



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:14 AM UTC

PDB ID : 3F8D / pdb_00003f8d
Title : Structure of Sulfolobus solfataricus Thioredoxin reductase Mutant C147A
Authors : Ruggiero, A.; Masullo, M.; Ruocco, M.R.; Arcari, P.; Zagari, A.; Vitagliano, L.
Deposited on : 2008-11-12
Resolution : 1.40 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 Phenix2.0
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

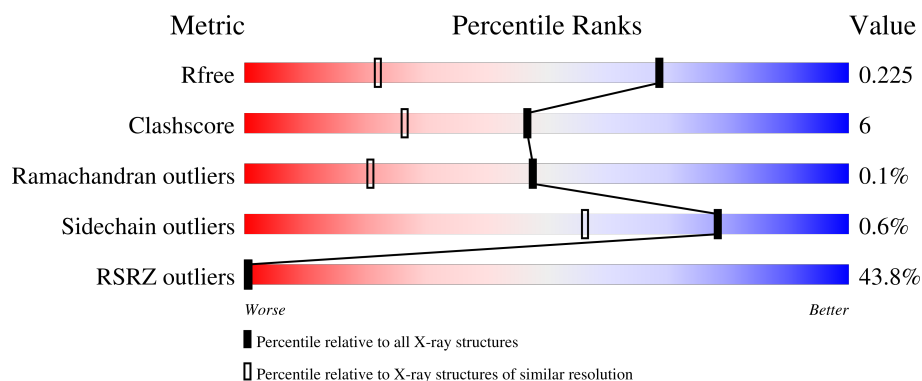
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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}	180053	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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	A	323	41% 86% 9% 5%
1	B	323	39% 85% 10% . .
1	C	323	46% 81% 13% 5%
1	D	323	39% 80% 12% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10030 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

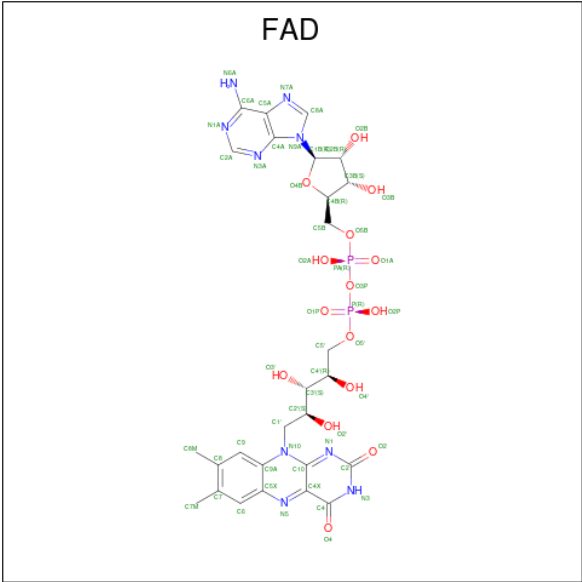
- Molecule 1 is a protein called Thioredoxin reductase (TrxB-3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2369	1524	395	445	5			
1	B	309	Total	C	N	O	S	0	0	0
			2377	1528	396	448	5			
1	C	307	Total	C	N	O	S	0	0	0
			2358	1518	391	444	5			
1	D	298	Total	C	N	O	S	0	0	0
			2287	1470	381	431	5			

There are 4 discrepancies between the modelled and reference sequences:

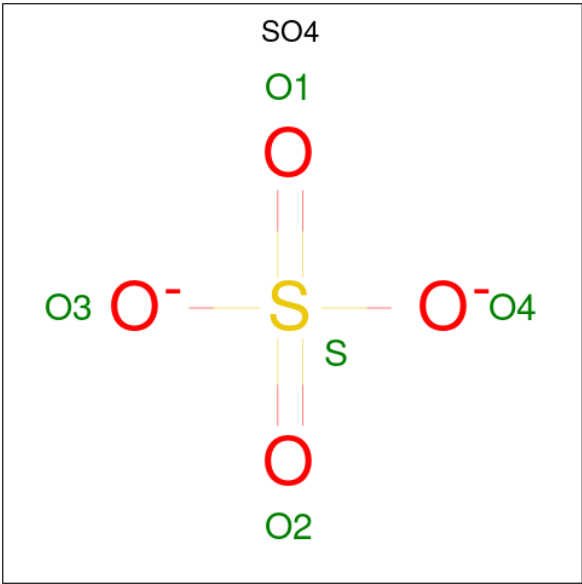
Chain	Residue	Modelled	Actual	Comment	Reference
A	147	ALA	CYS	engineered mutation	UNP Q97W27
B	147	ALA	CYS	engineered mutation	UNP Q97W27
C	147	ALA	CYS	engineered mutation	UNP Q97W27
D	147	ALA	CYS	engineered mutation	UNP Q97W27

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



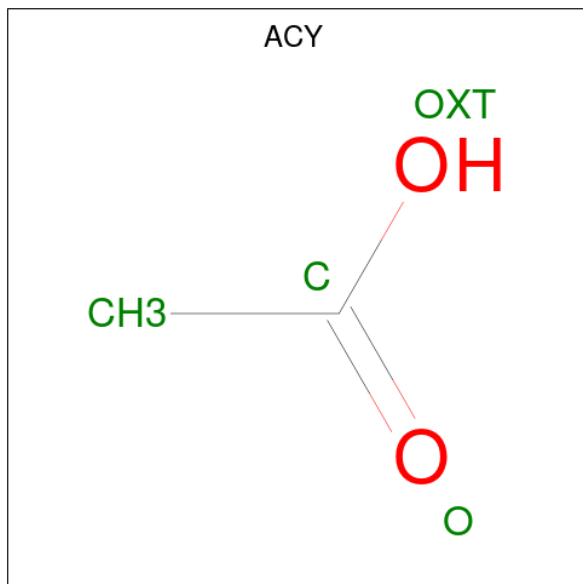
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	110	Total O 110 110	0	0
5	B	106	Total O 106 106	0	0
5	C	96	Total O 96 96	0	0

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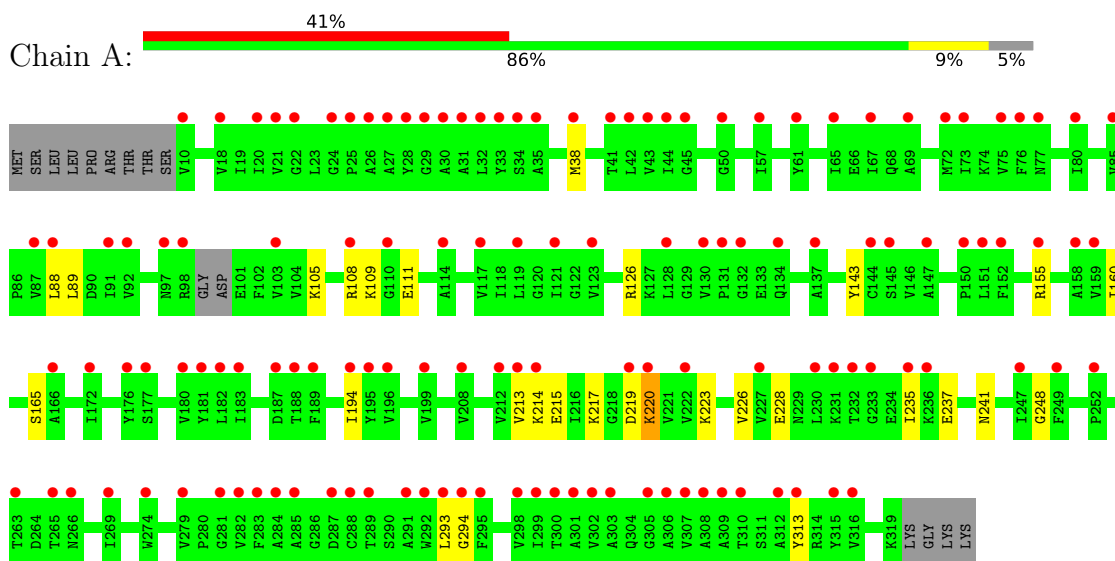
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	81	Total	O	0	0
			81	81		

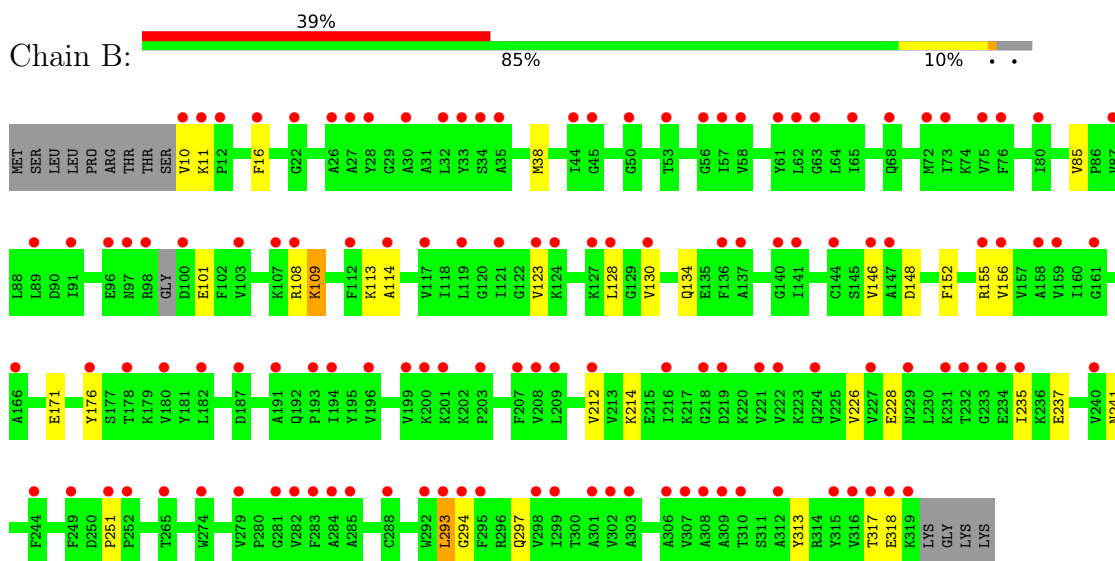
3 Residue-property plots [i](#)

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.

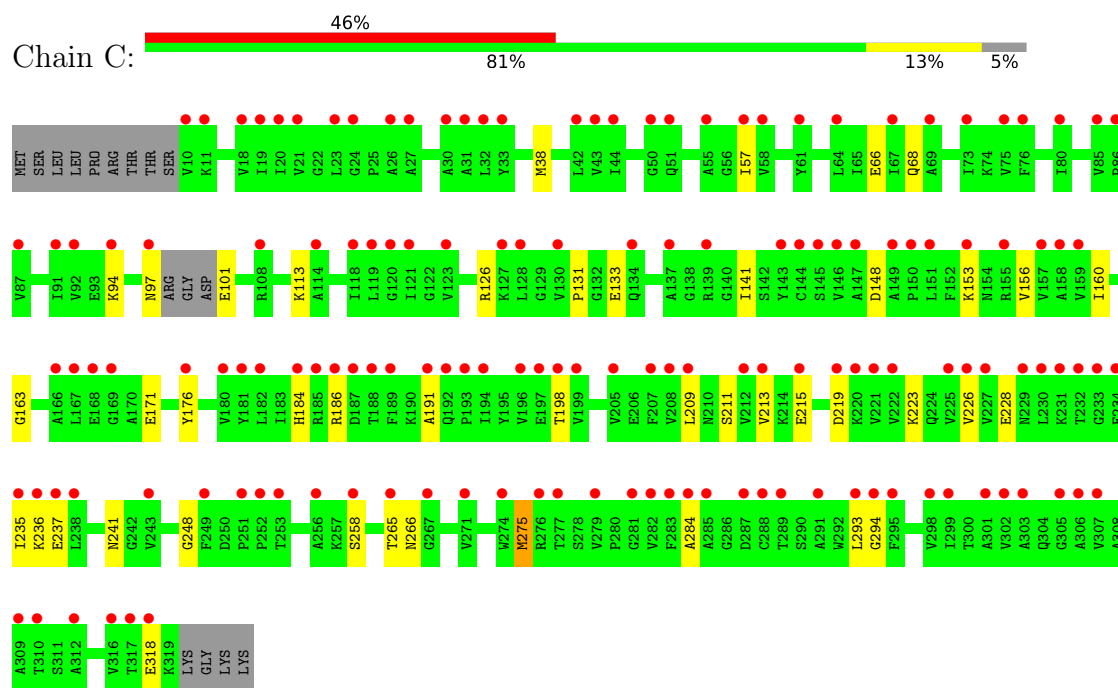
- Molecule 1: Thioredoxin reductase (TrxB-3)



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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.58Å 121.87Å 126.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.40 15.00 – 1.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-1.40) 97.3 (15.00-1.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.73 (at 1.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.206 , 0.226 0.211 , 0.225	Depositor DCC
R_{free} test set	814 reflections (0.35%)	wwPDB-VP
Wilson B-factor (Å ²)	13.6	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.47 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.008 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10030	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACY, FAD, SO4

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	0.78	0/2409	0.99	1/3255 (0.0%)
1	B	0.77	1/2417 (0.0%)	1.00	3/3266 (0.1%)
1	C	0.76	1/2398 (0.0%)	0.97	2/3241 (0.1%)
1	D	0.69	0/2326	0.97	2/3144 (0.1%)
All	All	0.75	2/9550 (0.0%)	0.98	8/12906 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	38	MET	SD-CE	-5.33	1.66	1.79
1	C	275	MET	SD-CE	-5.18	1.66	1.79

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	148	ASP	N-CA-C	6.35	121.19	113.38
1	B	148	ASP	N-CA-C	5.67	120.35	113.38
1	D	121	ILE	N-CA-C	5.43	119.05	112.80
1	A	220	LYS	N-CA-C	-5.35	106.92	113.50
1	B	85	VAL	CA-C-N	-5.30	114.46	119.76
1	B	85	VAL	C-N-CA	-5.30	114.46	119.76
1	C	148	ASP	N-CA-C	5.07	119.61	113.38
1	C	211	SER	N-CA-C	5.04	117.33	109.52

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	A	2369	0	2432	28	0
1	B	2377	0	2436	25	0
1	C	2358	0	2419	30	0
1	D	2287	0	2334	37	0
2	A	53	0	31	1	0
2	B	53	0	31	0	0
2	C	53	0	31	0	0
2	D	53	0	31	1	0
3	A	10	0	0	1	0
3	B	10	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	B	4	0	3	0	0
5	A	110	0	0	0	0
5	B	106	0	0	1	0
5	C	96	0	0	0	0
5	D	81	0	0	1	0
All	All	10030	0	9748	110	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 6.

All (110) 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:A:105:LYS:HE2	1:A:111:GLU:OE2	1.64	0.98
1:A:105:LYS:HG2	1:A:111:GLU:HG2	1.54	0.88
1:B:156:VAL:H	1:B:241:ASN:HD22	1.24	0.85
1:A:88:LEU:HD11	1:A:109:LYS:HD3	1.63	0.81
1:D:156:VAL:H	1:D:241:ASN:HD22	1.29	0.78
1:A:88:LEU:HD11	1:A:109:LYS:CD	2.14	0.77
1:A:219:ASP:OD1	1:A:223:LYS:HE3	1.88	0.74
1:B:134:GLN:HG2	5:B:5562:HOH:O	1.87	0.73
1:D:146:VAL:HG21	1:D:297:GLN:HE22	1.52	0.73
1:D:143:TYR:HB2	2:D:2004:FAD:HM72	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:LEU:HD23	1:A:294:GLY:N	2.06	0.70
1:C:293:LEU:HD13	1:C:294:GLY:N	2.05	0.70
1:C:38:MET:HG2	1:D:176:TYR:CZ	2.28	0.69
1:A:219:ASP:CG	1:A:220:LYS:H	2.01	0.68
1:B:146:VAL:HG21	1:B:297:GLN:HE22	1.57	0.68
1:D:293:LEU:HD13	1:D:294:GLY:N	2.08	0.68
1:C:293:LEU:HD13	1:C:293:LEU:C	2.19	0.67
1:C:318:GLU:HG2	1:D:194:ILE:HG12	1.77	0.66
1:C:126:ARG:NH1	1:C:248:GLY:HA3	2.12	0.65
1:D:194:ILE:HG23	1:D:195:TYR:HD1	1.62	0.65
1:B:214:LYS:CE	1:B:228:GLU:OE1	2.46	0.64
1:C:318:GLU:HG2	1:D:194:ILE:CG1	2.28	0.64
1:A:108:ARG:CZ	1:A:109:LYS:HE3	2.28	0.63
1:A:214:LYS:HE3	1:A:228:GLU:OE1	1.98	0.63
1:D:219:ASP:CG	1:D:220:LYS:H	2.07	0.62
1:D:219:ASP:CG	1:D:223:LYS:HE3	2.26	0.61
1:A:38:MET:HG2	1:B:176:TYR:CZ	2.37	0.59
1:C:171:GLU:OE1	1:C:198:THR:HG22	2.02	0.59
1:D:293:LEU:HD13	1:D:293:LEU:C	2.27	0.59
1:D:90:ASP:OD1	1:D:108:ARG:HD2	2.03	0.58
1:C:94:LYS:NZ	1:C:258:SER:O	2.35	0.58
1:B:128:LEU:HG	1:B:130:VAL:HG13	1.85	0.58
1:A:143:TYR:HB2	2:A:2001:FAD:HM72	1.86	0.57
1:B:156:VAL:H	1:B:241:ASN:ND2	2.00	0.57
1:A:215:GLU:HG2	1:A:217:LYS:HG2	1.89	0.55
1:D:156:VAL:H	1:D:241:ASN:ND2	2.01	0.55
1:D:139:ARG:HH21	1:D:220:LYS:HB3	1.72	0.54
1:A:226:VAL:HG22	1:A:237:GLU:HG2	1.89	0.54
1:D:13:GLY:HA3	1:D:111:GLU:O	2.07	0.54
1:A:194:ILE:HG12	1:B:318:GLU:HG2	1.89	0.54
1:C:101:GLU:OE2	1:C:113:LYS:HD3	2.09	0.53
1:C:160:ILE:HD11	1:C:213:VAL:HG21	1.90	0.53
1:D:139:ARG:NH2	1:D:220:LYS:HB3	2.24	0.53
1:A:88:LEU:HD11	1:A:109:LYS:HD2	1.90	0.52
1:A:293:LEU:HD23	1:A:293:LEU:C	2.34	0.52
1:B:109:LYS:N	1:B:109:LYS:HD2	2.25	0.52
1:C:265:THR:O	1:C:265:THR:HG22	2.10	0.52
1:B:226:VAL:HG22	1:B:237:GLU:HG2	1.92	0.52
1:B:214:LYS:HE2	1:B:228:GLU:HB3	1.92	0.51
1:C:160:ILE:CD1	1:C:213:VAL:HG21	2.41	0.51
1:A:214:LYS:HD2	1:A:235:ILE:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:VAL:HG22	1:C:237:GLU:HG2	1.92	0.51
1:B:152:PHE:HA	1:B:155:ARG:HD3	1.92	0.50
1:D:211:SER:HB3	1:D:227:VAL:CG1	2.42	0.50
1:D:219:ASP:OD1	1:D:223:LYS:HE3	2.11	0.49
1:C:163:GLY:C	1:C:191:ALA:HB2	2.37	0.49
1:C:293:LEU:C	1:C:293:LEU:CD1	2.85	0.49
1:A:89:LEU:O	1:A:108:ARG:NH2	2.45	0.49
1:B:108:ARG:C	1:B:109:LYS:HD2	2.38	0.48
1:D:194:ILE:HG23	1:D:195:TYR:CD1	2.45	0.48
1:D:13:GLY:O	1:D:112:PHE:CD2	2.67	0.47
1:D:219:ASP:CG	1:D:220:LYS:N	2.71	0.47
1:A:108:ARG:NE	1:A:109:LYS:HE3	2.28	0.47
1:A:194:ILE:CG1	1:B:318:GLU:HG2	2.45	0.47
1:C:219:ASP:N	1:C:219:ASP:OD1	2.46	0.47
1:A:219:ASP:CG	1:A:220:LYS:N	2.70	0.47
1:B:214:LYS:HE2	1:B:228:GLU:CB	2.46	0.46
1:D:133:GLU:HA	1:D:141:ILE:CD1	2.46	0.46
1:C:265:THR:O	1:C:265:THR:CG2	2.63	0.46
1:D:95:ILE:HD11	1:D:119:LEU:HD21	1.96	0.46
1:C:126:ARG:HH11	1:C:248:GLY:HA3	1.81	0.46
1:B:313:TYR:O	1:B:317:THR:HG23	2.16	0.46
1:D:160:ILE:HD11	1:D:213:VAL:HG21	1.98	0.45
1:B:101:GLU:OE2	1:B:113:LYS:HE2	2.17	0.45
1:C:38:MET:HG2	1:D:176:TYR:CE2	2.51	0.45
1:C:57:ILE:HD11	1:C:68:GLN:NE2	2.32	0.45
1:C:219:ASP:CG	1:C:223:LYS:NZ	2.75	0.45
1:B:16:PHE:O	1:B:114:ALA:HA	2.17	0.44
1:C:153:LYS:HG2	1:C:176:TYR:HD1	1.81	0.44
1:C:228:GLU:HB2	1:C:235:ILE:HD12	2.00	0.44
1:D:220:LYS:HE3	1:D:220:LYS:HB2	1.73	0.44
1:A:108:ARG:NH2	1:A:109:LYS:HE3	2.34	0.43
1:C:318:GLU:CG	1:D:194:ILE:HG12	2.48	0.43
1:A:155:ARG:HB3	1:A:241:ASN:HD22	1.83	0.43
1:B:214:LYS:HE3	1:B:228:GLU:OE1	2.18	0.43
1:A:293:LEU:C	1:A:293:LEU:CD2	2.92	0.42
1:D:134:GLN:NE2	5:D:5617:HOH:O	2.50	0.42
1:B:10:VAL:C	1:B:11:LYS:HD2	2.45	0.42
1:B:123:VAL:HG12	1:B:251:PRO:HA	2.00	0.42
1:D:13:GLY:O	1:D:112:PHE:HA	2.20	0.42
1:D:215:GLU:OE2	1:D:217:LYS:HG2	2.19	0.42
1:D:141:ILE:HD11	1:D:216:ILE:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:VAL:HG21	1:B:214:LYS:NZ	2.34	0.42
1:A:313:TYR:OH	1:B:171:GLU:HG3	2.19	0.42
1:C:131:PRO:HB2	1:C:215:GLU:HG3	2.02	0.42
1:C:66:GLU:OE2	1:D:82:LYS:HD2	2.19	0.42
1:C:184:HIS:HB3	1:C:209:LEU:HD23	2.01	0.42
1:D:171:GLU:OE2	1:D:202:LYS:HE3	2.20	0.42
1:D:13:GLY:O	1:D:112:PHE:HD2	2.03	0.41
1:D:191:ALA:O	1:D:192:GLN:C	2.63	0.41
1:B:228:GLU:HB2	1:B:235:ILE:CD1	2.51	0.41
1:A:126:ARG:NH1	1:A:248:GLY:HA3	2.35	0.41
1:A:160:ILE:HD11	1:A:213:VAL:HG21	2.03	0.41
1:C:133:GLU:HA	1:C:141:ILE:CD1	2.51	0.41
1:A:165:SER:OG	3:A:4159:SO4:O1	2.32	0.41
1:C:156:VAL:H	1:C:241:ASN:HD22	1.69	0.41
1:D:64:LEU:HD23	1:D:64:LEU:HA	1.91	0.41
1:D:219:ASP:OD1	1:D:220:LYS:N	2.54	0.40
1:B:293:LEU:HD23	1:B:294:GLY:N	2.36	0.40
1:C:275:MET:HB3	1:C:284:ALA:O	2.21	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	304/323 (94%)	296 (97%)	8 (3%)	0	100	100
1	B	305/323 (94%)	298 (98%)	7 (2%)	0	100	100
1	C	303/323 (94%)	297 (98%)	6 (2%)	0	100	100
1	D	294/323 (91%)	287 (98%)	6 (2%)	1 (0%)	36	16
All	All	1206/1292 (93%)	1178 (98%)	27 (2%)	1 (0%)	48	21

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	14	GLU

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	253/266 (95%)	253 (100%)	0	100	100
1	B	254/266 (96%)	252 (99%)	2 (1%)	73	48
1	C	252/266 (95%)	248 (98%)	4 (2%)	55	23
1	D	243/266 (91%)	243 (100%)	0	100	100
All	All	1002/1064 (94%)	996 (99%)	6 (1%)	78	56

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	109	LYS
1	B	293	LEU
1	C	97	ASN
1	C	186	ARG
1	C	236	LYS
1	C	266	ASN

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

Mol	Chain	Res	Type
1	A	210	ASN
1	A	241	ASN
1	A	297	GLN
1	B	241	ASN
1	B	297	GLN
1	C	241	ASN
1	D	134	GLN
1	D	224	GLN
1	D	241	ASN
1	D	297	GLN

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](#)

11 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	SO4	C	4163	-	4,4,4	1.80	2 (50%)	6,6,6	0.88	0
3	SO4	D	4162	-	4,4,4	1.83	2 (50%)	6,6,6	0.79	0
2	FAD	B	2002	-	58,58,58	1.50	8 (13%)	85,89,89	1.07	7 (8%)
3	SO4	B	4158	-	4,4,4	1.77	1 (25%)	6,6,6	0.83	0
3	SO4	A	4157	-	4,4,4	1.84	2 (50%)	6,6,6	0.85	0
2	FAD	A	2001	-	58,58,58	1.14	5 (8%)	85,89,89	1.07	5 (5%)
3	SO4	A	4159	-	4,4,4	1.77	2 (50%)	6,6,6	0.78	0
2	FAD	C	2003	-	58,58,58	1.40	8 (13%)	85,89,89	1.06	6 (7%)
4	ACY	B	1501	-	3,3,3	1.67	1 (33%)	3,3,3	1.25	0
2	FAD	D	2004	-	58,58,58	1.39	7 (12%)	85,89,89	1.12	9 (10%)
3	SO4	B	4161	-	4,4,4	1.82	2 (50%)	6,6,6	0.88	0

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	C	2003	-	-	2/34/50/50	0/6/6/6
2	FAD	A	2001	-	-	2/34/50/50	0/6/6/6
2	FAD	D	2004	-	-	1/34/50/50	0/6/6/6
2	FAD	B	2002	-	-	1/34/50/50	0/6/6/6

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2004	FAD	O2-C2	-4.77	1.15	1.24
2	B	2002	FAD	C4X-N5	4.51	1.40	1.30
2	B	2002	FAD	O2-C2	-4.22	1.16	1.24
2	D	2004	FAD	C4X-N5	4.12	1.39	1.30
2	B	2002	FAD	C9A-C5X	3.92	1.47	1.41
2	B	2002	FAD	C4'-C3'	-3.58	1.47	1.53
2	A	2001	FAD	C4X-N5	3.56	1.38	1.30
2	C	2003	FAD	C4'-C3'	-3.41	1.47	1.53
2	C	2003	FAD	P-O3P	-3.41	1.55	1.59
2	C	2003	FAD	C9A-C5X	3.34	1.46	1.41
2	D	2004	FAD	C9A-C5X	3.22	1.46	1.41
2	C	2003	FAD	C4X-N5	3.11	1.37	1.30
2	C	2003	FAD	O2-C2	-3.08	1.18	1.24
2	D	2004	FAD	C4'-C3'	-3.06	1.48	1.53
2	C	2003	FAD	C1'-C2'	2.98	1.56	1.52
2	A	2001	FAD	O2-C2	-2.95	1.18	1.24
3	D	4162	SO4	O1-S	2.95	1.62	1.44
3	A	4157	SO4	O1-S	2.94	1.62	1.44
3	B	4158	SO4	O1-S	2.93	1.62	1.44
3	B	4161	SO4	O1-S	2.92	1.62	1.44
3	C	4163	SO4	O1-S	2.92	1.62	1.44
3	A	4159	SO4	O1-S	2.85	1.61	1.44
2	B	2002	FAD	C2A-N1A	2.48	1.38	1.33
2	C	2003	FAD	O2'-C2'	2.47	1.48	1.43
4	B	1501	ACY	OXT-C	-2.39	1.19	1.30
2	B	2002	FAD	C5'-C4'	-2.35	1.48	1.51
2	A	2001	FAD	C4'-C3'	-2.34	1.49	1.53
2	B	2002	FAD	C4-N3	-2.33	1.34	1.38
2	A	2001	FAD	C9A-C5X	2.30	1.44	1.41
2	D	2004	FAD	C2A-N1A	2.17	1.37	1.33
2	D	2004	FAD	P-O3P	-2.16	1.57	1.59
3	A	4157	SO4	O3-S	-2.16	1.30	1.48
3	D	4162	SO4	O3-S	-2.11	1.30	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	FAD	C1'-C2'	2.10	1.55	1.52
3	B	4161	SO4	O3-S	-2.10	1.30	1.48
2	C	2003	FAD	C8-C7	2.08	1.46	1.40
3	C	4163	SO4	O3-S	-2.05	1.31	1.48
3	A	4159	SO4	O3-S	-2.04	1.31	1.48
2	D	2004	FAD	C8A-N7A	2.04	1.35	1.31
2	B	2002	FAD	C8A-N7A	2.00	1.35	1.31

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2004	FAD	C2B-C1B-N9A	3.19	121.24	113.30
2	D	2004	FAD	N3A-C2A-N1A	-3.14	123.83	128.58
2	B	2002	FAD	C4-C4X-N5	2.98	122.33	118.21
2	B	2002	FAD	N3A-C2A-N1A	-2.77	124.38	128.58
2	C	2003	FAD	C2B-C1B-N9A	2.71	120.03	113.30
2	D	2004	FAD	C4X-C10-N10	2.68	120.32	116.48
2	A	2001	FAD	C2B-C1B-N9A	2.67	119.94	113.30
2	B	2002	FAD	C4X-C10-N10	2.65	120.28	116.48
2	A	2001	FAD	C9A-C5X-N5	-2.56	119.74	122.45
2	B	2002	FAD	C2B-C1B-N9A	2.54	119.61	113.30
2	C	2003	FAD	O5'-C5'-C4'	-2.52	102.63	109.36
2	D	2004	FAD	C4-C4X-N5	2.51	121.67	118.21
2	D	2004	FAD	C4A-N9A-C8A	2.49	108.35	105.74
2	A	2001	FAD	N3A-C2A-N1A	-2.45	124.87	128.58
2	A	2001	FAD	O3P-PA-O1A	-2.28	103.85	110.70
2	D	2004	FAD	C10-C4X-N5	-2.27	120.17	124.81
2	C	2003	FAD	O3P-PA-O1A	-2.20	104.08	110.70
2	B	2002	FAD	C10-C4X-N5	-2.20	120.31	124.81
2	B	2002	FAD	O5'-C5'-C4'	-2.19	103.52	109.36
2	C	2003	FAD	C4'-C3'-C2'	-2.17	109.97	113.57
2	D	2004	FAD	O3P-PA-O1A	-2.11	104.36	110.70
2	D	2004	FAD	N9A-C8A-N7A	-2.11	110.95	113.94
2	C	2003	FAD	C9A-C5X-N5	-2.09	120.24	122.45
2	C	2003	FAD	C4X-C10-N10	2.03	119.39	116.48
2	A	2001	FAD	N9A-C8A-N7A	-2.03	111.06	113.94
2	B	2002	FAD	O3P-PA-O1A	-2.02	104.64	110.70
2	D	2004	FAD	C2A-N1A-C6A	2.01	122.02	118.73

There are no chirality outliers.

All (6) torsion outliers are listed below:

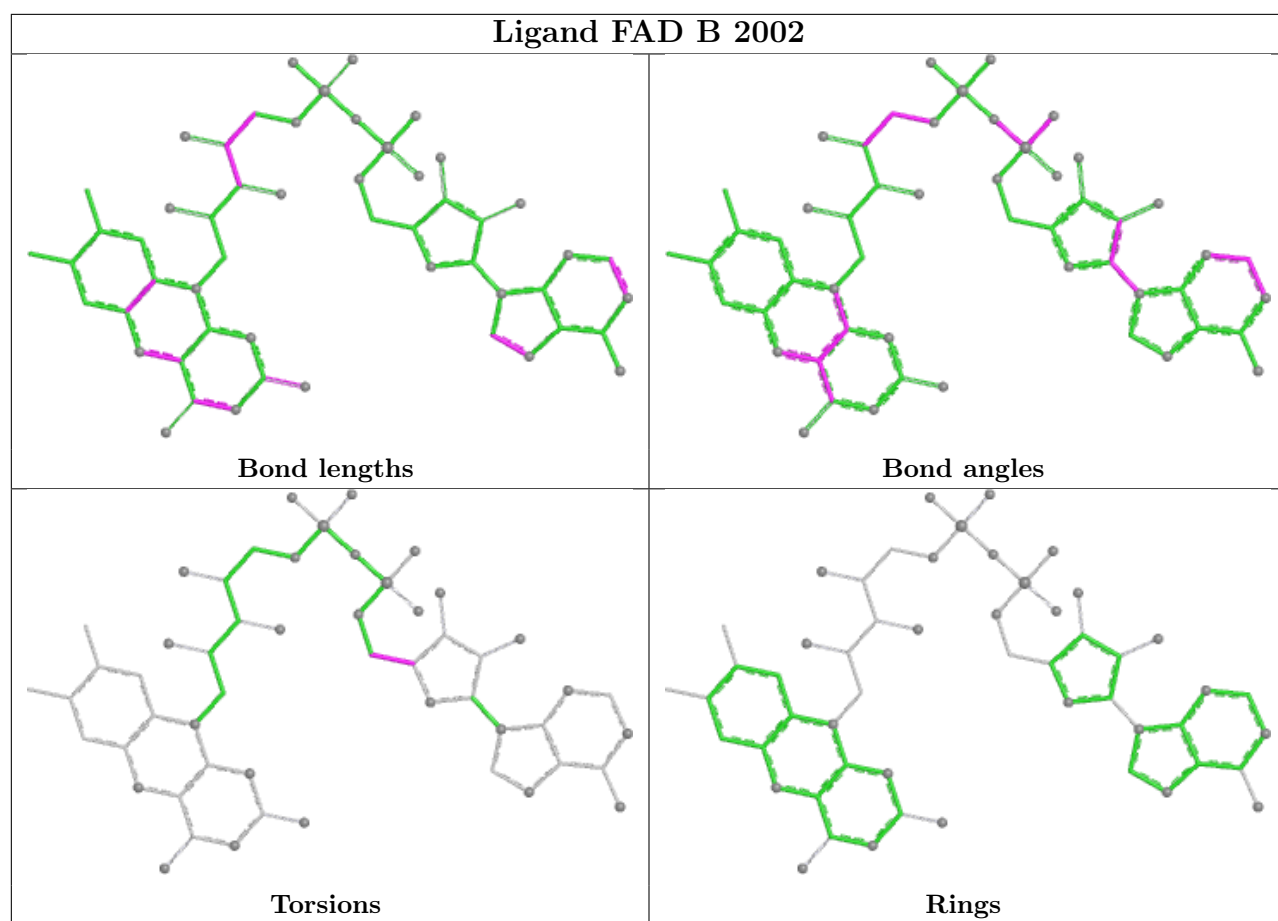
Mol	Chain	Res	Type	Atoms
2	A	2001	FAD	PA-O3P-P-O5'
2	C	2003	FAD	PA-O3P-P-O5'
2	B	2002	FAD	O4B-C4B-C5B-O5B
2	A	2001	FAD	O4B-C4B-C5B-O5B
2	C	2003	FAD	O4B-C4B-C5B-O5B
2	D	2004	FAD	O4B-C4B-C5B-O5B

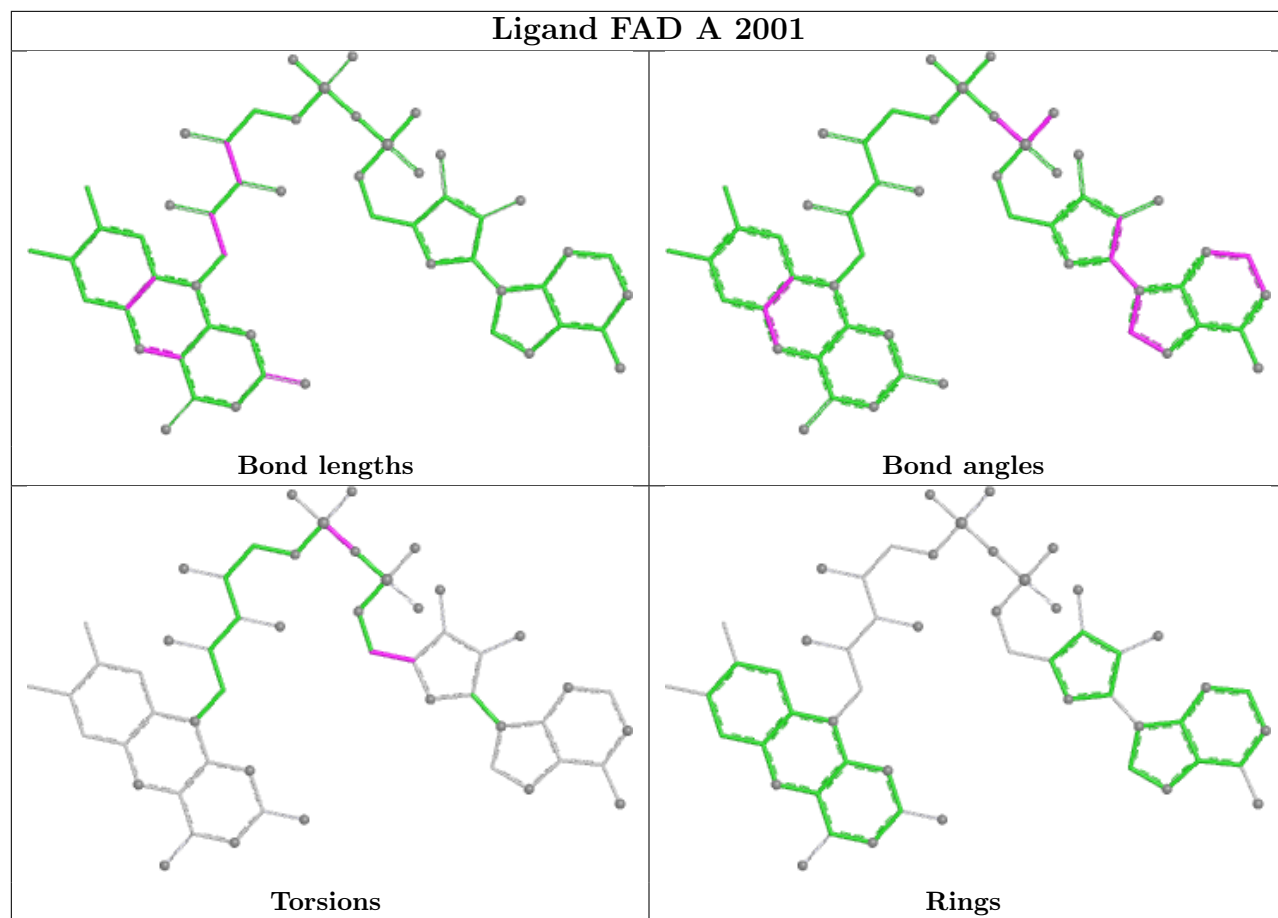
There are no ring outliers.

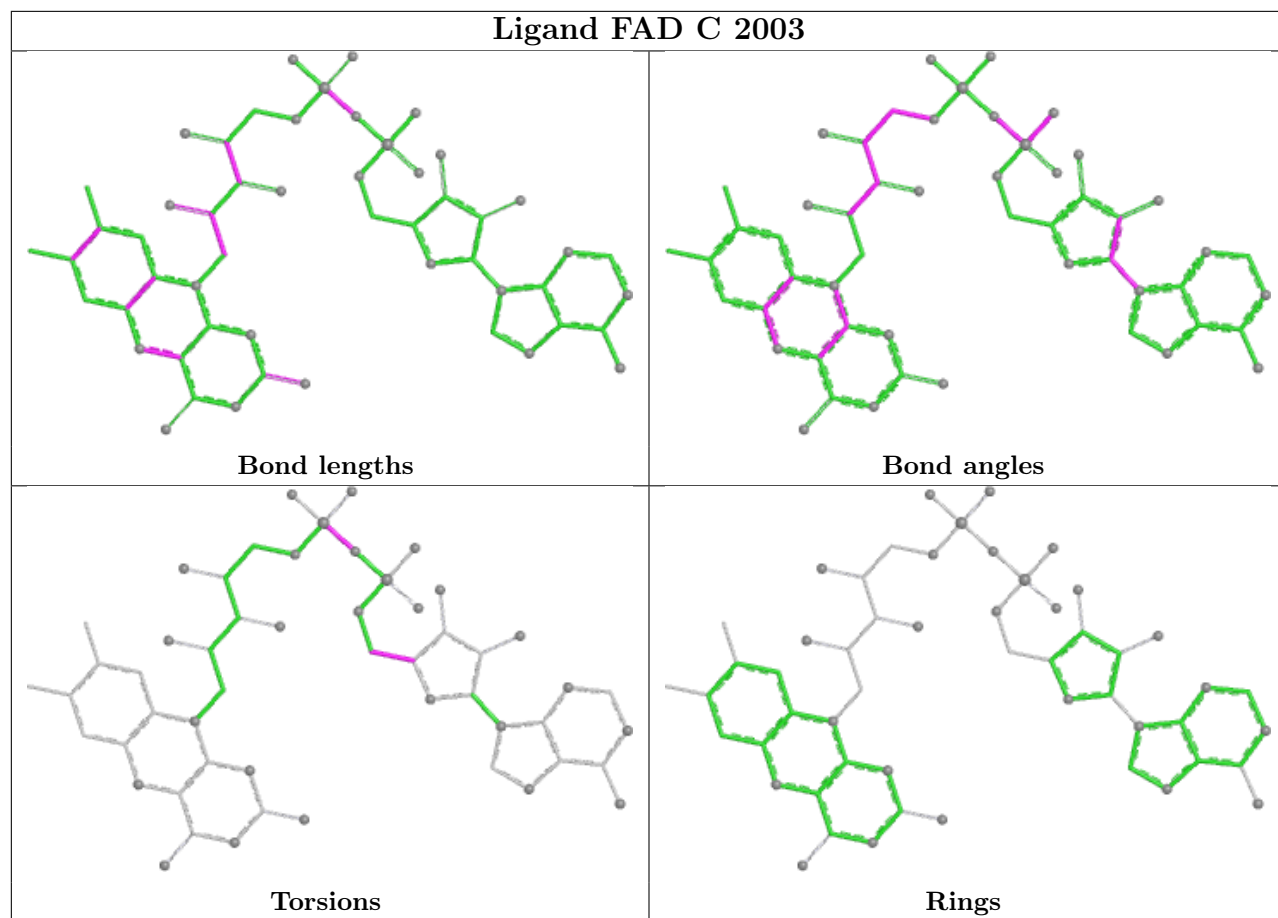
3 monomers are involved in 3 short contacts:

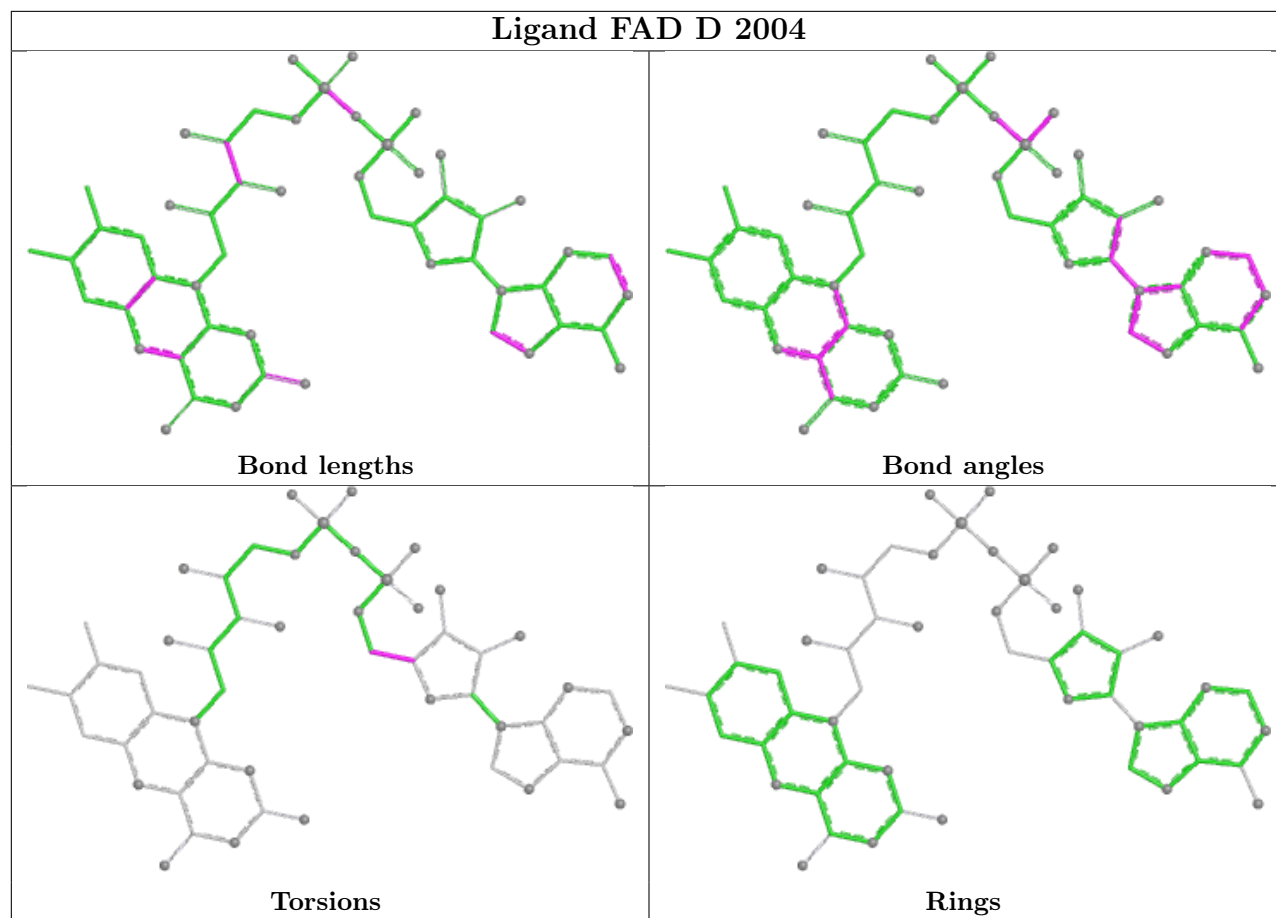
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	FAD	1	0
3	A	4159	SO4	1	0
2	D	2004	FAD	1	0

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	308/323 (95%)	1.88	132 (42%) 0 1	7, 15, 29, 38	0
1	B	309/323 (95%)	1.90	127 (41%) 0 1	8, 17, 30, 38	0
1	C	307/323 (95%)	2.01	149 (48%) 0 0	8, 16, 35, 41	0
1	D	298/323 (92%)	1.97	127 (42%) 0 1	8, 18, 38, 44	0
All	All	1222/1292 (94%)	1.94	535 (43%) 0 1	7, 17, 34, 44	0

All (535) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	13	GLY	10.9
1	C	233	GLY	4.7
1	B	232	THR	4.6
1	C	213	VAL	4.5
1	B	98	ARG	4.4
1	D	98	ARG	4.3
1	D	191	ALA	4.3
1	B	11	LYS	4.2
1	D	196	VAL	4.2
1	A	98	ARG	4.0
1	C	191	ALA	4.0
1	C	219	ASP	4.0
1	C	265	THR	4.0
1	D	139	ARG	4.0
1	D	186	ARG	3.9
1	D	197	GLU	3.8
1	D	212	VAL	3.7
1	B	282	VAL	3.7
1	C	189	PHE	3.7
1	C	134	GLN	3.7
1	D	100	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	235	ILE	3.7
1	C	232	THR	3.7
1	D	147	ALA	3.7
1	D	193	PRO	3.6
1	D	195	TYR	3.6
1	A	293	LEU	3.6
1	A	235	ILE	3.6
1	C	235	ILE	3.6
1	C	209	LEU	3.5
1	B	233	GLY	3.5
1	A	219	ASP	3.5
1	A	249	PHE	3.5
1	C	212	VAL	3.5
1	B	293	LEU	3.4
1	B	199	VAL	3.4
1	D	130	VAL	3.4
1	D	219	ASP	3.4
1	C	220	LYS	3.4
1	D	293	LEU	3.4
1	A	10	VAL	3.3
1	D	288	CYS	3.3
1	D	231	LYS	3.3
1	D	285	ALA	3.3
1	B	194	ILE	3.3
1	B	200	LYS	3.3
1	C	130	VAL	3.3
1	C	288	CYS	3.3
1	A	285	ALA	3.3
1	C	199	VAL	3.2
1	B	288	CYS	3.2
1	C	194	ILE	3.2
1	C	187	ASP	3.2
1	D	123	VAL	3.2
1	A	195	TYR	3.2
1	B	34	SER	3.2
1	A	265	THR	3.2
1	D	214	LYS	3.2
1	A	288	CYS	3.2
1	C	94	LYS	3.1
1	C	10	VAL	3.1
1	D	227	VAL	3.1
1	C	229	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	58	VAL	3.1
1	B	130	VAL	3.1
1	A	108	ARG	3.1
1	B	218	GLY	3.1
1	A	309	ALA	3.1
1	D	208	VAL	3.0
1	C	151	LEU	3.0
1	B	100	ASP	3.0
1	D	189	PHE	3.0
1	B	10	VAL	3.0
1	C	21	VAL	3.0
1	C	230	LEU	3.0
1	A	301	ALA	3.0
1	C	30	ALA	3.0
1	A	57	ILE	3.0
1	A	123	VAL	3.0
1	A	266	ASN	2.9
1	D	81	GLU	2.9
1	B	114	ALA	2.9
1	C	249	PHE	2.9
1	B	234	GLU	2.9
1	A	21	VAL	2.9
1	D	128	LEU	2.9
1	D	144	CYS	2.9
1	B	301	ALA	2.9
1	B	249	PHE	2.9
1	B	57	ILE	2.9
1	B	108	ARG	2.9
1	A	75	VAL	2.9
1	C	302	VAL	2.9
1	B	141	ILE	2.8
1	D	220	LYS	2.8
1	B	62	LEU	2.8
1	C	271	VAL	2.8
1	C	293	LEU	2.8
1	A	27	ALA	2.8
1	C	192	GLN	2.8
1	D	200	LYS	2.8
1	C	20	ILE	2.8
1	D	194	ILE	2.8
1	C	32	LEU	2.8
1	D	230	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	251	PRO	2.8
1	D	252	PRO	2.8
1	A	236	LYS	2.8
1	C	188	THR	2.8
1	D	178	THR	2.8
1	A	61	TYR	2.8
1	D	225	VAL	2.7
1	D	302	VAL	2.7
1	D	265	THR	2.7
1	D	317	THR	2.7
1	C	121	ILE	2.7
1	A	26	ALA	2.7
1	A	151	LEU	2.7
1	A	230	LEU	2.7
1	C	306	ALA	2.7
1	B	123	VAL	2.7
1	C	123	VAL	2.7
1	D	279	VAL	2.7
1	C	24	GLY	2.7
1	D	198	THR	2.7
1	C	150	PRO	2.7
1	D	203	PRO	2.7
1	A	30	ALA	2.7
1	A	147	ALA	2.7
1	B	312	ALA	2.7
1	C	147	ALA	2.7
1	C	284	ALA	2.7
1	B	107	LYS	2.7
1	A	269	ILE	2.7
1	D	207	PHE	2.7
1	B	144	CYS	2.7
1	A	303	ALA	2.6
1	C	149	ALA	2.6
1	C	303	ALA	2.6
1	C	309	ALA	2.6
1	D	24	GLY	2.6
1	D	308	ALA	2.6
1	B	28	TYR	2.6
1	B	146	VAL	2.6
1	B	156	VAL	2.6
1	B	187	ASP	2.6
1	B	302	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	75	VAL	2.6
1	D	146	VAL	2.6
1	D	155	ARG	2.6
1	C	193	PRO	2.6
1	A	231	LYS	2.6
1	A	67	ILE	2.6
1	C	305	GLY	2.6
1	D	121	ILE	2.6
1	B	112	PHE	2.6
1	C	26	ALA	2.6
1	C	285	ALA	2.6
1	D	309	ALA	2.6
1	D	312	ALA	2.6
1	C	198	THR	2.6
1	C	238	LEU	2.6
1	D	209	LEU	2.6
1	C	186	ARG	2.6
1	D	108	ARG	2.6
1	A	85	VAL	2.6
1	A	302	VAL	2.6
1	B	222	VAL	2.6
1	B	298	VAL	2.6
1	C	282	VAL	2.6
1	C	298	VAL	2.6
1	C	307	VAL	2.6
1	A	287	ASP	2.6
1	B	35	ALA	2.6
1	B	285	ALA	2.6
1	C	301	ALA	2.6
1	D	136	PHE	2.6
1	A	227	VAL	2.6
1	A	298	VAL	2.6
1	B	212	VAL	2.6
1	C	43	VAL	2.6
1	C	146	VAL	2.6
1	C	227	VAL	2.6
1	D	307	VAL	2.6
1	A	24	GLY	2.6
1	A	155	ARG	2.6
1	A	284	ALA	2.5
1	C	137	ALA	2.5
1	A	121	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	73	ILE	2.5
1	B	91	ILE	2.5
1	A	88	LEU	2.5
1	C	64	LEU	2.5
1	B	294	GLY	2.5
1	A	130	VAL	2.5
1	A	307	VAL	2.5
1	C	221	VAL	2.5
1	C	222	VAL	2.5
1	D	199	VAL	2.5
1	D	165	SER	2.5
1	D	68	GLN	2.5
1	A	20	ILE	2.5
1	B	292	TRP	2.5
1	C	299	ILE	2.5
1	D	65	ILE	2.5
1	D	292	TRP	2.5
1	B	33	TYR	2.5
1	D	93	GLU	2.5
1	C	226	VAL	2.5
1	D	316	VAL	2.5
1	B	303	ALA	2.5
1	C	114	ALA	2.5
1	A	194	ILE	2.5
1	A	299	ILE	2.5
1	B	121	ILE	2.5
1	B	216	ILE	2.5
1	C	80	ILE	2.5
1	A	110	GLY	2.5
1	B	96	GLU	2.5
1	B	140	GLY	2.5
1	C	215	GLU	2.5
1	A	33	TYR	2.5
1	B	61	TYR	2.5
1	B	16	PHE	2.5
1	B	207	PHE	2.5
1	B	231	LYS	2.5
1	C	86	PRO	2.5
1	C	153	LYS	2.5
1	C	97	ASN	2.5
1	C	139	ARG	2.5
1	A	159	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	310	THR	2.5
1	B	219	ASP	2.5
1	A	31	ALA	2.4
1	A	69	ALA	2.4
1	A	306	ALA	2.4
1	B	30	ALA	2.4
1	B	306	ALA	2.4
1	C	144	CYS	2.4
1	D	114	ALA	2.4
1	D	303	ALA	2.4
1	A	305	GLY	2.4
1	B	56	GLY	2.4
1	C	267	GLY	2.4
1	B	319	LYS	2.4
1	B	68	GLN	2.4
1	A	172	ILE	2.4
1	C	19	ILE	2.4
1	C	44	ILE	2.4
1	C	176	TYR	2.4
1	C	207	PHE	2.4
1	B	178	THR	2.4
1	A	196	VAL	2.4
1	B	307	VAL	2.4
1	C	159	VAL	2.4
1	D	58	VAL	2.4
1	A	34	SER	2.4
1	C	166	ALA	2.4
1	A	144	CYS	2.4
1	A	214	LYS	2.4
1	B	50	GLY	2.4
1	D	160	ILE	2.4
1	B	310	THR	2.4
1	D	201	LYS	2.4
1	A	158	ALA	2.4
1	D	26	ALA	2.4
1	A	18	VAL	2.4
1	B	75	VAL	2.4
1	B	316	VAL	2.4
1	C	18	VAL	2.4
1	C	180	VAL	2.4
1	C	196	VAL	2.4
1	D	221	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	271	VAL	2.4
1	B	97	ASN	2.4
1	A	182	LEU	2.4
1	A	300	THR	2.4
1	C	127	LYS	2.4
1	D	151	LEU	2.4
1	D	310	THR	2.4
1	A	176	TYR	2.4
1	C	143	TYR	2.4
1	C	181	TYR	2.4
1	A	22	GLY	2.4
1	C	294	GLY	2.4
1	D	283	PHE	2.4
1	B	137	ALA	2.3
1	C	312	ALA	2.3
1	D	306	ALA	2.3
1	A	187	ASP	2.3
1	A	274	TRP	2.3
1	A	279	VAL	2.3
1	A	316	VAL	2.3
1	C	87	VAL	2.3
1	C	208	VAL	2.3
1	D	180	VAL	2.3
1	D	127	LYS	2.3
1	A	44	ILE	2.3
1	A	183	ILE	2.3
1	B	44	ILE	2.3
1	C	42	LEU	2.3
1	A	35	ALA	2.3
1	A	137	ALA	2.3
1	C	31	ALA	2.3
1	C	158	ALA	2.3
1	D	301	ALA	2.3
1	A	283	PHE	2.3
1	A	180	VAL	2.3
1	A	208	VAL	2.3
1	B	193	PRO	2.3
1	B	221	VAL	2.3
1	C	85	VAL	2.3
1	C	316	VAL	2.3
1	D	282	VAL	2.3
1	D	274	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	47	THR	2.3
1	D	210	ASN	2.3
1	B	281	GLY	2.3
1	A	80	ILE	2.3
1	B	80	ILE	2.3
1	A	38	MET	2.3
1	B	284	ALA	2.3
1	D	27	ALA	2.3
1	A	76	PHE	2.3
1	A	295	PHE	2.3
1	B	295	PHE	2.3
1	D	249	PHE	2.3
1	A	25	PRO	2.3
1	B	252	PRO	2.3
1	A	97	ASN	2.3
1	A	117	VAL	2.3
1	B	117	VAL	2.3
1	B	227	VAL	2.3
1	C	243	VAL	2.3
1	D	75	VAL	2.3
1	A	233	GLY	2.3
1	A	294	GLY	2.3
1	B	209	LEU	2.3
1	C	128	LEU	2.3
1	D	23	LEU	2.3
1	D	28	TYR	2.3
1	D	37	TYR	2.3
1	D	313	TYR	2.3
1	A	312	ALA	2.2
1	C	256	ALA	2.2
1	D	149	ALA	2.2
1	B	12	PRO	2.2
1	D	131	PRO	2.2
1	C	310	THR	2.2
1	C	120	GLY	2.2
1	A	43	VAL	2.2
1	A	87	VAL	2.2
1	A	103	VAL	2.2
1	C	58	VAL	2.2
1	C	92	VAL	2.2
1	D	43	VAL	2.2
1	D	159	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	240	VAL	2.2
1	B	124	LYS	2.2
1	D	275	MET	2.2
1	C	237	GLU	2.2
1	D	64	LEU	2.2
1	D	20	ILE	2.2
1	A	181	TYR	2.2
1	C	33	TYR	2.2
1	A	166	ALA	2.2
1	B	309	ALA	2.2
1	C	51	GLN	2.2
1	C	185	ARG	2.2
1	D	251	PRO	2.2
1	A	232	THR	2.2
1	B	318	GLU	2.2
1	A	45	GLY	2.2
1	B	63	GLY	2.2
1	D	138	GLY	2.2
1	A	152	PHE	2.2
1	B	244	PHE	2.2
1	B	283	PHE	2.2
1	A	282	VAL	2.2
1	B	208	VAL	2.2
1	B	240	VAL	2.2
1	C	157	VAL	2.2
1	D	298	VAL	2.2
1	A	77	ASN	2.2
1	A	32	LEU	2.2
1	A	119	LEU	2.2
1	B	32	LEU	2.2
1	C	167	LEU	2.2
1	B	299	ILE	2.2
1	D	269	ILE	2.2
1	D	299	ILE	2.2
1	A	28	TYR	2.2
1	A	308	ALA	2.2
1	B	166	ALA	2.2
1	C	69	ALA	2.2
1	C	274	TRP	2.2
1	D	31	ALA	2.2
1	A	252	PRO	2.2
1	B	201	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	203	PRO	2.2
1	C	11	LYS	2.2
1	B	265	THR	2.2
1	B	317	THR	2.2
1	C	281	GLY	2.2
1	D	110	GLY	2.2
1	D	229	ASN	2.2
1	C	295	PHE	2.2
1	B	87	VAL	2.2
1	B	159	VAL	2.2
1	D	205	VAL	2.2
1	B	72	MET	2.2
1	C	184	HIS	2.2
1	B	89	LEU	2.1
1	B	119	LEU	2.1
1	B	251	PRO	2.1
1	A	132	GLY	2.1
1	B	161	GLY	2.1
1	C	91	ILE	2.1
1	D	245	ILE	2.1
1	A	313	TYR	2.1
1	D	315	TYR	2.1
1	C	276	ARG	2.1
1	B	274	TRP	2.1
1	B	229	ASN	2.1
1	A	220	LYS	2.1
1	C	236	LYS	2.1
1	A	189	PHE	2.1
1	C	76	PHE	2.1
1	A	92	VAL	2.1
1	A	213	VAL	2.1
1	B	180	VAL	2.1
1	D	21	VAL	2.1
1	D	157	VAL	2.1
1	C	108	ARG	2.1
1	C	155	ARG	2.1
1	A	50	GLY	2.1
1	A	281	GLY	2.1
1	C	145	SER	2.1
1	A	128	LEU	2.1
1	B	27	ALA	2.1
1	C	252	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	182	LEU	2.1
1	D	137	ALA	2.1
1	C	253	THR	2.1
1	C	317	THR	2.1
1	B	65	ILE	2.1
1	C	118	ILE	2.1
1	C	61	TYR	2.1
1	D	61	TYR	2.1
1	D	187	ASP	2.1
1	A	72	MET	2.1
1	C	231	LYS	2.1
1	A	134	GLN	2.1
1	B	224	GLN	2.1
1	C	50	GLY	2.1
1	C	197	GLU	2.1
1	C	283	PHE	2.1
1	A	199	VAL	2.1
1	B	103	VAL	2.1
1	C	205	VAL	2.1
1	C	279	VAL	2.1
1	D	18	VAL	2.1
1	D	213	VAL	2.1
1	A	289	THR	2.1
1	B	158	ALA	2.1
1	B	191	ALA	2.1
1	C	55	ALA	2.1
1	C	289	THR	2.1
1	D	30	ALA	2.1
1	A	42	LEU	2.1
1	C	23	LEU	2.1
1	D	119	LEU	2.1
1	A	73	ILE	2.1
1	C	67	ILE	2.1
1	D	80	ILE	2.1
1	D	247	ILE	2.1
1	D	224	GLN	2.1
1	C	234	GLU	2.1
1	A	145	SER	2.1
1	C	258	SER	2.1
1	D	72	MET	2.1
1	A	29	GLY	2.1
1	B	45	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	169	GLY	2.1
1	D	63	GLY	2.1
1	A	150	PRO	2.1
1	A	41	THR	2.0
1	B	53	THR	2.0
1	B	76	PHE	2.0
1	D	102	PHE	2.0
1	D	188	THR	2.0
1	B	279	VAL	2.0
1	C	225	VAL	2.0
1	A	114	ALA	2.0
1	B	26	ALA	2.0
1	C	291	ALA	2.0
1	D	284	ALA	2.0
1	C	182	LEU	2.0
1	D	173	LEU	2.0
1	C	318	GLU	2.0
1	A	65	ILE	2.0
1	A	91	ILE	2.0
1	A	247	ILE	2.0
1	A	315	TYR	2.0
1	B	176	TYR	2.0
1	B	315	TYR	2.0
1	C	57	ILE	2.0
1	C	73	ILE	2.0
1	B	22	GLY	2.0
1	D	294	GLY	2.0
1	B	127	LYS	2.0
1	D	223	LYS	2.0
1	A	131	PRO	2.0
1	A	188	THR	2.0
1	A	263	THR	2.0
1	B	155	ARG	2.0
1	C	277	THR	2.0
1	A	292	TRP	2.0
1	C	168	GLU	2.0
1	D	84	GLU	2.0
1	A	291	ALA	2.0
1	B	147	ALA	2.0
1	B	308	ALA	2.0
1	C	27	ALA	2.0
1	D	291	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	212	VAL	2.0
1	A	222	VAL	2.0
1	B	136	PHE	2.0
1	B	196	VAL	2.0
1	B	128	LEU	2.0
1	C	119	LEU	2.0
1	D	39	LEU	2.0
1	A	177	SER	2.0
1	C	287	ASP	2.0
1	D	33	TYR	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.

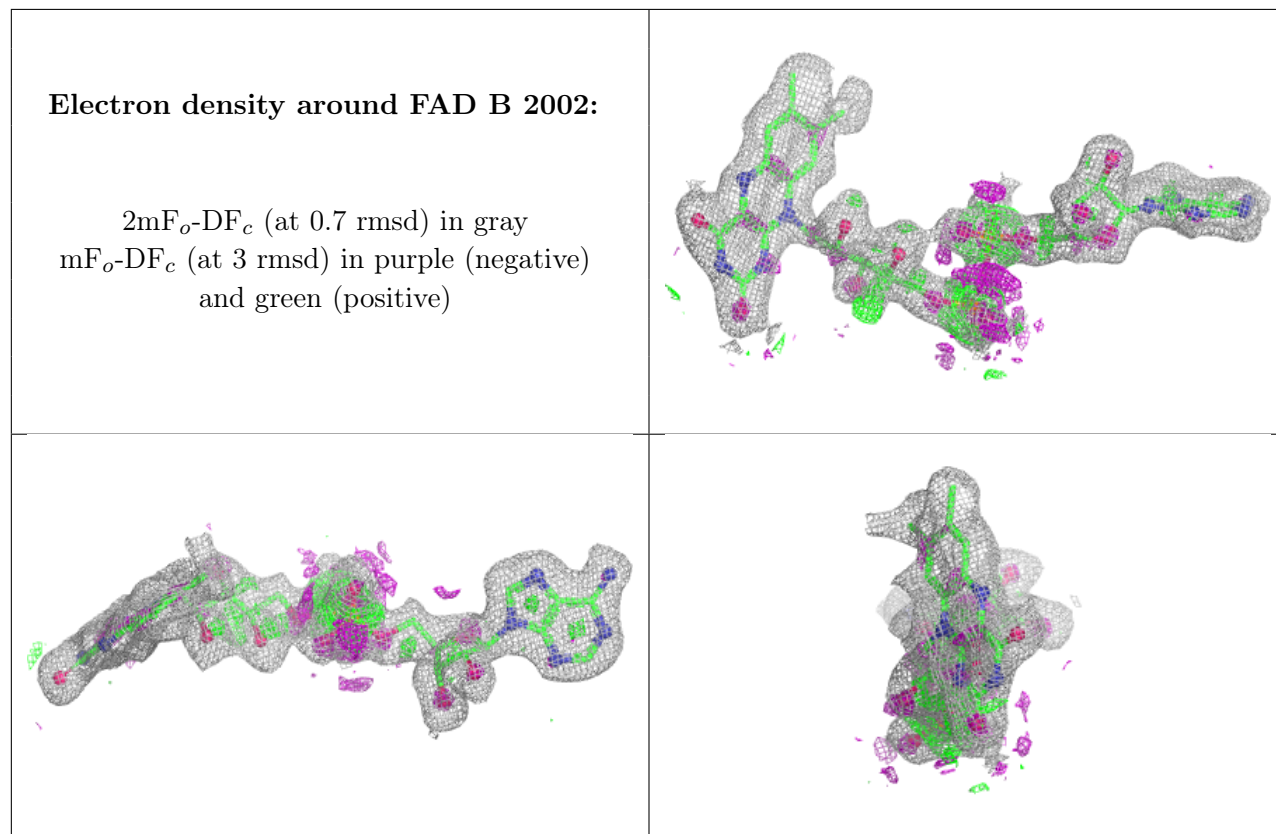
6.4 Ligands [i](#)

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(Å ²)	Q<0.9
4	ACY	B	1501	4/4	0.72	0.15	17,17,17,18	0
2	FAD	B	2002	53/53	0.81	0.13	9,14,20,22	0
2	FAD	C	2003	53/53	0.81	0.14	8,12,22,25	0
2	FAD	A	2001	53/53	0.81	0.14	8,11,18,21	0
2	FAD	D	2004	53/53	0.83	0.13	9,13,20,22	0
3	SO4	A	4159	5/5	0.86	0.16	37,40,42,42	0
3	SO4	D	4162	5/5	0.89	0.13	41,42,43,43	0
3	SO4	B	4158	5/5	0.89	0.14	32,36,39,40	0
3	SO4	C	4163	5/5	0.90	0.12	44,44,45,45	0
3	SO4	A	4157	5/5	0.92	0.13	43,43,44,44	0
3	SO4	B	4161	5/5	0.92	0.12	30,37,39,39	0

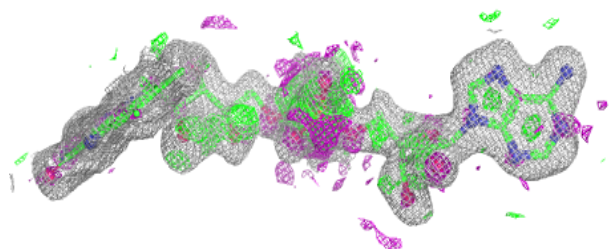
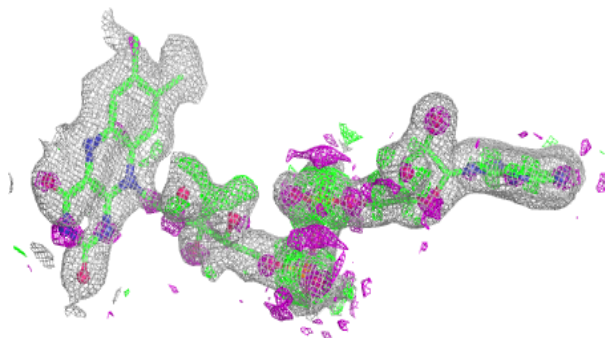
The following is a graphical depiction of the model fit to experimental electron density of all

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.

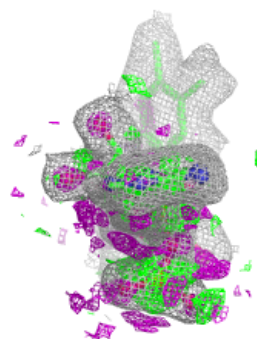
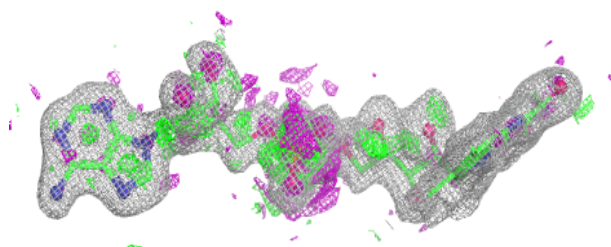
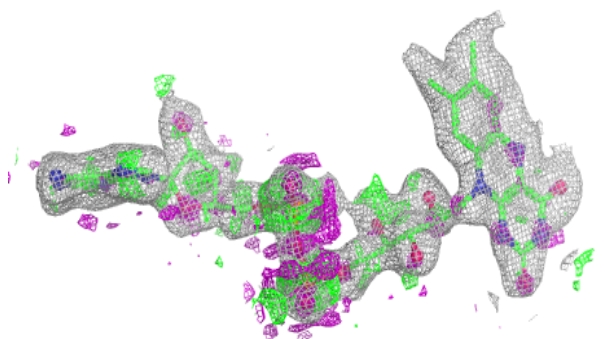


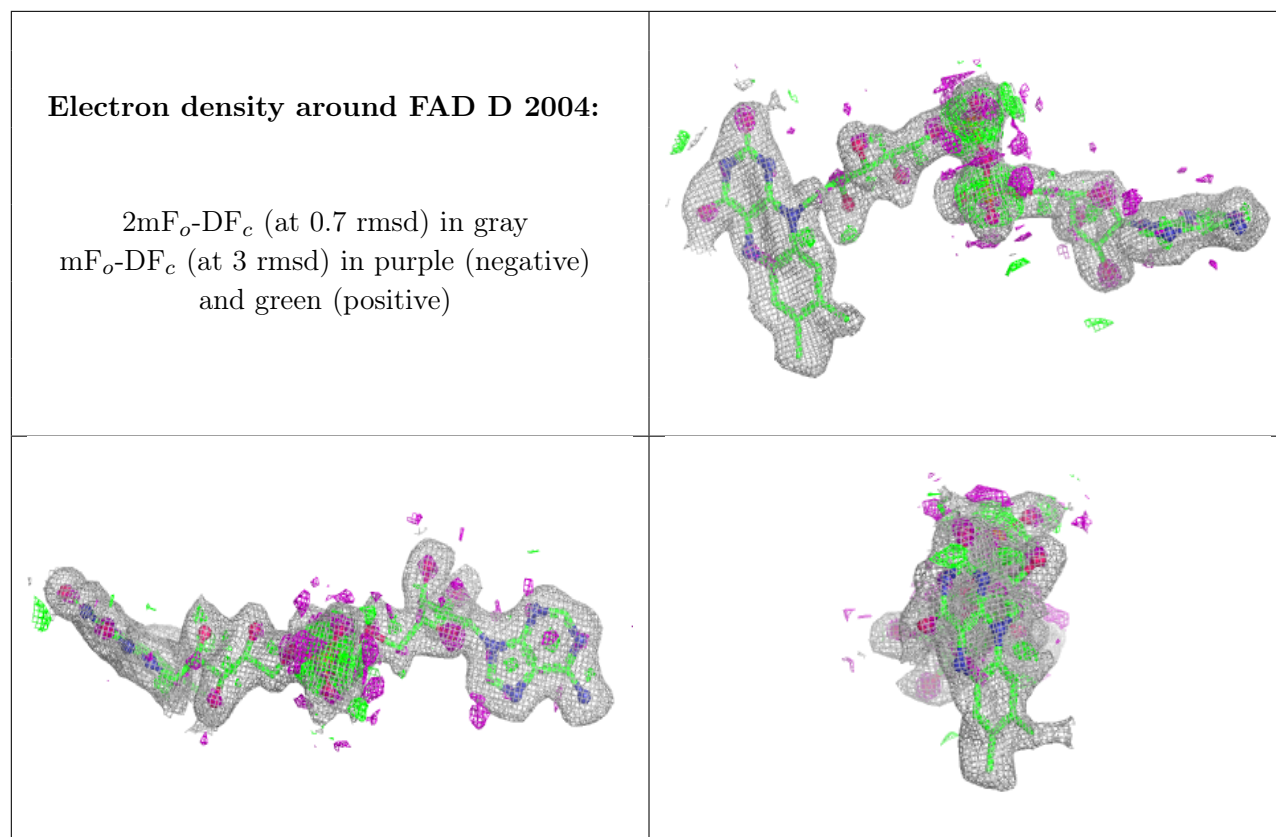
Electron density around FAD C 2003:

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

**Electron density around FAD A 2001:**

$2mF_o-DF_c$ (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.