



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:17 AM UTC

PDB ID : 5X1Y / pdb_00005x1y
Title : Structure of mercuric reductase from Lysinibacillus sphaericus
Authors : Khan, F.; Suguna, K.
Deposited on : 2017-01-28
Resolution : 3.48 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

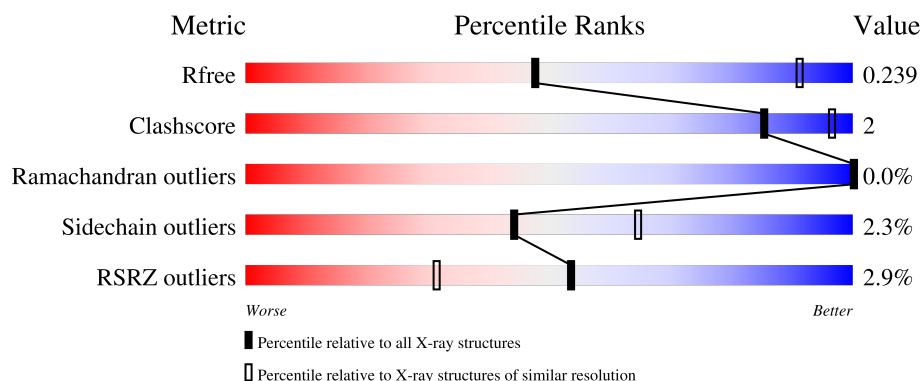
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.48 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	1083 (3.52-3.44)
Clashscore	190562	1139 (3.52-3.44)
Ramachandran outliers	187476	1111 (3.52-3.44)
Sidechain outliers	187428	1112 (3.52-3.44)
RSRZ outliers	180081	1082 (3.52-3.44)

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	554	3% 77% 5% 18%
1	B	554	2% 76% 6% 18%
1	C	554	3% 76% 6% 18%
1	D	554	2% 76% 6% 18%
1	E	554	2% 76% 6% 18%

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Mol	Chain	Length	Quality of chain
1	F	554	3% 77% • 18%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 40020 atoms, of which 19925 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 Mercuric reductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	454	Total	C	H	N	O	S	0	0	0
			6464	2070	3199	537	650	8			
1	A	453	Total	C	H	N	O	S	0	0	0
			6603	2096	3305	546	649	7			
1	C	453	Total	C	H	N	O	S	0	0	0
			6612	2098	3310	546	651	7			
1	D	453	Total	C	H	N	O	S	0	0	0
			6609	2097	3307	546	651	8			
1	E	453	Total	C	H	N	O	S	0	0	0
			6592	2094	3297	543	651	7			
1	F	453	Total	C	H	N	O	S	0	0	0
			6641	2107	3326	546	654	8			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	547	LEU	-	expression tag	UNP D9J041
B	548	GLU	-	expression tag	UNP D9J041
B	549	HIS	-	expression tag	UNP D9J041
B	550	HIS	-	expression tag	UNP D9J041
B	551	HIS	-	expression tag	UNP D9J041
B	552	HIS	-	expression tag	UNP D9J041
B	553	HIS	-	expression tag	UNP D9J041
B	554	HIS	-	expression tag	UNP D9J041
A	547	LEU	-	expression tag	UNP D9J041
A	548	GLU	-	expression tag	UNP D9J041
A	549	HIS	-	expression tag	UNP D9J041
A	550	HIS	-	expression tag	UNP D9J041
A	551	HIS	-	expression tag	UNP D9J041
A	552	HIS	-	expression tag	UNP D9J041
A	553	HIS	-	expression tag	UNP D9J041
A	554	HIS	-	expression tag	UNP D9J041
C	547	LEU	-	expression tag	UNP D9J041

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Chain	Residue	Modelled	Actual	Comment	Reference
C	548	GLU	-	expression tag	UNP D9J041
C	549	HIS	-	expression tag	UNP D9J041
C	550	HIS	-	expression tag	UNP D9J041
C	551	HIS	-	expression tag	UNP D9J041
C	552	HIS	-	expression tag	UNP D9J041
C	553	HIS	-	expression tag	UNP D9J041
C	554	HIS	-	expression tag	UNP D9J041
D	547	LEU	-	expression tag	UNP D9J041
D	548	GLU	-	expression tag	UNP D9J041
D	549	HIS	-	expression tag	UNP D9J041
D	550	HIS	-	expression tag	UNP D9J041
D	551	HIS	-	expression tag	UNP D9J041
D	552	HIS	-	expression tag	UNP D9J041
D	553	HIS	-	expression tag	UNP D9J041
D	554	HIS	-	expression tag	UNP D9J041
E	547	LEU	-	expression tag	UNP D9J041
E	548	GLU	-	expression tag	UNP D9J041
E	549	HIS	-	expression tag	UNP D9J041
E	550	HIS	-	expression tag	UNP D9J041
E	551	HIS	-	expression tag	UNP D9J041
E	552	HIS	-	expression tag	UNP D9J041
E	553	HIS	-	expression tag	UNP D9J041
E	554	HIS	-	expression tag	UNP D9J041
F	547	LEU	-	expression tag	UNP D9J041
F	548	GLU	-	expression tag	UNP D9J041
F	549	HIS	-	expression tag	UNP D9J041
F	550	HIS	-	expression tag	UNP D9J041
F	551	HIS	-	expression tag	UNP D9J041
F	552	HIS	-	expression tag	UNP D9J041
F	553	HIS	-	expression tag	UNP D9J041
F	554	HIS	-	expression tag	UNP D9J041

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

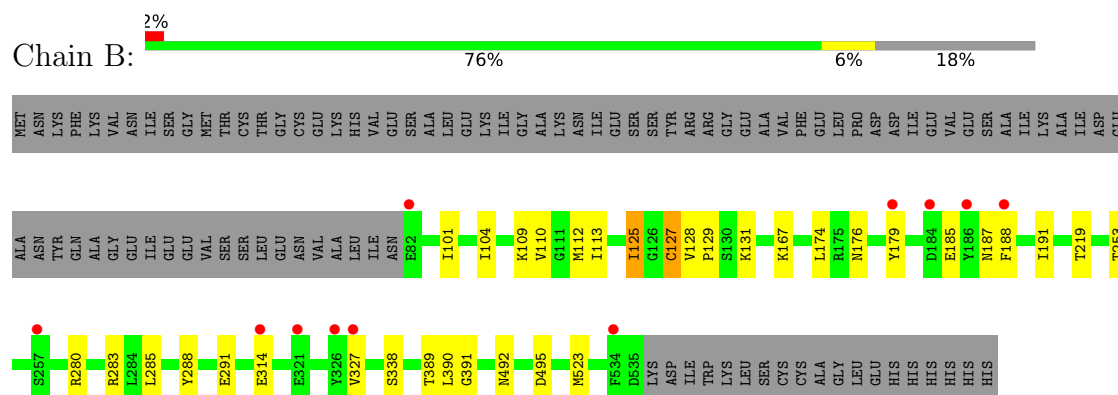


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total 83	C 27	H 30	N 9	O 15	P 2	0	0
2	A	1	Total 83	C 27	H 30	N 9	O 15	P 2	0	0
2	C	1	Total 83	C 27	H 30	N 9	O 15	P 2	0	0
2	D	1	Total 83	C 27	H 30	N 9	O 15	P 2	0	0
2	E	1	Total 83	C 27	H 30	N 9	O 15	P 2	0	0
2	F	1	Total 84	C 27	H 31	N 9	O 15	P 2	0	0

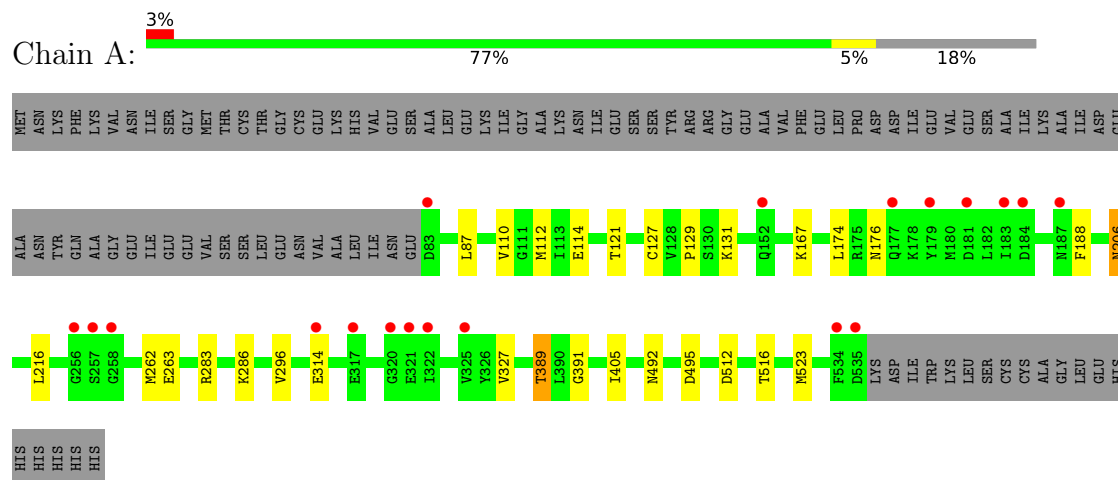
3 Residue-property plots [i](#)

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.

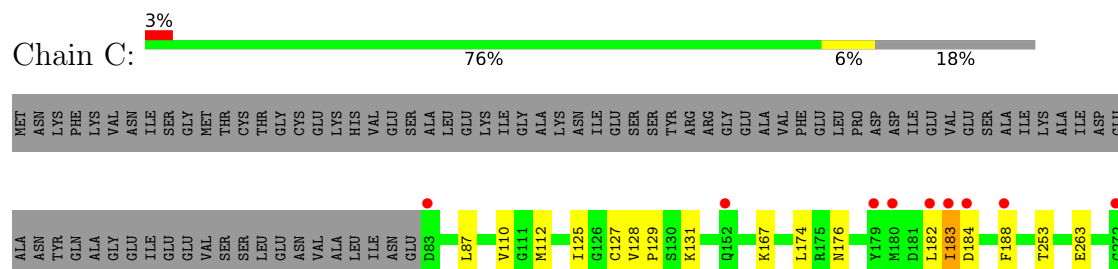
• Molecule 1: Mercuric reductase



• Molecule 1: Mercuric reductase

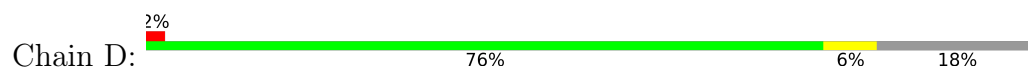


• Molecule 1: Mercuric reductase

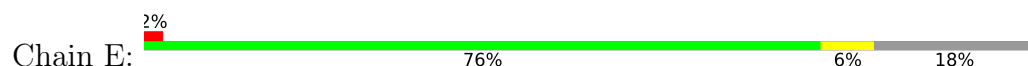




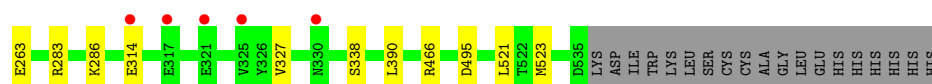
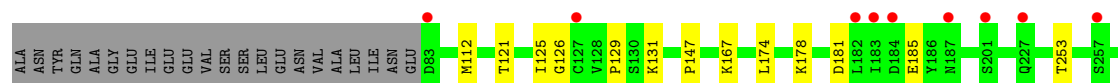
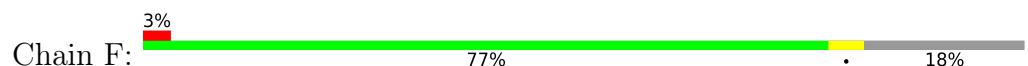
• Molecule 1: Mercuric reductase



• Molecule 1: Mercuric reductase



• Molecule 1: Mercuric reductase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	236.38Å 150.27Å 122.78Å 90.00° 92.62° 90.00°	Depositor
Resolution (Å)	87.07 – 3.48 87.07 – 3.48	Depositor EDS
% Data completeness (in resolution range)	99.9 (87.07-3.48) 100.0 (87.07-3.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 3.49Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.191 , 0.240 0.192 , 0.239	Depositor DCC
R_{free} test set	2763 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	64.6	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 66.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	40020	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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: 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	0.15	0/3339	0.31	0/4537
1	B	0.16	0/3306	0.32	0/4505
1	C	0.16	0/3343	0.31	0/4542
1	D	0.16	0/3343	0.32	0/4541
1	E	0.16	0/3336	0.31	0/4534
1	F	0.14	0/3357	0.31	0/4560
All	All	0.15	0/20024	0.31	0/27219

There are no bond length outliers.

There are no bond angle outliers.

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	3298	3305	3305	16	0
1	B	3265	3199	3199	18	0
1	C	3302	3310	3309	18	0
1	D	3302	3307	3307	16	0
1	E	3295	3297	3296	14	0
1	F	3315	3326	3325	12	0
2	A	53	30	31	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	53	30	31	0	0
2	C	53	30	31	0	0
2	D	53	30	31	0	0
2	E	53	30	31	1	0
2	F	53	31	31	0	0
All	All	20095	19925	19927	87	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 (87) 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:F:253:THR:HG1	1:F:338:SER:HG	1.05	0.83
1:C:283:ARG:NH2	1:C:286:LYS:O	2.20	0.74
1:D:283:ARG:NH2	1:D:286:LYS:O	2.26	0.68
1:E:283:ARG:NH2	1:E:286:LYS:O	2.30	0.64
1:A:114:GLU:OE1	2:A:601:FAD:O2B	2.13	0.63
1:E:253:THR:OG1	1:E:338:SER:OG	1.98	0.63
1:A:131:LYS:NZ	1:A:263:GLU:OE1	2.32	0.62
1:B:389:THR:O	1:B:391:GLY:N	2.33	0.62
1:C:131:LYS:NZ	1:C:263:GLU:OE1	2.35	0.59
1:F:283:ARG:NH2	1:F:286:LYS:O	2.36	0.58
1:A:492:ASN:ND2	1:A:495:ASP:OD2	2.37	0.58
1:E:121:THR:O	1:E:126:GLY:N	2.36	0.58
1:E:131:LYS:NZ	1:E:263:GLU:OE1	2.38	0.57
1:C:253:THR:OG1	1:C:338:SER:OG	2.08	0.53
1:D:131:LYS:NZ	1:D:263:GLU:OE1	2.42	0.53
1:B:314:GLU:H	1:B:327:VAL:CB	2.24	0.51
1:B:495:ASP:OD2	1:C:492:ASN:ND2	2.43	0.51
1:B:492:ASN:ND2	1:C:495:ASP:OD2	2.43	0.51
1:F:181:ASP:N	1:F:181:ASP:OD1	2.41	0.51
1:D:314:GLU:H	1:D:327:VAL:CB	2.23	0.51
1:F:131:LYS:NZ	1:F:263:GLU:OE1	2.45	0.49
1:C:389:THR:O	1:C:391:GLY:N	2.46	0.49
1:D:253:THR:OG1	1:D:338:SER:OG	1.90	0.49
1:A:121:THR:OG1	2:A:601:FAD:O2A	2.27	0.49
1:F:185:GLU:OE1	1:F:185:GLU:N	2.46	0.49
1:C:129:PRO:HB3	1:C:167:LYS:HD2	1.95	0.48
1:A:283:ARG:NH2	1:A:286:LYS:O	2.46	0.48
1:F:121:THR:O	1:F:126:GLY:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:GLU:OE2	1:C:291:GLU:N	2.40	0.48
1:B:128:VAL:HB	1:B:129:PRO:HD3	1.96	0.48
1:C:253:THR:HG1	1:C:338:SER:HG	1.28	0.47
1:A:314:GLU:H	1:A:327:VAL:CB	2.27	0.47
1:A:389:THR:O	1:A:391:GLY:N	2.46	0.47
1:E:386:GLY:O	1:E:389:THR:HG22	2.15	0.47
1:A:216:LEU:HD13	1:A:405:ILE:HG21	1.98	0.46
1:D:323:LYS:O	1:D:324:ARG:HD2	2.15	0.46
1:C:128:VAL:HB	1:C:129:PRO:HD3	1.97	0.46
1:C:110:VAL:O	1:C:188:PHE:HA	2.15	0.46
1:E:314:GLU:H	1:E:327:VAL:CB	2.29	0.45
1:E:110:VAL:O	1:E:188:PHE:HA	2.15	0.45
1:A:129:PRO:HB3	1:A:167:LYS:HD2	1.97	0.45
1:D:129:PRO:HB3	1:D:167:LYS:HD2	1.99	0.45
1:B:104:ILE:HG12	1:B:187:ASN:CB	2.46	0.45
1:F:129:PRO:HB3	1:F:167:LYS:HD2	1.97	0.45
1:B:113:ILE:HA	1:B:191:ILE:O	2.16	0.45
1:B:176:ASN:HB3	1:A:176:ASN:HB3	1.97	0.45
1:B:109:LYS:NZ	1:A:206:ASN:O	2.46	0.45
1:E:128:VAL:HB	1:E:129:PRO:HD3	1.98	0.45
1:C:176:ASN:HB3	1:D:176:ASN:HB3	1.98	0.45
1:F:181:ASP:O	1:F:185:GLU:HB2	2.17	0.45
1:E:93:GLY:HA3	2:E:601:FAD:O1A	2.18	0.44
1:E:185:GLU:O	1:E:187:ASN:N	2.47	0.44
1:B:127:CYS:O	1:B:131:LYS:HD3	2.18	0.44
1:E:511:GLU:O	1:E:515:GLU:HG2	2.17	0.44
1:B:125:ILE:HD12	1:B:125:ILE:O	2.18	0.43
1:D:110:VAL:HG23	1:D:188:PHE:HB2	2.01	0.42
1:D:188:PHE:CD1	1:D:188:PHE:C	2.96	0.42
1:F:314:GLU:H	1:F:327:VAL:CB	2.32	0.42
1:C:183:ILE:HG23	1:C:184:ASP:H	1.84	0.42
1:C:87:LEU:HB3	1:C:110:VAL:HG12	2.01	0.42
1:E:298:LYS:NZ	1:E:302:GLU:OE2	2.53	0.42
1:D:511:GLU:O	1:D:515:GLU:HG2	2.20	0.42
1:B:291:GLU:OE2	1:B:291:GLU:N	2.42	0.41
1:C:405:ILE:HD11	1:C:417:ILE:HD11	2.02	0.41
1:D:396:TYR:OH	1:D:423:PRO:O	2.27	0.41
1:B:110:VAL:HG23	1:B:188:PHE:CB	2.50	0.41
1:A:512:ASP:O	1:A:516:THR:HG23	2.20	0.41
1:C:314:GLU:H	1:C:327:VAL:CB	2.33	0.41
1:B:129:PRO:HB3	1:B:167:LYS:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:VAL:HG23	1:A:188:PHE:HB2	2.02	0.41
1:A:188:PHE:CD1	1:A:188:PHE:C	2.99	0.41
1:E:184:ASP:HB2	1:E:187:ASN:CB	2.51	0.41
1:D:492:ASN:ND2	1:F:495:ASP:OD2	2.54	0.41
1:E:110:VAL:HG23	1:E:188:PHE:CB	2.51	0.41
1:F:147:PRO:HB2	1:F:466:ARG:HD2	2.02	0.41
1:C:110:VAL:HG23	1:C:188:PHE:HB2	2.01	0.41
1:D:97:PHE:O	1:D:101:ILE:HG12	2.21	0.41
1:B:253:THR:OG1	1:B:338:SER:OG	2.01	0.41
1:B:285:LEU:HB3	1:B:288:TYR:CD1	2.56	0.41
1:A:262:MET:HE1	1:A:296:VAL:HG21	2.02	0.41
1:C:87:LEU:O	1:C:110:VAL:HA	2.21	0.41
1:D:131:LYS:CG	1:F:521:LEU:HD13	2.50	0.41
1:B:176:ASN:HA	1:B:179:TYR:HD2	1.86	0.41
1:D:159:ASP:OD2	1:D:162:SER:OG	2.36	0.40
1:A:87:LEU:O	1:A:110:VAL:HA	2.20	0.40
1:B:101:ILE:CD1	1:B:185:GLU:HG3	2.52	0.40
1:D:110:VAL:HG23	1:D:188:PHE:CB	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	451/554 (81%)	427 (95%)	24 (5%)	0	100	100
1	B	452/554 (82%)	429 (95%)	22 (5%)	1 (0%)	43	74
1	C	451/554 (81%)	426 (94%)	25 (6%)	0	100	100
1	D	451/554 (81%)	424 (94%)	27 (6%)	0	100	100
1	E	451/554 (81%)	428 (95%)	23 (5%)	0	100	100
1	F	451/554 (81%)	430 (95%)	21 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2707/3324 (81%)	2564 (95%)	142 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	390	LEU

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	342/458 (75%)	336 (98%)	6 (2%)	51	69
1	B	332/458 (72%)	324 (98%)	8 (2%)	43	64
1	C	343/458 (75%)	333 (97%)	10 (3%)	37	61
1	D	343/458 (75%)	334 (97%)	9 (3%)	40	63
1	E	342/458 (75%)	333 (97%)	9 (3%)	40	63
1	F	346/458 (76%)	340 (98%)	6 (2%)	53	69
All	All	2048/2748 (74%)	2000 (98%)	48 (2%)	44	64

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	112	MET
1	B	125	ILE
1	B	127	CYS
1	B	174	LEU
1	B	219	THR
1	B	280	ARG
1	B	283	ARG
1	B	523	MET
1	A	112	MET
1	A	127	CYS
1	A	174	LEU

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Mol	Chain	Res	Type
1	A	206	ASN
1	A	389	THR
1	A	523	MET
1	C	112	MET
1	C	125	ILE
1	C	127	CYS
1	C	174	LEU
1	C	182	LEU
1	C	183	ILE
1	C	282	GLU
1	C	390	LEU
1	C	454	LEU
1	C	523	MET
1	D	84	ASN
1	D	112	MET
1	D	127	CYS
1	D	158	VAL
1	D	174	LEU
1	D	282	GLU
1	D	389	THR
1	D	390	LEU
1	D	523	MET
1	E	112	MET
1	E	127	CYS
1	E	158	VAL
1	E	174	LEU
1	E	182	LEU
1	E	232	GLU
1	E	389	THR
1	E	390	LEU
1	E	523	MET
1	F	112	MET
1	F	125	ILE
1	F	174	LEU
1	F	178	LYS
1	F	390	LEU
1	F	523	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	270	HIS

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Mol	Chain	Res	Type
1	B	367	ASN
1	B	492	ASN
1	C	146	ASN
1	D	492	ASN
1	E	166	GLN
1	E	393	GLN
1	F	84	ASN
1	F	367	ASN
1	F	492	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](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FAD	D	601	-	58,58,58	1.50	9 (15%)	85,89,89	1.60	15 (17%)
2	FAD	C	601	-	58,58,58	1.48	8 (13%)	85,89,89	1.62	16 (18%)
2	FAD	F	601	-	58,58,58	1.48	8 (13%)	85,89,89	1.60	20 (23%)
2	FAD	B	601	-	58,58,58	1.46	8 (13%)	85,89,89	1.60	17 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	A	601	-	58,58,58	1.50	9 (15%)	85,89,89	1.70	18 (21%)
2	FAD	E	601	-	58,58,58	1.48	9 (15%)	85,89,89	1.64	18 (21%)

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	D	601	-	-	2/34/50/50	0/6/6/6
2	FAD	C	601	-	-	4/34/50/50	0/6/6/6
2	FAD	F	601	-	-	5/34/50/50	0/6/6/6
2	FAD	B	601	-	-	2/34/50/50	0/6/6/6
2	FAD	A	601	-	-	5/34/50/50	0/6/6/6
2	FAD	E	601	-	-	4/34/50/50	0/6/6/6

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	C9A-C5X	5.87	1.50	1.41
2	C	601	FAD	C9A-C5X	5.59	1.50	1.41
2	B	601	FAD	C9A-C5X	5.54	1.50	1.41
2	E	601	FAD	C9A-C5X	5.53	1.50	1.41
2	F	601	FAD	C9A-C5X	5.48	1.50	1.41
2	D	601	FAD	C9A-C5X	5.46	1.50	1.41
2	F	601	FAD	C5A-C4A	4.51	1.47	1.39
2	D	601	FAD	C5A-C4A	4.48	1.47	1.39
2	E	601	FAD	C5A-C4A	4.47	1.47	1.39
2	A	601	FAD	C5A-C4A	4.42	1.47	1.39
2	C	601	FAD	C5A-C4A	4.36	1.46	1.39
2	B	601	FAD	C5A-C4A	4.34	1.46	1.39
2	F	601	FAD	C8-C7	3.33	1.49	1.40
2	C	601	FAD	C8-C7	3.33	1.49	1.40
2	D	601	FAD	C8-C7	3.32	1.48	1.40
2	A	601	FAD	C8-C7	3.26	1.48	1.40
2	B	601	FAD	C8-C7	3.22	1.48	1.40
2	E	601	FAD	C8-C7	3.18	1.48	1.40
2	C	601	FAD	C5A-C6A	2.73	1.48	1.41
2	A	601	FAD	C5A-C6A	2.62	1.48	1.41
2	E	601	FAD	C5A-C6A	2.59	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	601	FAD	C5A-C6A	2.58	1.48	1.41
2	A	601	FAD	C4-N3	-2.53	1.34	1.38
2	B	601	FAD	C5A-C6A	2.53	1.48	1.41
2	D	601	FAD	C5A-C6A	2.53	1.48	1.41
2	D	601	FAD	C5X-N5	-2.53	1.34	1.39
2	D	601	FAD	C4-N3	-2.49	1.34	1.38
2	D	601	FAD	C5A-N7A	-2.46	1.34	1.39
2	B	601	FAD	C5A-N7A	-2.45	1.34	1.39
2	C	601	FAD	C4-N3	-2.44	1.34	1.38
2	F	601	FAD	C8A-N7A	2.42	1.36	1.31
2	C	601	FAD	C8A-N7A	2.42	1.36	1.31
2	F	601	FAD	C4-N3	-2.40	1.34	1.38
2	A	601	FAD	C8A-N7A	2.39	1.36	1.31
2	B	601	FAD	C4-N3	-2.37	1.34	1.38
2	E	601	FAD	C8A-N7A	2.36	1.36	1.31
2	E	601	FAD	C5A-N7A	-2.35	1.34	1.39
2	D	601	FAD	C8A-N7A	2.35	1.36	1.31
2	B	601	FAD	C8A-N7A	2.34	1.36	1.31
2	C	601	FAD	C5A-N7A	-2.32	1.34	1.39
2	F	601	FAD	C5A-N7A	-2.30	1.34	1.39
2	C	601	FAD	C5X-N5	-2.28	1.35	1.39
2	E	601	FAD	C4-N3	-2.28	1.34	1.38
2	A	601	FAD	C10-N10	2.26	1.42	1.37
2	A	601	FAD	C5A-N7A	-2.24	1.35	1.39
2	E	601	FAD	C5X-N5	-2.20	1.35	1.39
2	B	601	FAD	C5X-N5	-2.18	1.35	1.39
2	A	601	FAD	C5X-N5	-2.12	1.35	1.39
2	F	601	FAD	C10-N10	2.02	1.41	1.37
2	D	601	FAD	C10-N10	2.01	1.41	1.37
2	E	601	FAD	C10-N10	2.01	1.41	1.37

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	C5A-C4A-N3A	-6.08	118.35	126.72
2	C	601	FAD	C5A-C4A-N3A	-6.03	118.41	126.72
2	A	601	FAD	C5A-C4A-N3A	-6.01	118.44	126.72
2	E	601	FAD	C5A-C4A-N3A	-5.92	118.56	126.72
2	D	601	FAD	C5A-C4A-N3A	-5.90	118.59	126.72
2	F	601	FAD	C5A-C4A-N3A	-5.74	118.81	126.72
2	A	601	FAD	N3A-C4A-N9A	5.05	135.76	127.17
2	E	601	FAD	N3A-C4A-N9A	4.85	135.41	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	FAD	N3A-C4A-N9A	4.83	135.39	127.17
2	B	601	FAD	N3A-C4A-N9A	4.83	135.38	127.17
2	C	601	FAD	N3A-C4A-N9A	4.74	135.22	127.17
2	F	601	FAD	N3A-C4A-N9A	4.64	135.06	127.17
2	A	601	FAD	N3A-C2A-N1A	-4.17	122.27	128.58
2	A	601	FAD	C2A-N3A-C4A	4.17	122.01	111.83
2	C	601	FAD	C2A-N3A-C4A	3.99	121.57	111.83
2	E	601	FAD	C2A-N3A-C4A	3.94	121.45	111.83
2	B	601	FAD	C2A-N3A-C4A	3.91	121.38	111.83
2	F	601	FAD	C2A-N3A-C4A	3.84	121.20	111.83
2	D	601	FAD	C2A-N3A-C4A	3.77	121.03	111.83
2	F	601	FAD	N3A-C2A-N1A	-3.73	122.94	128.58
2	C	601	FAD	C4A-C5A-N7A	-3.72	106.32	110.58
2	E	601	FAD	N3A-C2A-N1A	-3.71	122.97	128.58
2	C	601	FAD	N3A-C2A-N1A	-3.67	123.03	128.58
2	B	601	FAD	N3A-C2A-N1A	-3.63	123.09	128.58
2	B	601	FAD	C4A-C5A-N7A	-3.58	106.48	110.58
2	D	601	FAD	N3A-C2A-N1A	-3.52	123.26	128.58
2	F	601	FAD	C4A-C5A-N7A	-3.46	106.63	110.58
2	A	601	FAD	C4A-C5A-N7A	-3.37	106.72	110.58
2	D	601	FAD	C4A-C5A-N7A	-3.36	106.73	110.58
2	A	601	FAD	C4A-N9A-C8A	3.36	109.26	105.74
2	E	601	FAD	C4A-C5A-N7A	-3.29	106.82	110.58
2	A	601	FAD	C4X-C10-N1	-3.29	116.53	124.59
2	D	601	FAD	C4A-N9A-C8A	3.07	108.97	105.74
2	C	601	FAD	C4A-N9A-C8A	3.07	108.96	105.74
2	D	601	FAD	C4X-C10-N1	-3.05	117.12	124.59
2	B	601	FAD	C4X-C10-N1	-3.03	117.16	124.59
2	F	601	FAD	C4X-C10-N1	-3.02	117.17	124.59
2	A	601	FAD	C4X-C10-N10	3.02	120.81	116.48
2	F	601	FAD	C4A-N9A-C8A	3.02	108.91	105.74
2	E	601	FAD	C4X-C10-N1	-3.00	117.22	124.59
2	C	601	FAD	C4X-C10-N10	2.99	120.75	116.48
2	C	601	FAD	C4X-C10-N1	-2.98	117.28	124.59
2	E	601	FAD	C4A-N9A-C8A	2.98	108.87	105.74
2	E	601	FAD	C4X-C10-N10	2.97	120.73	116.48
2	C	601	FAD	C5A-N7A-C8A	2.93	108.06	103.45
2	B	601	FAD	C4A-N9A-C8A	2.88	108.76	105.74
2	F	601	FAD	C4X-C10-N10	2.86	120.58	116.48
2	B	601	FAD	C4X-C10-N10	2.85	120.56	116.48
2	A	601	FAD	C5A-N7A-C8A	2.82	107.88	103.45
2	D	601	FAD	C4X-C10-N10	2.79	120.47	116.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	C5A-N7A-C8A	2.78	107.81	103.45
2	F	601	FAD	C5A-N7A-C8A	2.73	107.74	103.45
2	D	601	FAD	C9A-N10-C10	-2.68	116.67	120.75
2	D	601	FAD	C5A-N7A-C8A	2.67	107.64	103.45
2	E	601	FAD	C5A-N7A-C8A	2.66	107.63	103.45
2	A	601	FAD	C10-N1-C2	2.63	122.54	116.85
2	D	601	FAD	O4-C4-C4X	-2.62	119.62	126.53
2	A	601	FAD	C9A-N10-C10	-2.61	116.77	120.75
2	C	601	FAD	N9A-C8A-N7A	-2.57	110.29	113.94
2	A	601	FAD	N9A-C8A-N7A	-2.53	110.34	113.94
2	E	601	FAD	C9A-N10-C10	-2.50	116.94	120.75
2	E	601	FAD	O4-C4-C4X	-2.47	120.00	126.53
2	F	601	FAD	C10-N1-C2	2.47	122.19	116.85
2	F	601	FAD	C4-C4X-N5	2.44	121.58	118.21
2	B	601	FAD	C10-N1-C2	2.44	122.14	116.85
2	B	601	FAD	O4-C4-C4X	-2.44	120.09	126.53
2	C	601	FAD	C9A-N10-C10	-2.38	117.12	120.75
2	E	601	FAD	C1'-N10-C9A	2.36	125.22	120.63
2	D	601	FAD	C10-N1-C2	2.36	121.96	116.85
2	A	601	FAD	C4-N3-C2	-2.36	121.46	125.64
2	F	601	FAD	N9A-C8A-N7A	-2.35	110.60	113.94
2	E	601	FAD	C10-N1-C2	2.35	121.94	116.85
2	D	601	FAD	C4-N3-C2	-2.34	121.48	125.64
2	D	601	FAD	N9A-C8A-N7A	-2.32	110.64	113.94
2	F	601	FAD	O4B-C1B-N9A	2.32	112.54	108.09
2	E	601	FAD	N9A-C8A-N7A	-2.31	110.66	113.94
2	B	601	FAD	N9A-C8A-N7A	-2.31	110.66	113.94
2	B	601	FAD	C4-N3-C2	-2.30	121.56	125.64
2	C	601	FAD	C10-N1-C2	2.29	121.82	116.85
2	E	601	FAD	C4-N3-C2	-2.28	121.59	125.64
2	A	601	FAD	O4-C4-C4X	-2.26	120.56	126.53
2	C	601	FAD	C1'-N10-C9A	2.24	124.99	120.63
2	C	601	FAD	O4-C4-C4X	-2.24	120.62	126.53
2	F	601	FAD	C4-N3-C2	-2.24	121.67	125.64
2	F	601	FAD	O4-C4-C4X	-2.22	120.67	126.53
2	C	601	FAD	C6A-C5A-N7A	2.18	136.30	132.09
2	A	601	FAD	C6A-C5A-N7A	2.16	136.26	132.09
2	A	601	FAD	C4X-C4-N3	2.16	118.76	113.25
2	B	601	FAD	C9A-N10-C10	-2.12	117.51	120.75
2	E	601	FAD	O2-C2-N1	-2.12	118.28	121.80
2	F	601	FAD	C6A-C5A-N7A	2.11	136.16	132.09
2	B	601	FAD	C1'-N10-C9A	2.11	124.73	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	C4-C4X-N5	2.10	121.11	118.21
2	C	601	FAD	C4-N3-C2	-2.09	121.93	125.64
2	F	601	FAD	C2A-N1A-C6A	2.08	122.16	118.73
2	A	601	FAD	C2A-N1A-C6A	2.07	122.14	118.73
2	B	601	FAD	C4X-C4-N3	2.05	118.48	113.25
2	E	601	FAD	C4'-C3'-C2'	-2.05	110.16	113.57
2	A	601	FAD	C1'-N10-C9A	2.04	124.59	120.63
2	F	601	FAD	C4X-C4-N3	2.03	118.43	113.25
2	D	601	FAD	C4X-C4-N3	2.03	118.42	113.25
2	F	601	FAD	C1'-N10-C9A	2.01	124.54	120.63
2	E	601	FAD	C2A-N1A-C6A	2.01	122.02	118.73
2	F	601	FAD	C10-C4X-N5	-2.00	120.72	124.81

There are no chirality outliers.

All (22) torsion outliers are listed below:

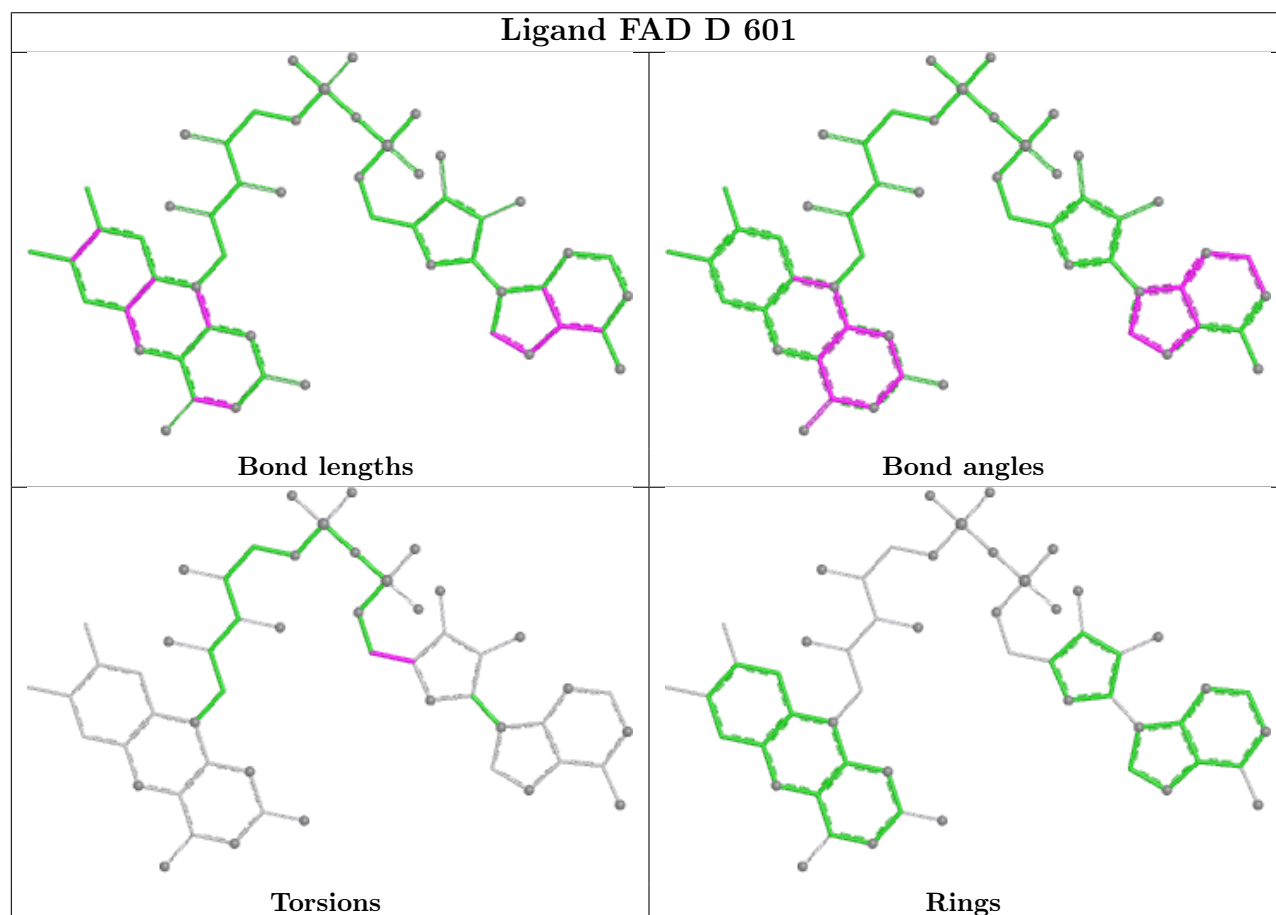
Mol	Chain	Res	Type	Atoms
2	A	601	FAD	C5B-O5B-PA-O1A
2	A	601	FAD	C5B-O5B-PA-O2A
2	A	601	FAD	C5B-O5B-PA-O3P
2	E	601	FAD	C3'-C4'-C5'-O5'
2	E	601	FAD	O4'-C4'-C5'-O5'
2	E	601	FAD	PA-O3P-P-O5'
2	F	601	FAD	C5B-O5B-PA-O1A
2	F	601	FAD	C5B-O5B-PA-O2A
2	F	601	FAD	C5B-O5B-PA-O3P
2	F	601	FAD	C3B-C4B-C5B-O5B
2	B	601	FAD	O4B-C4B-C5B-O5B
2	F	601	FAD	O4B-C4B-C5B-O5B
2	B	601	FAD	C3B-C4B-C5B-O5B
2	C	601	FAD	O4B-C4B-C5B-O5B
2	C	601	FAD	C3B-C4B-C5B-O5B
2	D	601	FAD	O4B-C4B-C5B-O5B
2	D	601	FAD	C3B-C4B-C5B-O5B
2	E	601	FAD	C4B-C5B-O5B-PA
2	A	601	FAD	C3B-C4B-C5B-O5B
2	C	601	FAD	PA-O3P-P-O5'
2	A	601	FAD	P-O3P-PA-O2A
2	C	601	FAD	P-O3P-PA-O2A

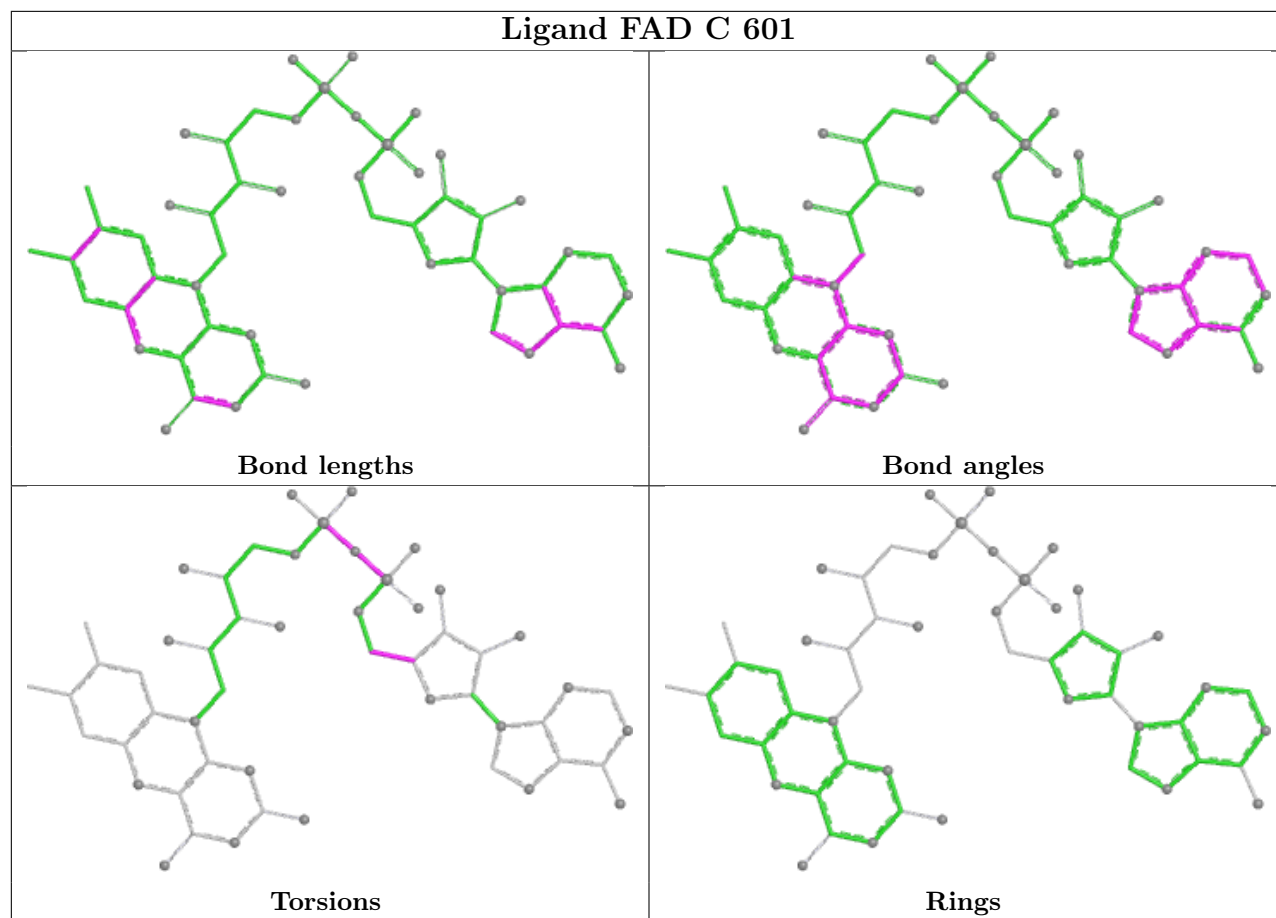
There are no ring outliers.

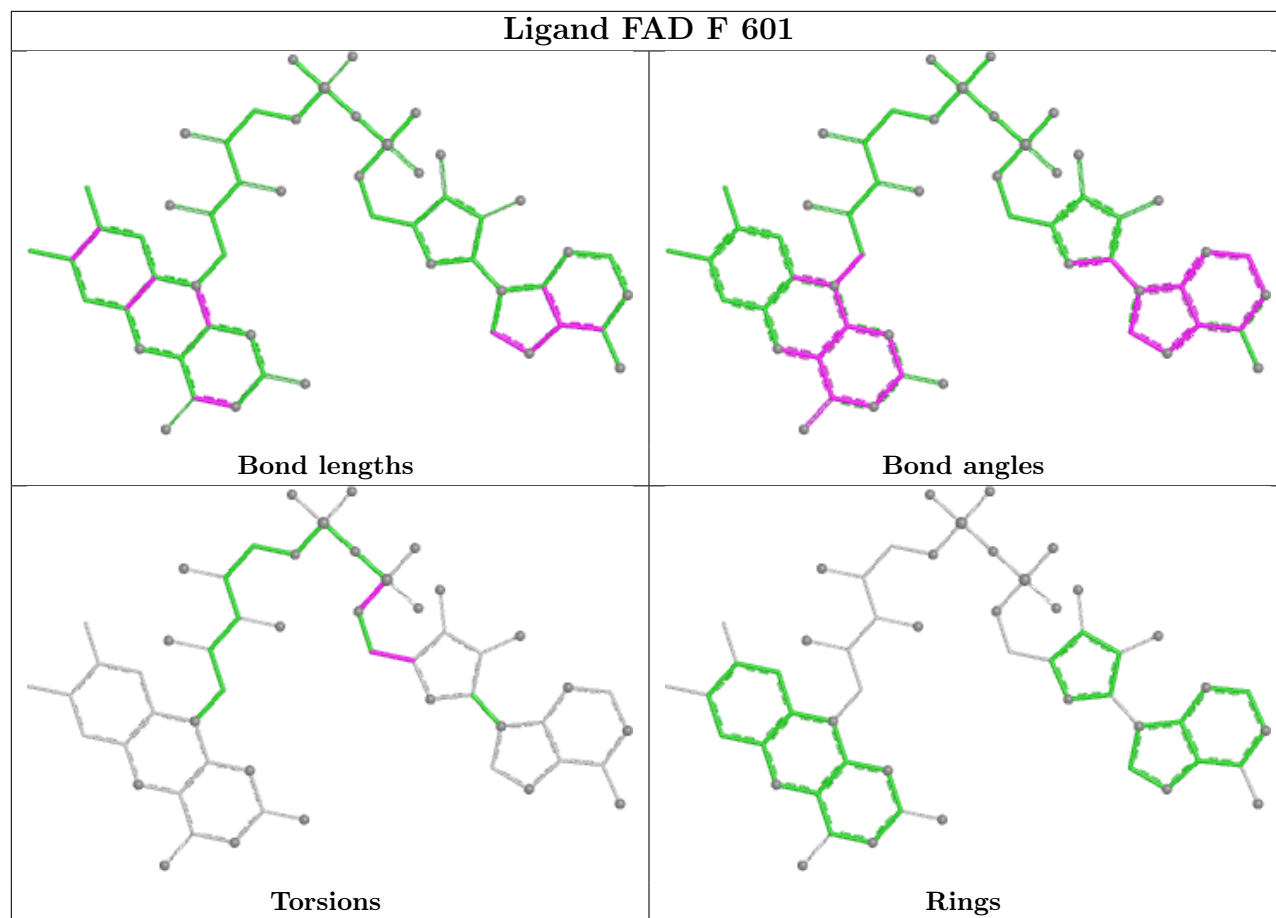
2 monomers are involved in 3 short contacts:

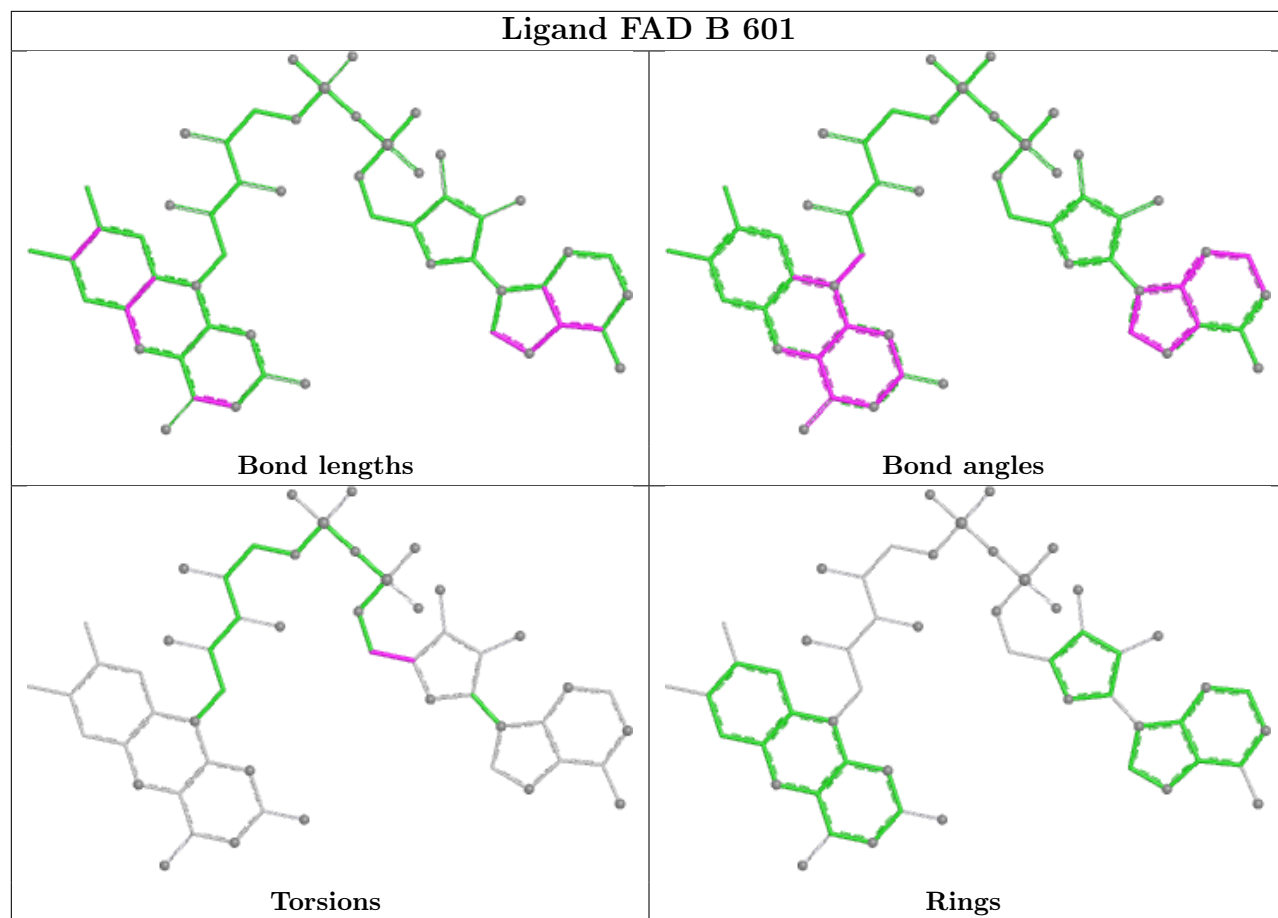
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	FAD	2	0
2	E	601	FAD	1	0

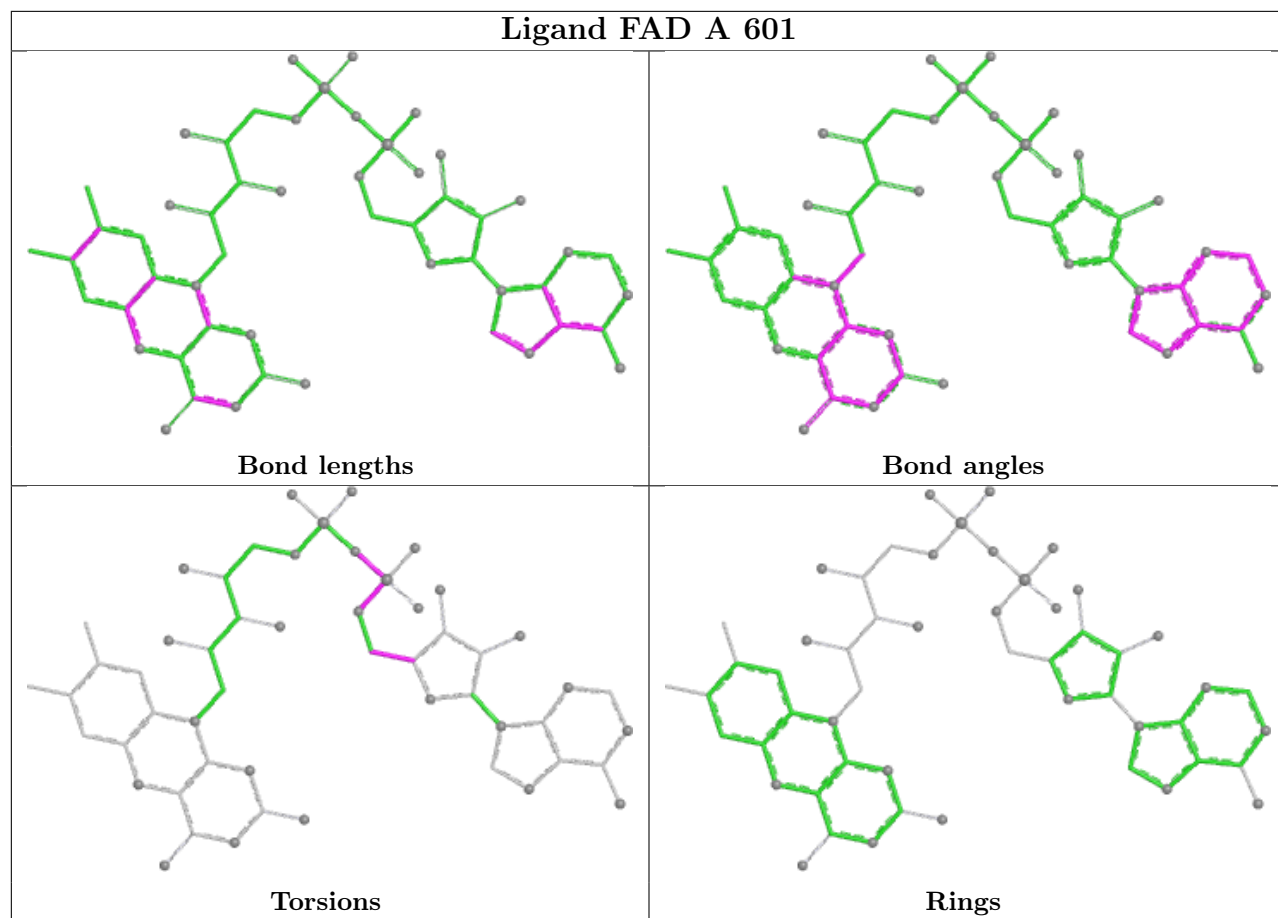
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

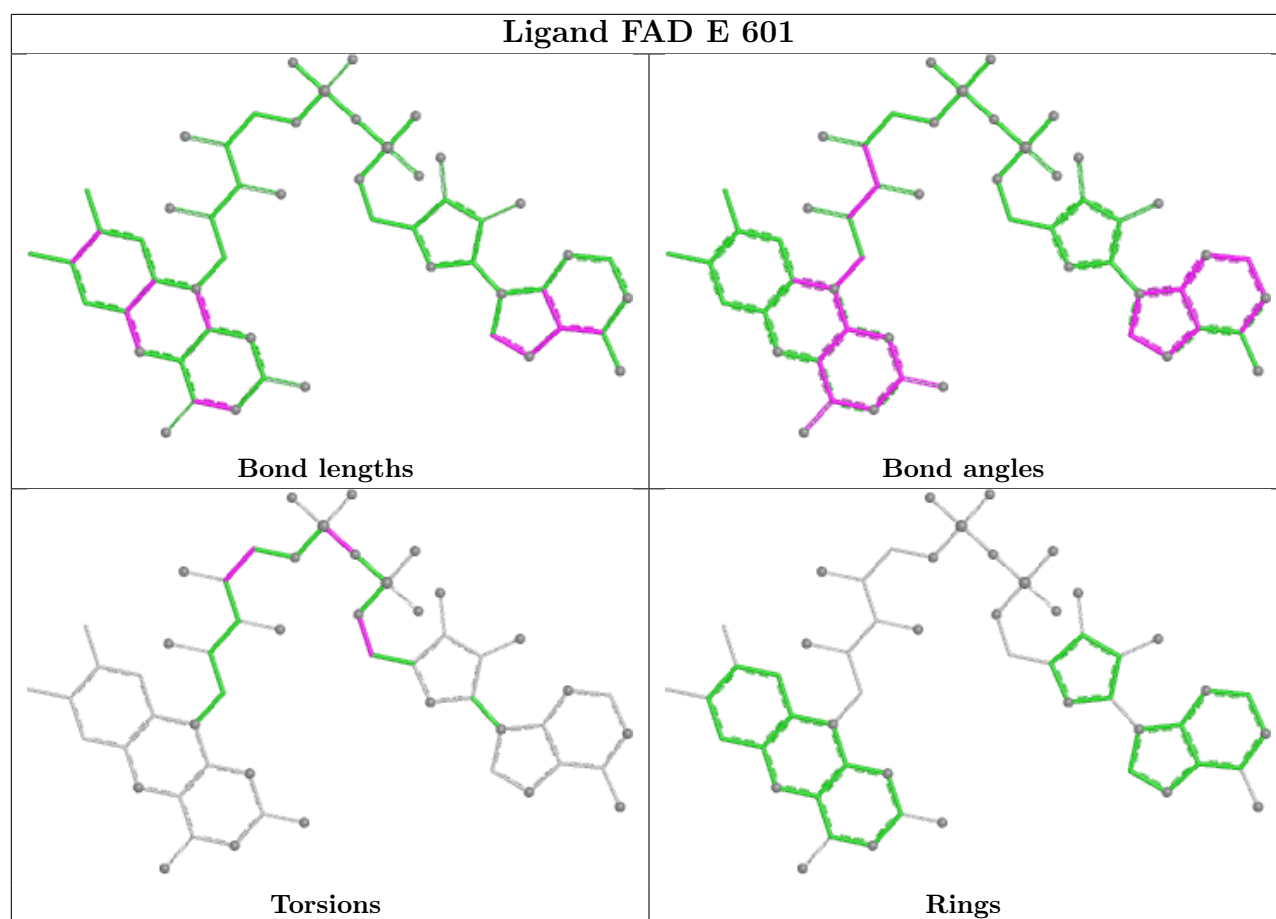












5.7 Other polymers [i](#)

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	453/554 (81%)	0.15	19 (4%) 40 23	35, 61, 87, 122	0
1	B	454/554 (81%)	0.06	11 (2%) 59 36	31, 57, 81, 100	0
1	C	453/554 (81%)	0.19	16 (3%) 47 27	37, 63, 96, 122	0
1	D	453/554 (81%)	0.10	9 (1%) 65 40	36, 59, 88, 105	0
1	E	453/554 (81%)	0.10	11 (2%) 59 36	39, 59, 86, 110	0
1	F	453/554 (81%)	0.16	14 (3%) 51 30	42, 67, 101, 141	0
All	All	2719/3324 (81%)	0.13	80 (2%) 53 31	31, 61, 92, 141	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	83	ASP	4.8
1	E	180	MET	4.2
1	C	179	TYR	4.1
1	D	187	ASN	4.0
1	F	83	ASP	3.6
1	B	257	SER	3.6
1	E	186	TYR	3.5
1	F	183	ILE	3.3
1	D	188	PHE	3.3
1	F	314	GLU	3.2
1	A	184	ASP	3.2
1	C	321	GLU	3.1
1	F	127	CYS	3.1
1	A	187	ASN	3.0
1	F	317	GLU	3.0
1	A	181	ASP	3.0
1	C	188	PHE	3.0
1	C	180	MET	3.0
1	A	258	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	535	ASP	2.8
1	E	321	GLU	2.8
1	A	179	TYR	2.8
1	A	257	SER	2.8
1	F	201	SER	2.8
1	C	184	ASP	2.8
1	E	330	ASN	2.7
1	D	182	LEU	2.6
1	A	183	ILE	2.6
1	F	182	LEU	2.6
1	D	179	TYR	2.6
1	F	184	ASP	2.6
1	E	187	ASN	2.5
1	D	314	GLU	2.5
1	E	83	ASP	2.5
1	B	186	TYR	2.5
1	B	314	GLU	2.5
1	C	183	ILE	2.4
1	C	314	GLU	2.4
1	A	534	PHE	2.4
1	A	83	ASP	2.4
1	C	330	ASN	2.4
1	F	330	ASN	2.4
1	D	186	TYR	2.4
1	A	322	ILE	2.4
1	F	187	ASN	2.4
1	A	320	GLY	2.4
1	B	188	PHE	2.4
1	E	181	ASP	2.4
1	A	152	GLN	2.4
1	D	177	GLN	2.4
1	B	184	ASP	2.3
1	A	535	ASP	2.3
1	E	127	CYS	2.3
1	F	321	GLU	2.3
1	D	257	SER	2.3
1	E	183	ILE	2.3
1	B	326	TYR	2.3
1	B	321	GLU	2.3
1	A	321	GLU	2.3
1	A	314	GLU	2.2
1	A	317	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	327	VAL	2.2
1	B	534	PHE	2.2
1	F	227	GLN	2.2
1	C	152	GLN	2.2
1	B	82	GLU	2.2
1	B	179	TYR	2.1
1	E	179	TYR	2.1
1	A	177	GLN	2.1
1	E	257	SER	2.1
1	F	257	SER	2.1
1	D	83	ASP	2.1
1	A	325	VAL	2.1
1	A	256	GLY	2.1
1	B	327	VAL	2.1
1	F	325	VAL	2.1
1	C	182	LEU	2.0
1	C	315	ARG	2.0
1	C	272	GLY	2.0
1	C	322	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

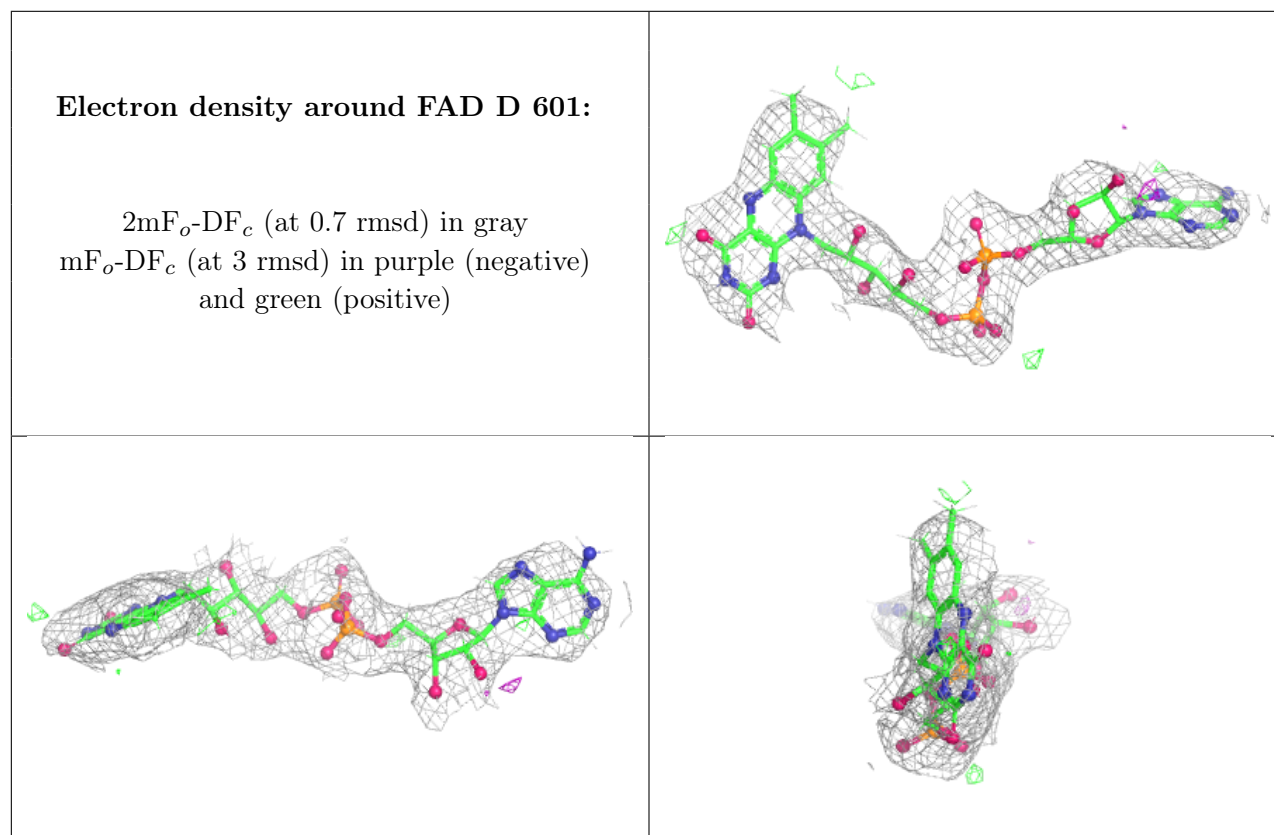
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	D	601	53/53	0.95	0.10	28,49,72,83	0
2	FAD	E	601	53/53	0.95	0.11	32,56,83,85	0
2	FAD	F	601	53/53	0.95	0.10	40,56,78,85	0
2	FAD	C	601	53/53	0.96	0.09	33,50,69,88	0

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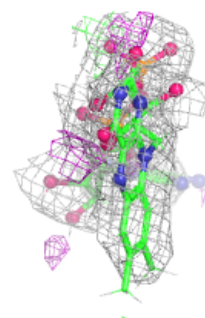
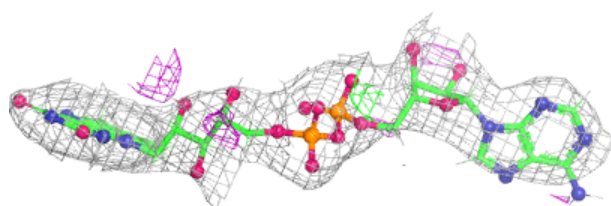
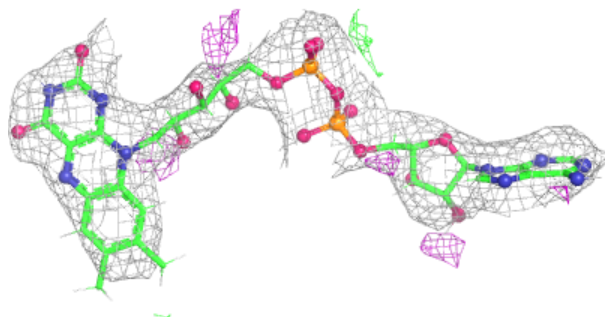
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	A	601	53/53	0.96	0.09	36,51,70,79	0
2	FAD	B	601	53/53	0.97	0.09	33,50,67,79	0

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.

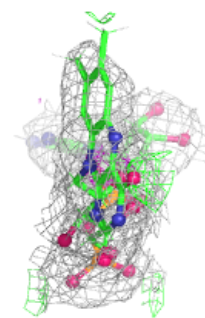
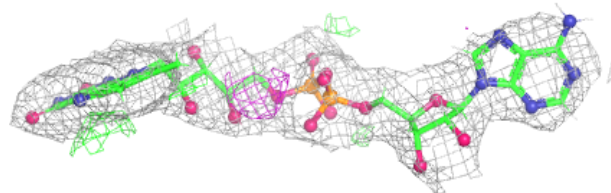


Electron density around FAD E 601:

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

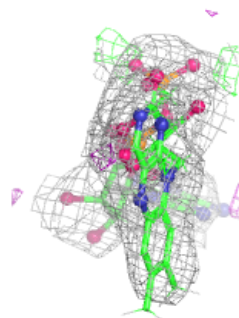
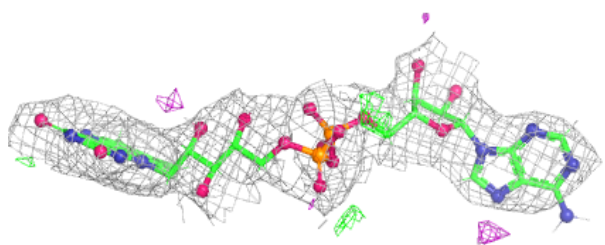
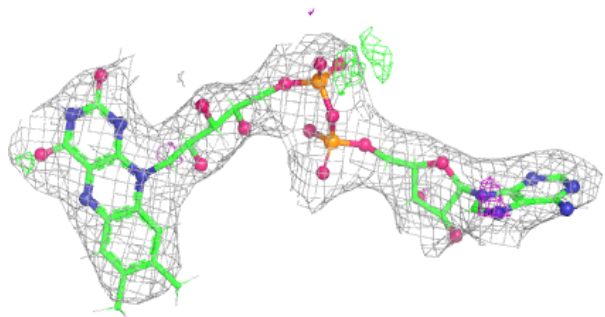
**Electron density around FAD F 601:**

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

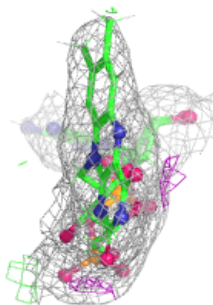
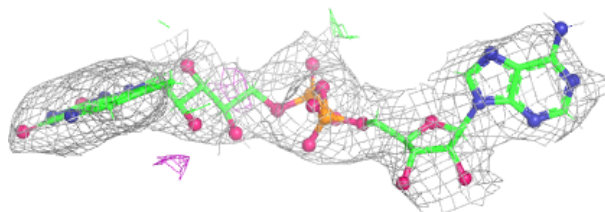
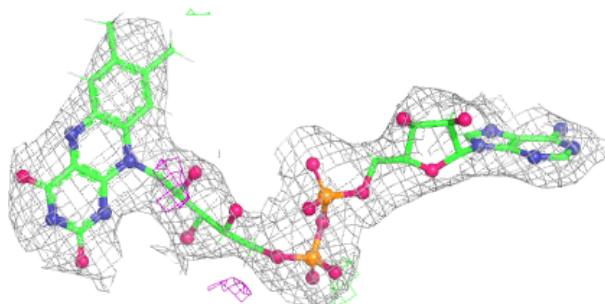


Electron density around FAD C 601:

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

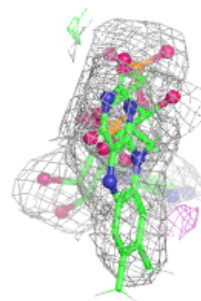
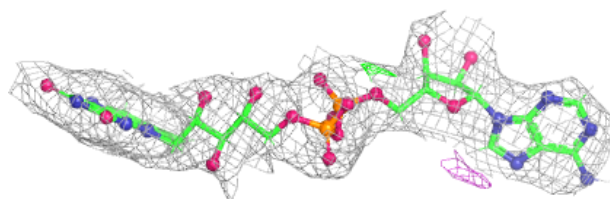
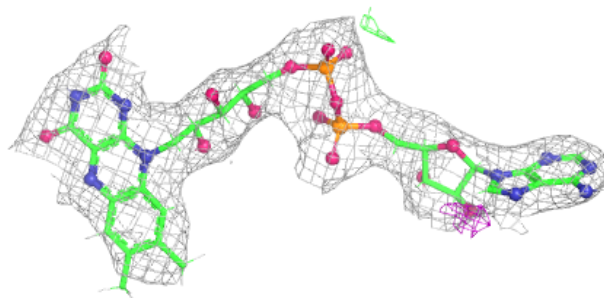
**Electron density around FAD A 601:**

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



Electron density around FAD B 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.