50	0
2	FAD	A	401	53/53	0.98	0.05	18,27,44,50	0
2	FAD	B	500	53/53	0.98	0.05	20,30,46,48	0
3	CA	A	402	1/1	0.99	0.08	40,40,40,40	0
3	CA	B	502	1/1	0.99	0.07	40,40,40,40	0

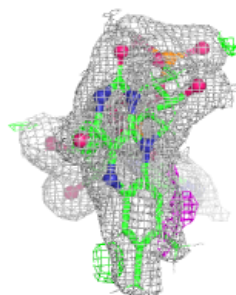
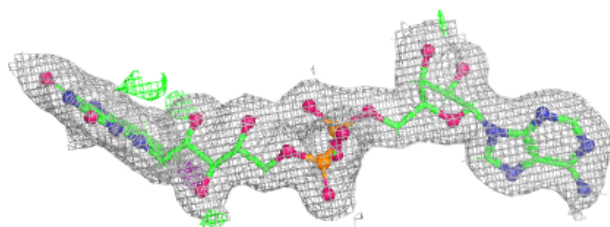
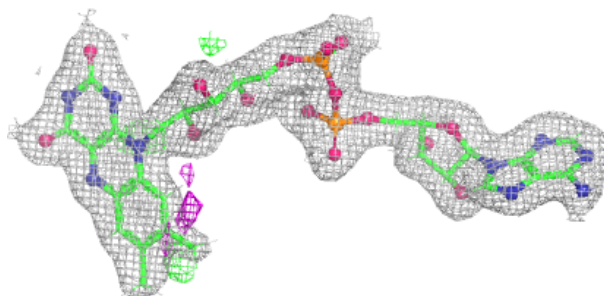
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD C 500:

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

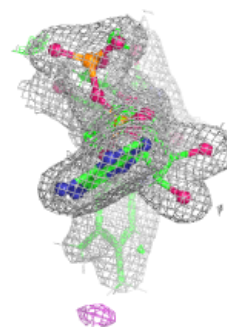
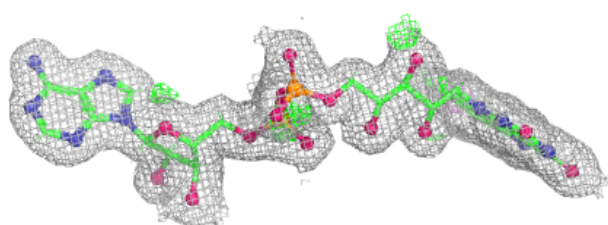
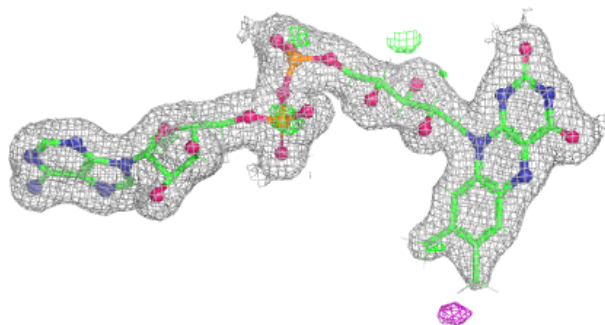
**Electron density around FAD D 401:**

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

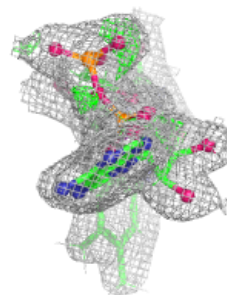
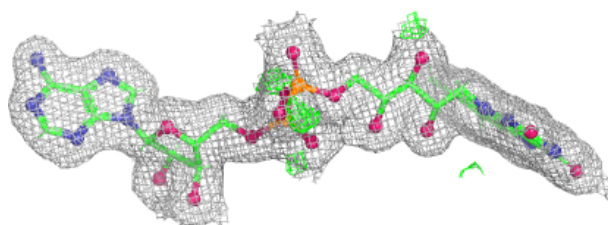
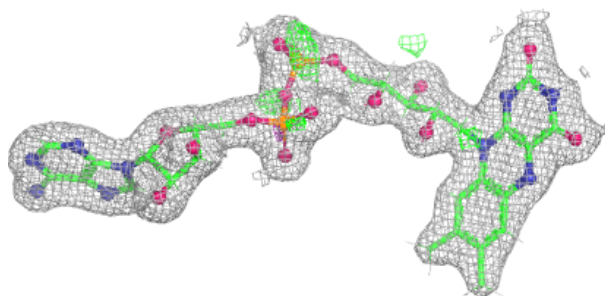


Electron density around FAD A 401:

$2mF_o-DF_c$ (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.