



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 30, 2025 – 07:12 pm BST

PDB ID : 9H9C / pdb_00009h9c
Title : Crystal structure of thioredoxin reductase from *Cryptosporidium parvum* in the "activated in" conformation
Authors : Gabriele, F.; Palmera, M.; Ardini, M.; Bogard, J.; Chen, X.M.; Williams, D.L.; Angelucci, F.
Deposited on : 2024-10-30
Resolution : 2.40 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 Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

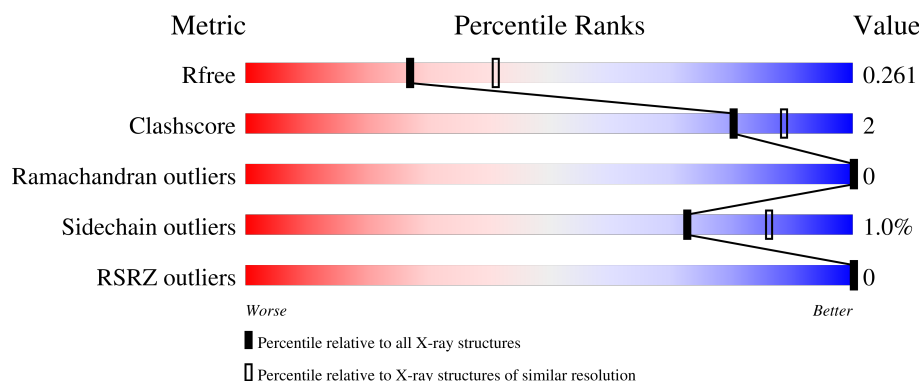
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.40 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}	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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	AAA	521	
1	BBB	521	
1	CCC	521	
1	DDD	521	

2 Entry composition [i](#)

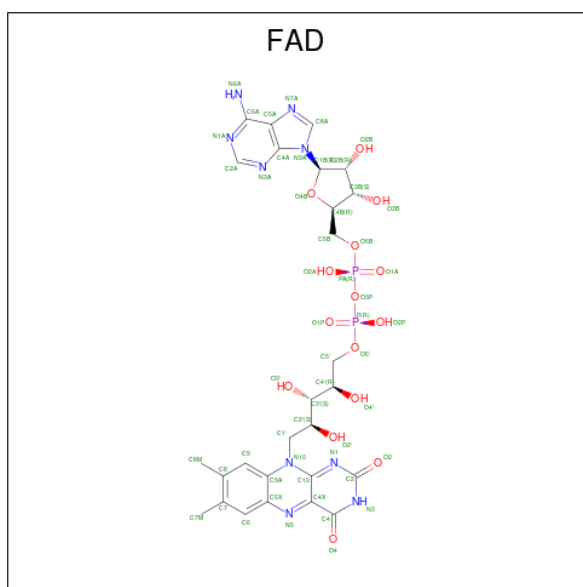
There are 4 unique types of molecules in this entry. The entry contains 15653 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Putative thioredoxin reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	498	Total	C	N	O	S	0	3	0
			3788	2417	629	726	16			
1	BBB	495	Total	C	N	O	S	0	2	0
			3767	2406	627	719	15			
1	CCC	498	Total	C	N	O	S	0	5	0
			3799	2424	632	726	17			
1	DDD	496	Total	C	N	O	S	0	1	0
			3768	2407	626	720	15			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



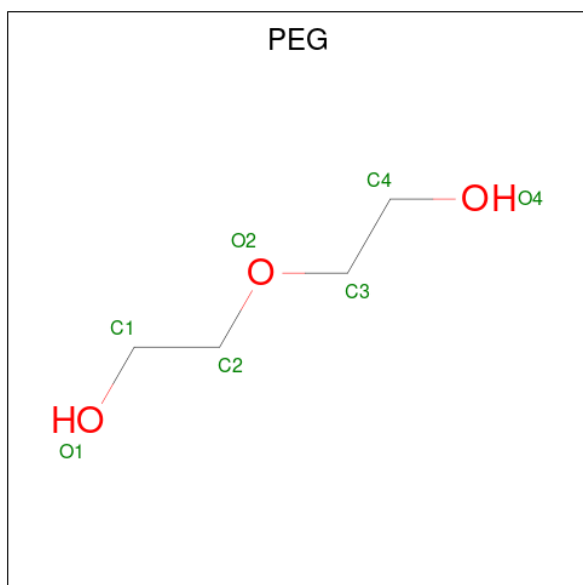
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	N	O	P	0
			53	27	9	15	2	
2	BBB	1	Total	C	N	O	P	0
			53	27	9	15	2	

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

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	C	O	0	0
			7	4	3		
3	BBB	1	Total	C	O	0	0
			7	4	3		
3	BBB	1	Total	C	O	0	0
			7	4	3		
3	CCC	1	Total	C	O	0	0
			7	4	3		
3	DDD	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	89	Total	O	0	0
			89	89		
4	BBB	94	Total	O	0	0
			94	94		

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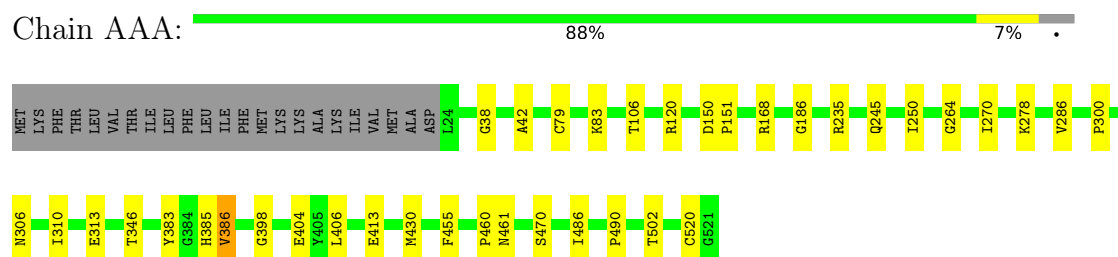
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	CCC	64	Total 64	O 64	0	0
4	DDD	37	Total 37	O 37	0	0

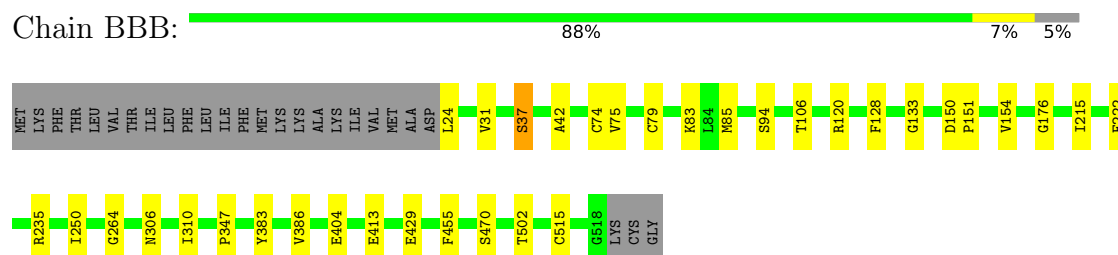
3 Residue-property plots [i](#)

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.

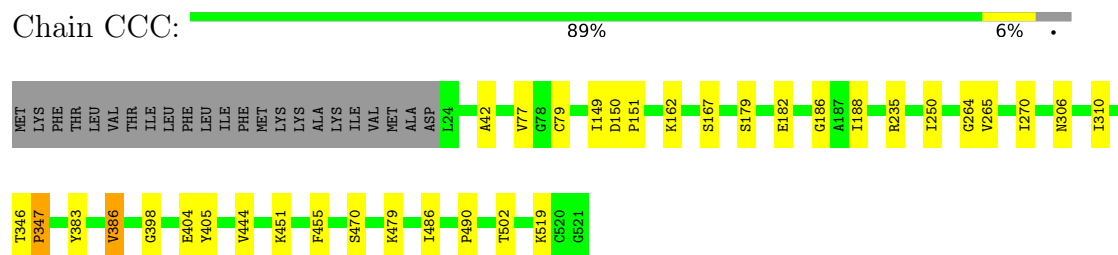
- Molecule 1: Putative thioredoxin reductase



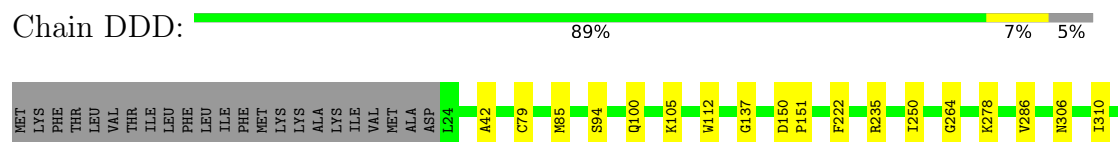
- Molecule 1: Putative thioredoxin reductase



- Molecule 1: Putative thioredoxin reductase



- Molecule 1: Putative thioredoxin reductase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.87Å 72.54Å 188.46Å 90.00° 90.61° 90.00°	Depositor
Resolution (Å)	39.91 – 2.40 39.91 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.91-2.40) 96.6 (39.91-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.223 , 0.257 0.225 , 0.261	Depositor DCC
R_{free} test set	3930 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 7.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.115 for k,h,-l 0.165 for -k,-h,-l 0.199 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15653	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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: PEG, 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	AAA	1.13	5/3870 (0.1%)	1.41	7/5231 (0.1%)
1	BBB	1.11	3/3849 (0.1%)	1.40	7/5205 (0.1%)
1	CCC	1.10	4/3887 (0.1%)	1.39	7/5253 (0.1%)
1	DDD	1.08	0/3847	1.38	5/5202 (0.1%)
All	All	1.10	12/15453 (0.1%)	1.40	26/20891 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	460	PRO	C-O	-6.93	1.15	1.23
1	BBB	347	PRO	C-O	-6.50	1.15	1.24
1	CCC	386	VAL	C-O	6.23	1.30	1.23
1	AAA	386	VAL	C-O	6.12	1.30	1.23
1	AAA	300	PRO	C-O	-5.91	1.16	1.23
1	BBB	176	GLY	C-O	5.73	1.30	1.23
1	CCC	347	PRO	C-O	-5.69	1.16	1.24
1	BBB	75	VAL	C-O	5.60	1.30	1.24
1	CCC	77	VAL	C-O	-5.57	1.17	1.24
1	CCC	265	VAL	C-O	5.21	1.29	1.24
1	AAA	385	HIS	CE1-NE2	5.11	1.37	1.32
1	AAA	486	ILE	C-O	5.05	1.29	1.24

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	313	GLU	CB-CG-CD	6.38	123.44	112.60
1	BBB	128	PHE	CA-CB-CG	-6.09	107.71	113.80
1	CCC	42	ALA	CA-C-N	5.47	127.55	120.44
1	CCC	42	ALA	C-N-CA	5.47	127.55	120.44
1	DDD	398	GLY	CA-C-N	5.45	127.85	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DDD	398	GLY	C-N-CA	5.45	127.85	120.38
1	AAA	42	ALA	CA-C-N	5.42	127.49	120.44
1	AAA	42	ALA	C-N-CA	5.42	127.49	120.44
1	CCC	149	ILE	N-CA-C	-5.41	107.16	111.81
1	BBB	42	ALA	CA-C-N	5.30	127.33	120.44
1	BBB	42	ALA	C-N-CA	5.30	127.33	120.44
1	DDD	42	ALA	CA-C-N	5.23	127.24	120.44
1	DDD	42	ALA	C-N-CA	5.23	127.24	120.44
1	AAA	38	GLY	CA-C-N	5.19	125.70	119.94
1	AAA	38	GLY	C-N-CA	5.19	125.70	119.94
1	BBB	215	ILE	CA-C-N	5.17	125.83	119.99
1	BBB	215	ILE	C-N-CA	5.17	125.83	119.99
1	DDD	423	GLU	CB-CA-C	5.13	120.15	109.95
1	CCC	398	GLY	CA-C-N	5.09	127.35	120.38
1	CCC	398	GLY	C-N-CA	5.09	127.35	120.38
1	CCC	486	ILE	CA-C-N	5.07	125.72	120.60
1	CCC	486	ILE	C-N-CA	5.07	125.72	120.60
1	AAA	398	GLY	CA-C-N	5.05	127.30	120.38
1	AAA	398	GLY	C-N-CA	5.05	127.30	120.38
1	BBB	37	SER	CA-C-N	5.00	125.39	119.94
1	BBB	37	SER	C-N-CA	5.00	125.39	119.94

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	3788	0	3789	21	0
1	BBB	3767	0	3772	22	0
1	CCC	3799	0	3804	17	0
1	DDD	3768	0	3772	22	0
2	AAA	53	0	31	0	0
2	BBB	53	0	31	0	0
2	CCC	53	0	31	0	0
2	DDD	53	0	31	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	AAA	7	0	10	0	0
3	BBB	14	0	20	1	0
3	CCC	7	0	10	0	0
3	DDD	7	0	10	0	0
4	AAA	89	0	0	6	0
4	BBB	94	0	0	4	0
4	CCC	64	0	0	2	0
4	DDD	37	0	0	2	0
All	All	15653	0	15311	76	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 2.

All (76) 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:DDD:100:GLN:HE22	1:DDD:105:LYS:HD2	1.01	1.11
1:DDD:100:GLN:HE22	1:DDD:105:LYS:CD	1.77	0.97
1:DDD:100:GLN:NE2	1:DDD:105:LYS:HD2	1.78	0.97
4:AAA:771:HOH:O	1:BBB:106:THR:HB	1.77	0.83
1:AAA:430:MET:HE1	1:CCC:179:SER:HB3	1.65	0.78
1:AAA:430:MET:HE1	1:CCC:179:SER:CB	2.13	0.77
1:BBB:429:GLU:HG3	4:BBB:732:HOH:O	1.85	0.75
1:AAA:83:LYS:HE2	1:BBB:413:GLU:OE2	1.88	0.73
1:BBB:133:GLY:O	4:BBB:701:HOH:O	2.06	0.73
1:AAA:106:THR:HB	4:AAA:771:HOH:O	1.96	0.65
1:DDD:137:GLY:HA2	4:DDD:732:HOH:O	1.98	0.63
1:BBB:74[B]:CYS:HB3	4:BBB:724:HOH:O	1.99	0.63
4:CCC:712:HOH:O	1:DDD:513:GLY:HA3	1.98	0.63
1:BBB:120[B]:ARG:CZ	3:BBB:603:PEG:H12	2.30	0.60
1:AAA:430:MET:CE	1:CCC:179:SER:HB3	2.33	0.59
1:AAA:120:ARG:HD3	4:AAA:785:HOH:O	2.03	0.57
1:DDD:137:GLY:CA	4:DDD:732:HOH:O	2.52	0.57
1:BBB:235:ARG:O	1:BBB:264:GLY:HA2	2.06	0.56
1:AAA:278:LYS:HE2	1:AAA:286:VAL:HG11	1.88	0.56
1:BBB:85:MET:CE	1:BBB:222:PHE:CE1	2.89	0.55
1:CCC:235:ARG:O	1:CCC:264:GLY:HA2	2.07	0.55
1:AAA:404:GLU:O	1:AAA:502:THR:HA	2.08	0.53
1:DDD:235:ARG:O	1:DDD:264:GLY:HA2	2.09	0.52
1:AAA:235:ARG:O	1:AAA:264:GLY:HA2	2.09	0.52
1:BBB:85:MET:HE3	1:BBB:222:PHE:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:120:ARG:CD	4:AAA:785:HOH:O	2.56	0.52
1:BBB:404:GLU:O	1:BBB:502:THR:HA	2.10	0.52
1:CCC:404:GLU:O	1:CCC:502:THR:HA	2.10	0.52
1:DDD:404:GLU:O	1:DDD:502:THR:HA	2.10	0.52
1:BBB:150:ASP:HB2	1:BBB:151:PRO:HD2	1.92	0.51
1:DDD:386:VAL:HG11	1:DDD:470:SER:HA	1.92	0.51
1:DDD:85:MET:CE	1:DDD:222:PHE:CE1	2.94	0.51
1:BBB:31:VAL:HG11	1:BBB:154:VAL:HG21	1.92	0.50
1:CCC:162:LYS:HD3	4:CCC:746:HOH:O	2.11	0.49
1:AAA:386:VAL:HG11	1:AAA:470:SER:HA	1.94	0.48
1:DDD:250:ILE:HD11	1:DDD:383:TYR:HB2	1.97	0.46
1:BBB:250:ILE:HD11	1:BBB:383:TYR:HB2	1.98	0.46
1:DDD:85:MET:HE3	1:DDD:222:PHE:CE1	2.51	0.46
1:BBB:85:MET:HE2	1:BBB:222:PHE:CE1	2.51	0.45
1:CCC:250:ILE:HD11	1:CCC:383:TYR:HB2	1.99	0.45
1:CCC:386:VAL:HG11	1:CCC:470:SER:HA	1.99	0.44
1:AAA:150:ASP:HB2	1:AAA:151:PRO:CD	2.48	0.43
1:AAA:186:GLY:HA3	1:AAA:270:ILE:O	2.18	0.43
1:BBB:306:ASN:O	1:BBB:310:ILE:HG12	2.17	0.43
1:BBB:429:GLU:CG	4:BBB:732:HOH:O	2.53	0.43
1:AAA:245:GLN:HE22	1:AAA:406:LEU:CD1	2.32	0.43
1:CCC:347:PRO:HG2	1:DDD:487:GLY:O	2.18	0.43
1:AAA:455:PHE:CD1	1:AAA:455:PHE:C	2.97	0.43
1:BBB:150:ASP:HB2	1:BBB:151:PRO:CD	2.48	0.43
1:DDD:278:LYS:HE3	1:DDD:286:VAL:HG11	1.99	0.43
1:AAA:250:ILE:HD11	1:AAA:383:TYR:HB2	2.00	0.43
1:BBB:386:VAL:HG11	1:BBB:470:SER:HA	2.00	0.43
1:DDD:306:ASN:O	1:DDD:310:ILE:HG12	2.19	0.43
1:DDD:336:GLY:HA3	2:DDD:601:FAD:O2P	2.19	0.42
1:AAA:150:ASP:HB2	1:AAA:151:PRO:HD2	2.01	0.42
1:AAA:306:ASN:O	1:AAA:310:ILE:HG12	2.18	0.42
1:CCC:306:ASN:O	1:CCC:310:ILE:HG12	2.19	0.42
1:AAA:413:GLU:OE2	1:BBB:83:LYS:HE2	2.20	0.42
1:DDD:85:MET:HE1	1:DDD:112:TRP:CH2	2.55	0.42
1:DDD:150:ASP:HB2	1:DDD:151:PRO:CD	2.49	0.42
1:BBB:455:PHE:CD1	1:BBB:455:PHE:C	2.98	0.42
1:BBB:24:LEU:HD12	1:BBB:24:LEU:HA	1.94	0.41
1:DDD:85:MET:HE2	1:DDD:222:PHE:CE1	2.54	0.41
1:DDD:405:TYR:CG	1:DDD:479:LYS:HE3	2.55	0.41
1:CCC:150:ASP:HB2	1:CCC:151:PRO:CD	2.50	0.41
1:CCC:186:GLY:HA3	1:CCC:270:ILE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:405:TYR:CG	1:CCC:479:LYS:HE3	2.55	0.41
1:CCC:455:PHE:CD1	1:CCC:455:PHE:C	2.98	0.41
1:DDD:150:ASP:HB2	1:DDD:151:PRO:HD2	2.02	0.41
1:CCC:150:ASP:HB2	1:CCC:151:PRO:HD2	2.02	0.41
1:DDD:455:PHE:CD1	1:DDD:455:PHE:C	2.98	0.41
1:AAA:461:ASN:HA	4:AAA:719:HOH:O	2.20	0.41
1:CCC:444:VAL:HA	1:CCC:451:LYS:O	2.20	0.41
1:CCC:182:GLU:HG2	1:CCC:188:ILE:HD11	2.03	0.40
1:AAA:168:ARG:NE	4:AAA:722:HOH:O	2.54	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	AAA	499/521 (96%)	476 (95%)	23 (5%)	0	100	100
1	BBB	495/521 (95%)	473 (96%)	22 (4%)	0	100	100
1	CCC	501/521 (96%)	481 (96%)	20 (4%)	0	100	100
1	DDD	495/521 (95%)	475 (96%)	20 (4%)	0	100	100
All	All	1990/2084 (96%)	1905 (96%)	85 (4%)	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	AAA	409/427 (96%)	404 (99%)	5 (1%)	67	82
1	BBB	406/427 (95%)	403 (99%)	3 (1%)	81	91
1	CCC	411/427 (96%)	406 (99%)	5 (1%)	67	82
1	DDD	406/427 (95%)	401 (99%)	5 (1%)	67	82
All	All	1632/1708 (96%)	1614 (99%)	18 (1%)	73	84

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	79	CYS
1	AAA	346	THR
1	AAA	490	PRO
1	AAA	520[A]	CYS
1	AAA	520[B]	CYS
1	BBB	79	CYS
1	BBB	94	SER
1	BBB	515	CYS
1	CCC	79	CYS
1	CCC	167	SER
1	CCC	346	THR
1	CCC	490	PRO
1	CCC	519	LYS
1	DDD	79	CYS
1	DDD	94	SER
1	DDD	400	ASP
1	DDD	490	PRO
1	DDD	515	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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	PEG	CCC	602	-	6,6,6	0.24	0	5,5,5	0.14	0
3	PEG	DDD	602	-	6,6,6	0.25	0	5,5,5	0.16	0
2	FAD	AAA	601	-	53,58,58	0.72	0	68,89,89	0.83	1 (1%)
3	PEG	BBB	602	-	6,6,6	0.26	0	5,5,5	0.13	0
3	PEG	BBB	603	-	6,6,6	0.25	0	5,5,5	0.21	0
2	FAD	BBB	601	-	53,58,58	0.73	0	68,89,89	0.87	4 (5%)
3	PEG	AAA	602	-	6,6,6	0.21	0	5,5,5	0.16	0
2	FAD	DDD	601	-	53,58,58	0.66	0	68,89,89	0.78	2 (2%)
2	FAD	CCC	601	-	53,58,58	0.66	1 (1%)	68,89,89	0.85	4 (5%)

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	PEG	CCC	602	-	-	2/4/4/4	-
3	PEG	DDD	602	-	-	2/4/4/4	-
2	FAD	AAA	601	-	-	4/30/50/50	0/6/6/6
3	PEG	BBB	602	-	-	1/4/4/4	-
3	PEG	BBB	603	-	-	2/4/4/4	-
2	FAD	BBB	601	-	-	8/30/50/50	0/6/6/6
3	PEG	AAA	602	-	-	1/4/4/4	-
2	FAD	DDD	601	-	-	3/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	CCC	601	-	-	6/30/50/50	0/6/6/6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	CCC	601	FAD	C2-N1	-2.14	1.31	1.36

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	DDD	601	FAD	O4B-C1B-C2B	-2.81	102.82	106.93
2	BBB	601	FAD	O4B-C1B-C2B	-2.57	103.17	106.93
2	AAA	601	FAD	O4B-C1B-C2B	-2.44	103.36	106.93
2	CCC	601	FAD	C4-N3-C2	-2.19	121.59	125.64
2	CCC	601	FAD	O4B-C1B-C2B	-2.14	103.80	106.93
2	CCC	601	FAD	N3-C2-N1	2.11	123.53	119.38
2	BBB	601	FAD	O2P-P-O1P	2.07	122.47	112.24
2	BBB	601	FAD	C4X-C4-N3	2.02	118.33	113.19
2	BBB	601	FAD	O3B-C3B-C4B	-2.02	105.21	111.05
2	CCC	601	FAD	C5A-C6A-N6A	2.02	123.42	120.35
2	DDD	601	FAD	C5A-C6A-N6A	2.01	123.40	120.35

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	BBB	601	FAD	C5'-O5'-P-O2P
2	DDD	601	FAD	PA-O3P-P-O5'
2	DDD	601	FAD	O4B-C4B-C5B-O5B
3	DDD	602	PEG	O2-C3-C4-O4
3	BBB	603	PEG	O2-C3-C4-O4
3	CCC	602	PEG	O2-C3-C4-O4
2	DDD	601	FAD	C3B-C4B-C5B-O5B
3	CCC	602	PEG	O1-C1-C2-O2
2	AAA	601	FAD	PA-O3P-P-O5'
2	BBB	601	FAD	PA-O3P-P-O5'
2	CCC	601	FAD	PA-O3P-P-O5'
3	AAA	602	PEG	O1-C1-C2-O2
2	BBB	601	FAD	C5'-O5'-P-O3P
2	AAA	601	FAD	P-O3P-PA-O2A
2	BBB	601	FAD	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	BBB	601	FAD	C5'-O5'-P-O1P
3	DDD	602	PEG	C1-C2-O2-C3
3	BBB	603	PEG	O1-C1-C2-O2
2	CCC	601	FAD	O4B-C4B-C5B-O5B
3	BBB	602	PEG	C1-C2-O2-C3
2	CCC	601	FAD	P-O3P-PA-O2A
2	BBB	601	FAD	O4'-C4'-C5'-O5'
2	CCC	601	FAD	C5'-O5'-P-O3P
2	BBB	601	FAD	O4B-C4B-C5B-O5B
2	AAA	601	FAD	P-O3P-PA-O1A
2	CCC	601	FAD	PA-O3P-P-O2P
2	CCC	601	FAD	C5'-O5'-P-O1P
2	AAA	601	FAD	O4B-C4B-C5B-O5B
2	BBB	601	FAD	C1'-C2'-C3'-O3'

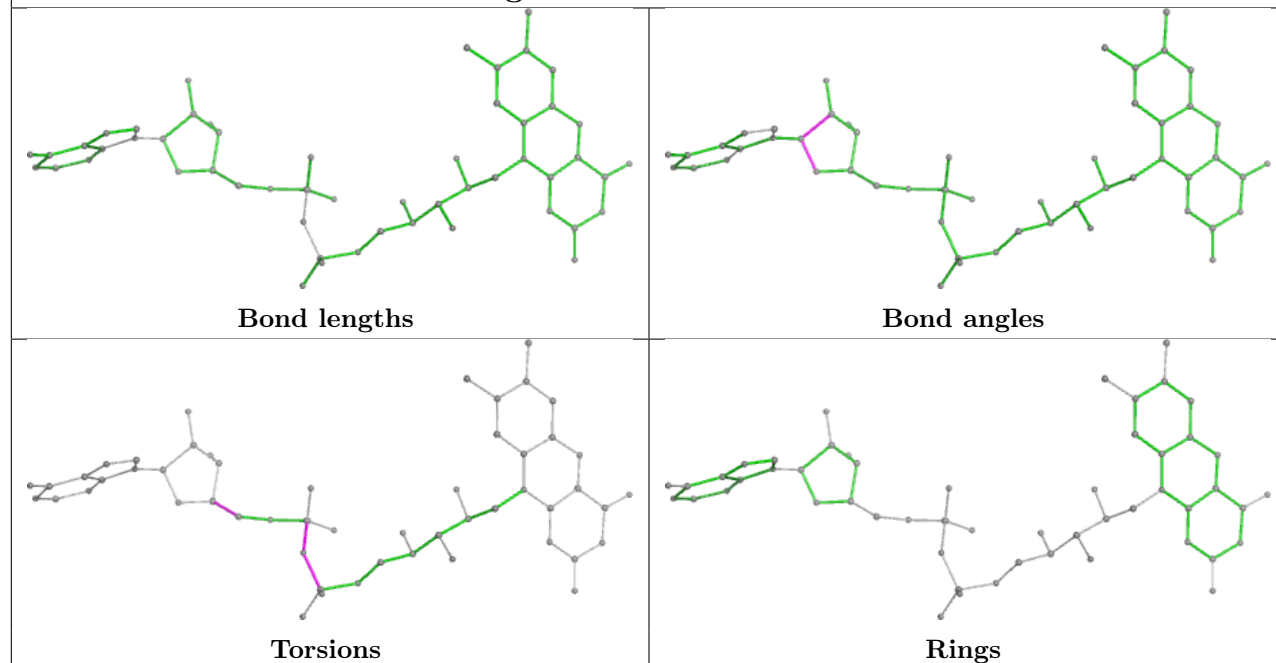
There are no ring outliers.

2 monomers are involved in 2 short contacts:

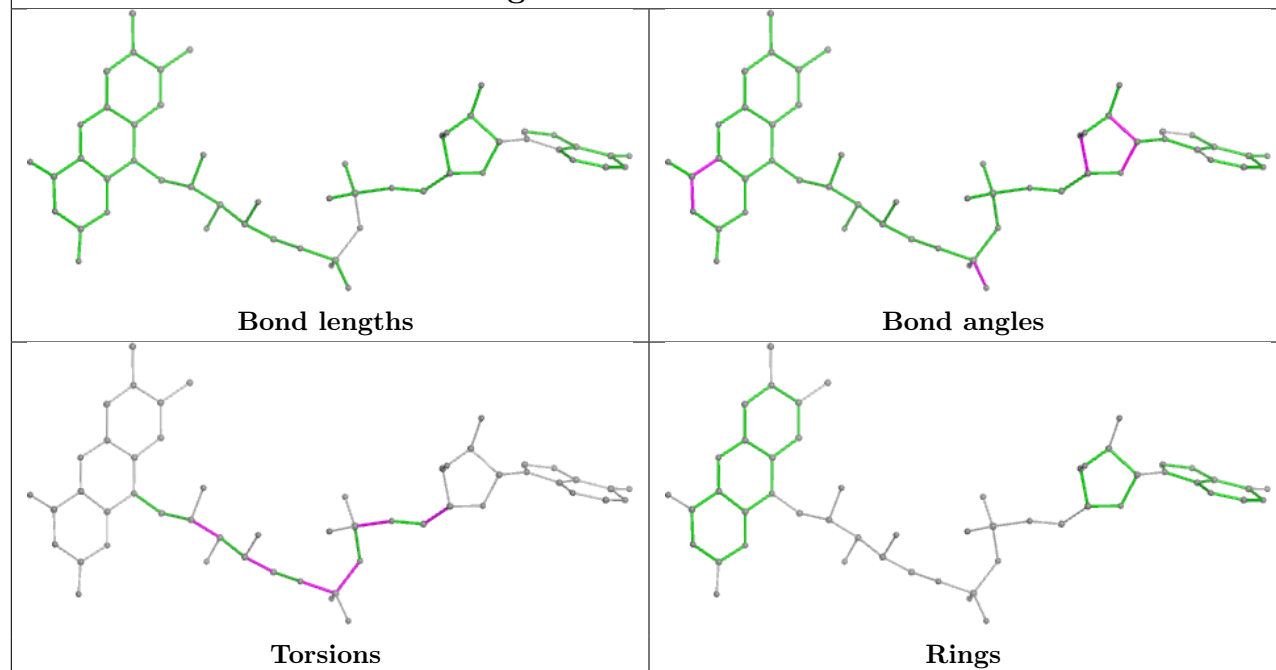
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	BBB	603	PEG	1	0
2	DDD	601	FAD	1	0

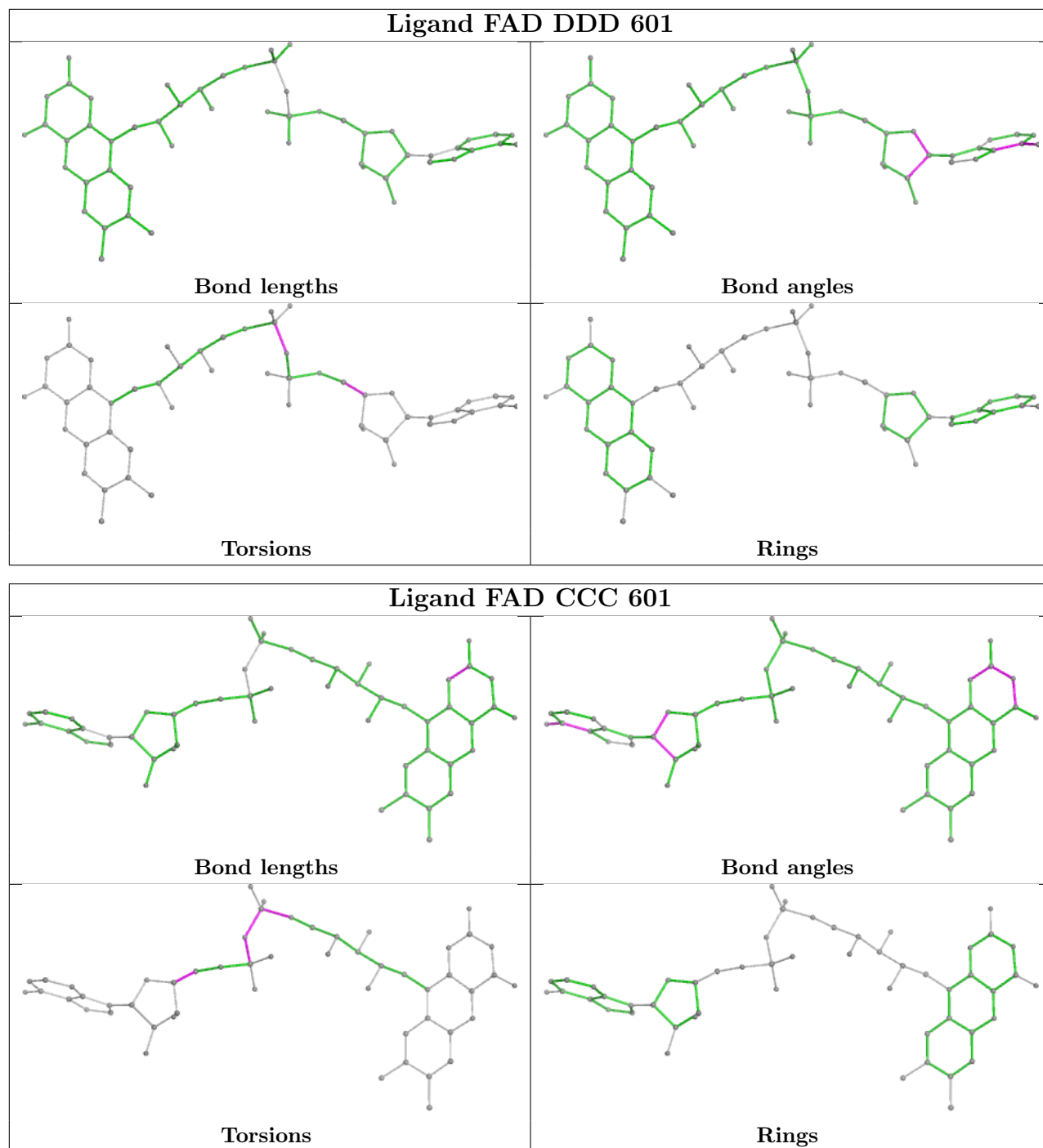
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand FAD AAA 601



Ligand FAD BBB 601





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	AAA	498/521 (95%)	-1.55	0 100 100	15, 37, 64, 104	3 (0%)
1	BBB	495/521 (95%)	-1.58	0 100 100	16, 35, 61, 95	2 (0%)
1	CCC	498/521 (95%)	-1.50	0 100 100	14, 40, 71, 99	5 (1%)
1	DDD	496/521 (95%)	-1.35	0 100 100	22, 50, 84, 114	2 (0%)
All	All	1987/2084 (95%)	-1.49	0 100 100	14, 39, 75, 114	12 (0%)

There are no RSRZ outliers to report.

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 monosaccharides 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(Å ²)	Q<0.9
3	PEG	BBB	602	7/7	0.96	0.07	60,69,75,76	0
3	PEG	AAA	602	7/7	0.98	0.06	65,73,76,80	0
3	PEG	BBB	603	7/7	0.98	0.07	59,65,67,67	0
3	PEG	CCC	602	7/7	0.98	0.05	58,70,75,75	0

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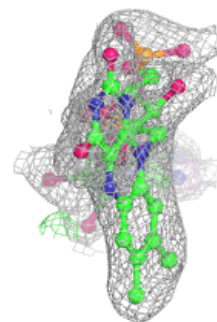
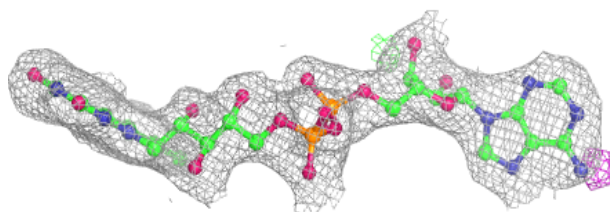
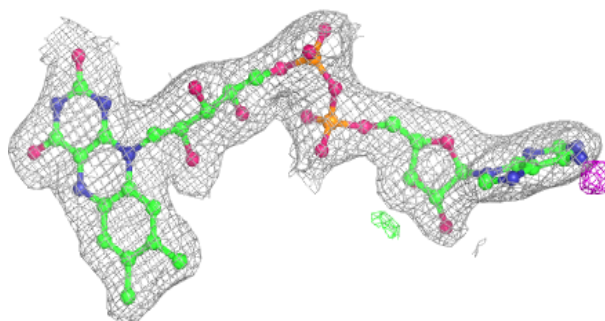
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PEG	DDD	602	7/7	0.98	0.07	59,72,80,82	0
2	FAD	BBB	601	53/53	0.99	0.02	17,19,22,22	0
2	FAD	CCC	601	53/53	0.99	0.03	20,26,36,39	0
2	FAD	DDD	601	53/53	0.99	0.03	31,36,45,48	0
2	FAD	AAA	601	53/53	0.99	0.02	13,24,34,35	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.

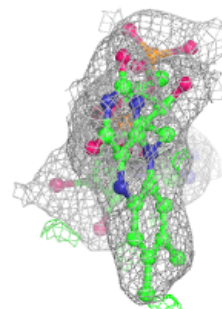
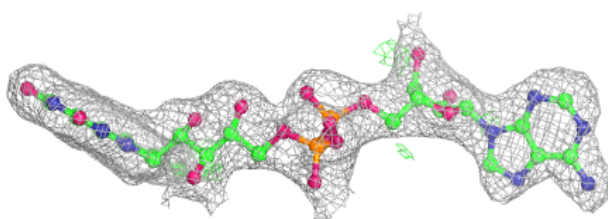
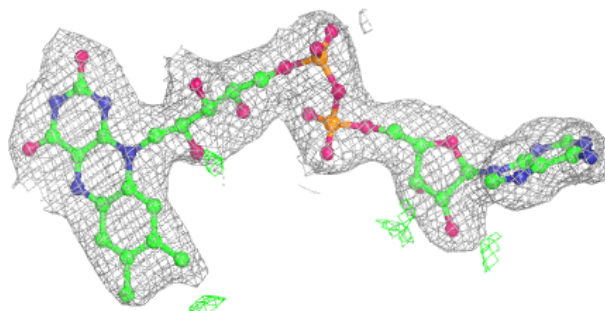
Electron density around FAD BBB 601:

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

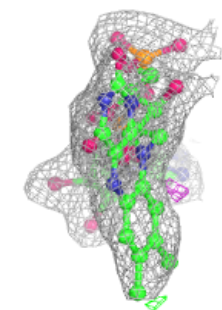
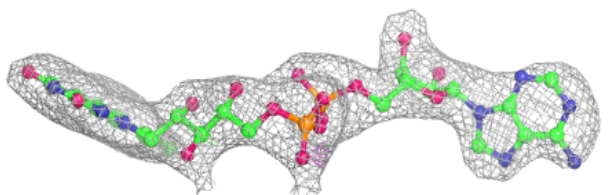
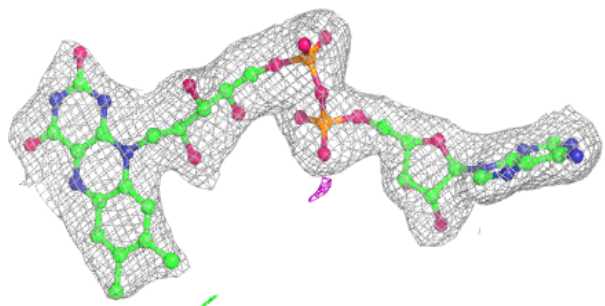


Electron density around FAD CCC 601:

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

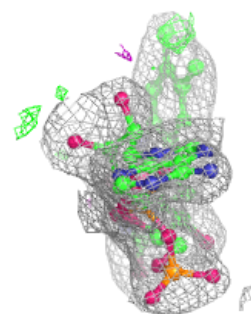
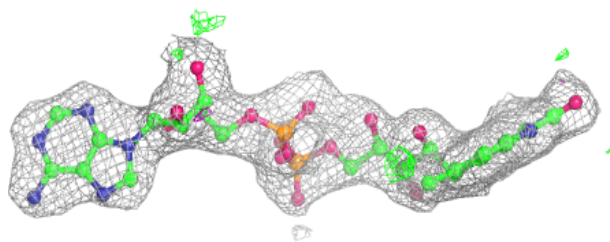
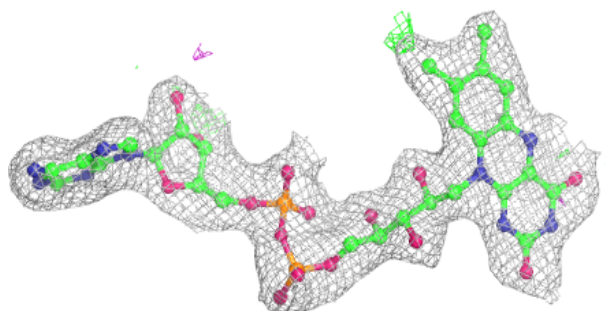
**Electron density around FAD DDD 601:**

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



Electron density around FAD AAA 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.