



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:13 PM UTC

PDB ID : 2C12 / pdb_00002c12
Title : Crystal Structure of Nitroalkane Oxidase in Complex with Spermine, a Competitive Inhibitor
Authors : Nagpal, A.; Valley, M.P.; Fitzpatrick, P.F.; Orville, A.M.
Deposited on : 2005-09-10
Resolution : 2.07 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

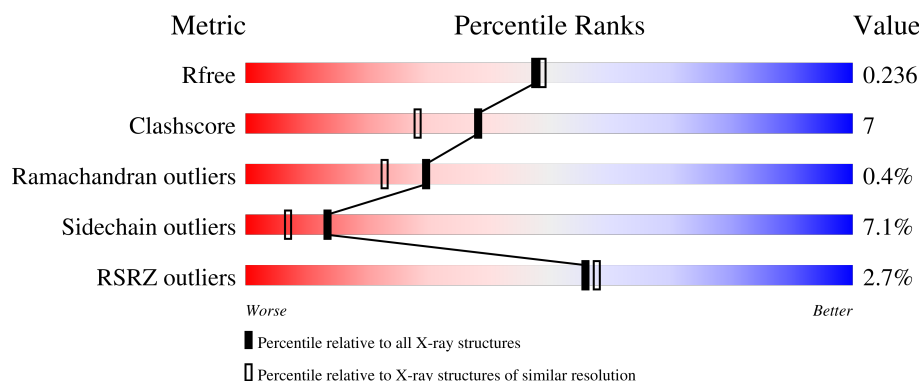
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	439	2% 84% 11% ..
1	B	439	3% 79% 15% ..
1	C	439	4% 82% 12% ..
1	D	439	2% 85% 12% ..
1	E	439	2% 86% 9% ..

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Mol	Chain	Length	Quality of chain
1	F	439	3% 82% 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SPM	C	1434	-	-	X	-
5	PE4	B	1436	-	-	X	-
5	PE4	F	1435	-	-	X	-

2 Entry composition ⓘ

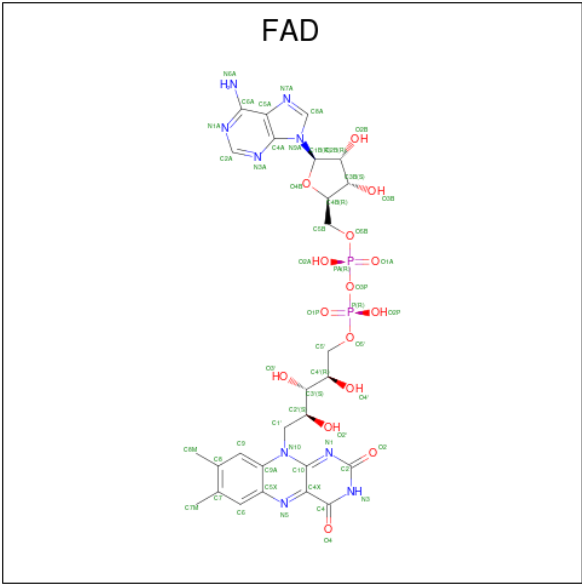
There are 6 unique types of molecules in this entry. The entry contains 21487 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NITROALKANE OXIDASE.

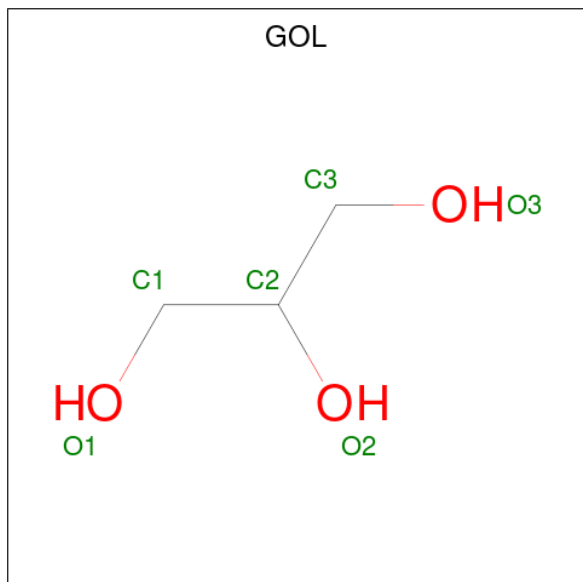
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	1	0
			3309	2096	567	625	21			
1	B	430	Total	C	N	O	S	0	1	0
			3309	2096	567	625	21			
1	C	430	Total	C	N	O	S	0	1	0
			3309	2096	567	625	21			
1	D	430	Total	C	N	O	S	0	3	0
			3313	2097	568	627	21			
1	E	430	Total	C	N	O	S	0	1	0
			3309	2096	567	625	21			
1	F	430	Total	C	N	O	S	0	1	0
			3309	2096	567	625	21			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



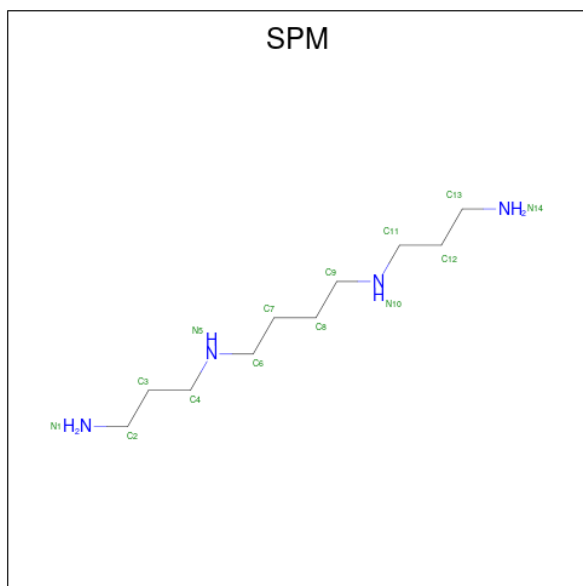
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).



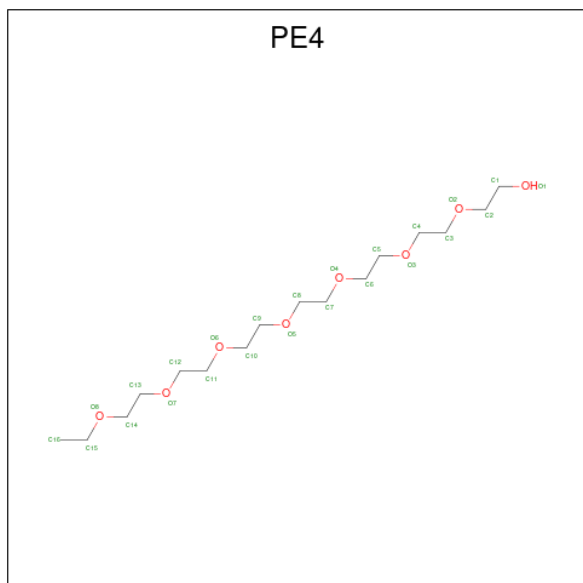
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	N	0	0
			14	10	4		
4	C	1	Total	C	N	0	0
			14	10	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	N	0	0
			14	10	4		
4	F	1	Total	C	N	0	0
			14	10	4		

- Molecule 5 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (CCD ID: PE4) (formula: C₁₆H₃₄O₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			24	16	8		
5	F	1	Total	C	O	0	0
			24	16	8		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	195	Total	O	0	0
			195	195		
6	B	207	Total	O	0	0
			207	207		
6	C	164	Total	O	0	0
			164	164		
6	D	159	Total	O	0	0
			159	159		
6	E	187	Total	O	0	0
			187	187		

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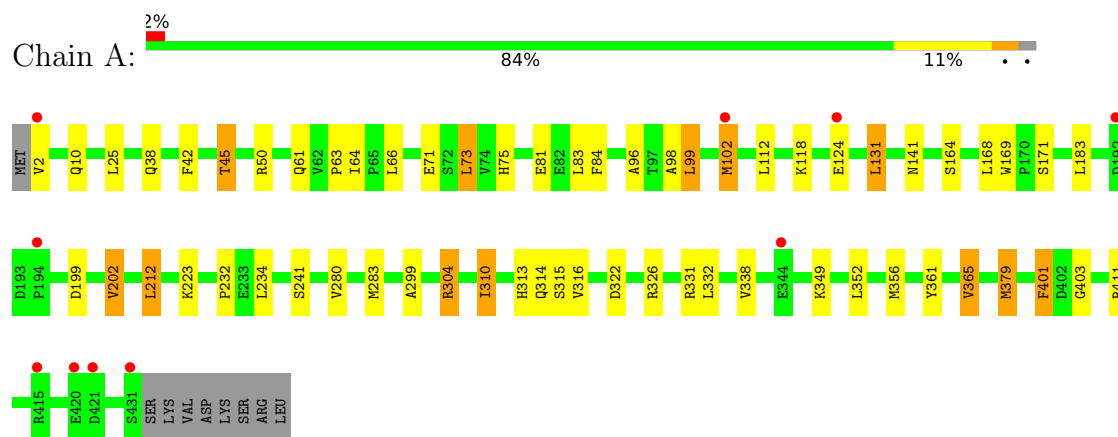
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	205	Total 205	O 205	0	0

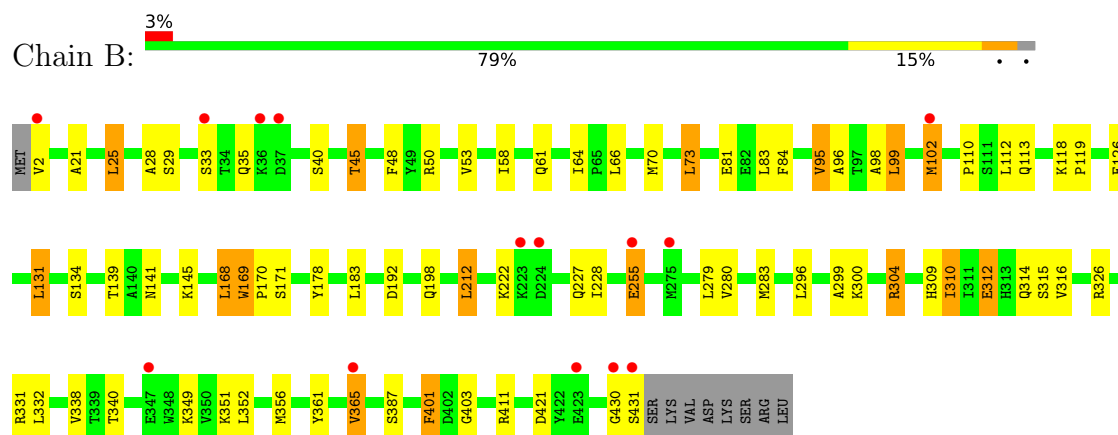
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

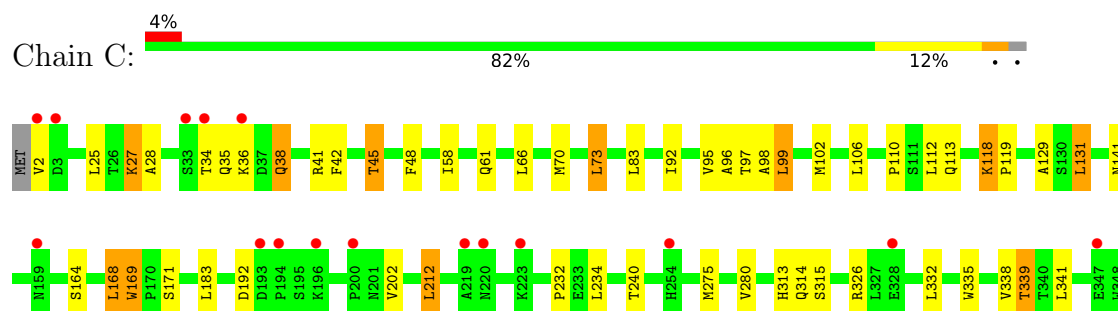
• Molecule 1: NITROALKANE OXIDASE

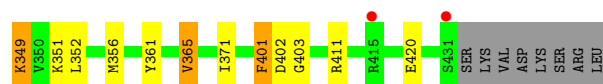


• Molecule 1: NITROALKANE OXIDASE

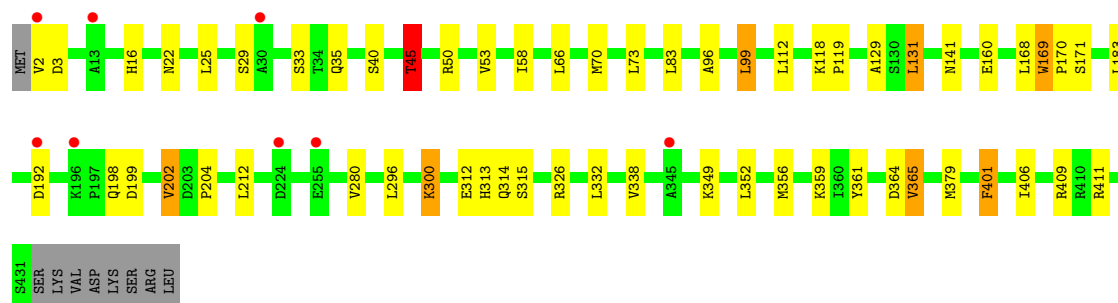
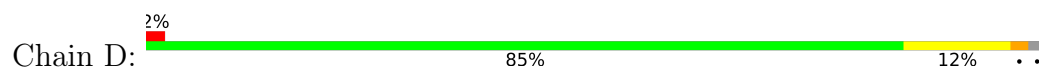


• Molecule 1: NITROALKANE OXIDASE

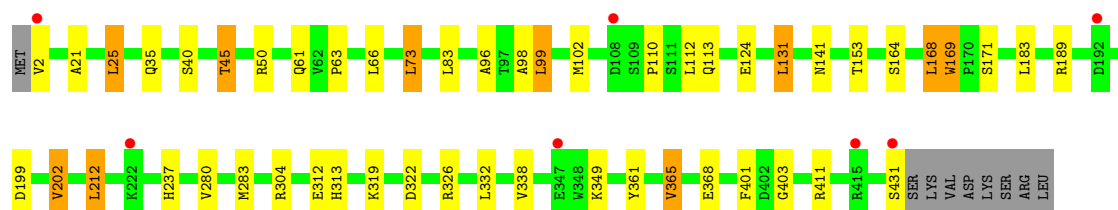
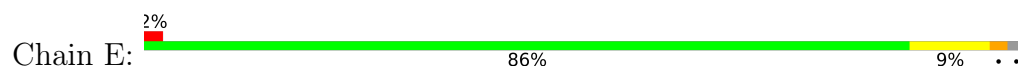




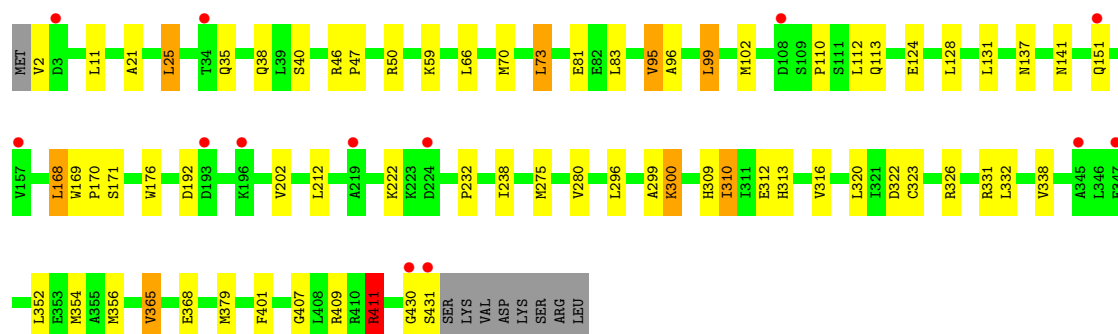
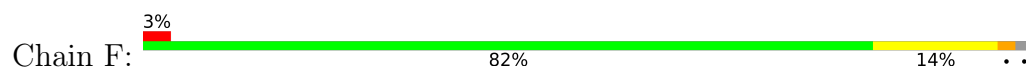
● Molecule 1: NITROALKANE OXIDASE



● Molecule 1: NITROALKANE OXIDASE



● Molecule 1: NITROALKANE OXIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	103.39Å 103.39Å 485.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.07 50.00 – 2.07	Depositor EDS
% Data completeness (in resolution range)	97.8 (50.00-2.07) 97.8 (50.00-2.07)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.71 (at 2.07Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.188 , 0.225 0.199 , 0.236	Depositor DCC
R_{free} test set	9048 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 34.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21487	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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: SPM, GOL, FAD, PE4

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	0.82	2/3384 (0.1%)	0.90	2/4592 (0.0%)
1	B	0.72	1/3384 (0.0%)	0.91	0/4592
1	C	0.71	0/3384	0.88	1/4592 (0.0%)
1	D	0.70	1/3398 (0.0%)	0.86	1/4611 (0.0%)
1	E	0.71	1/3384 (0.0%)	0.87	2/4592 (0.0%)
1	F	0.72	0/3384	0.90	2/4592 (0.0%)
All	All	0.73	5/20318 (0.0%)	0.89	8/27571 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	379	MET	SD-CE	-21.78	1.25	1.79
1	D	379	MET	SD-CE	7.07	1.97	1.79
1	B	64	ILE	CA-CB	5.87	1.57	1.54
1	A	64	ILE	CA-CB	5.67	1.57	1.53
1	E	283	MET	SD-CE	-5.49	1.65	1.79

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	411	ARG	CB-CG-CD	6.02	125.15	111.30
1	C	38	GLN	CB-CA-C	-5.33	102.51	110.88
1	D	45	THR	N-CA-CB	-5.20	102.79	110.53
1	A	63	PRO	CA-C-N	5.15	123.49	120.24
1	A	63	PRO	C-N-CA	5.15	123.49	120.24
1	E	63	PRO	CA-C-N	5.09	123.45	120.24
1	E	63	PRO	C-N-CA	5.09	123.45	120.24
1	F	411	ARG	CG-CD-NE	5.00	123.00	112.00

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	3309	0	3320	50	0
1	B	3309	0	3320	64	0
1	C	3309	0	3320	48	0
1	D	3313	0	3323	34	0
1	E	3309	0	3320	28	0
1	F	3309	0	3320	42	0
2	A	53	0	31	5	0
2	B	53	0	31	11	0
2	C	53	0	31	4	0
2	D	53	0	31	2	0
2	E	53	0	31	2	0
2	F	53	0	31	5	0
3	A	6	0	8	0	0
3	B	12	0	16	0	0
3	C	24	0	32	1	0
3	D	24	0	32	2	0
3	E	18	0	24	1	0
3	F	6	0	8	3	0
4	B	14	0	26	5	0
4	C	14	0	26	9	0
4	D	14	0	26	1	0
4	F	14	0	26	8	0
5	B	24	0	34	16	0
5	F	24	0	34	9	0
6	A	195	0	0	4	0
6	B	207	0	0	15	0
6	C	164	0	0	7	0
6	D	159	0	0	5	0
6	E	187	0	0	6	0
6	F	205	0	0	12	0
All	All	21487	0	20401	280	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (280) 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)
5:B:1436:PE4:H141	6:B:2206:HOH:O	1.29	1.27
6:A:2191:HOH:O	1:B:310:ILE:HG21	1.35	1.23
1:C:141:ASN:HD21	2:C:1433:FAD:H61A	1.19	0.91
1:A:10:GLN:HG3	1:A:75:HIS:CE1	2.09	0.87
5:F:1435:PE4:H142	6:F:2203:HOH:O	1.75	0.87
1:F:354:MET:SD	6:F:2152:HOH:O	2.34	0.86
1:B:141:ASN:HD21	2:B:1432:FAD:H61A	1.21	0.85
1:D:141:ASN:HD21	2:D:1433:FAD:H61A	1.25	0.83
4:C:1434:SPM:H41	6:C:2164:HOH:O	1.77	0.82
1:A:141:ASN:HD21	2:A:1432:FAD:H61A	1.27	0.81
1:C:70:MET:HE1	4:C:1434:SPM:N14	1.99	0.78
1:A:379:MET:HE1	1:B:401:PHE:CB	2.14	0.77
1:E:141:ASN:HD21	2:E:1432:FAD:H61A	1.31	0.76
1:A:379:MET:HE3	2:B:1432:FAD:H9	1.69	0.75
1:F:137:ASN:OD1	1:F:151:GLN:OE1	2.05	0.74
1:E:73:LEU:HB3	1:E:338:VAL:HB	1.69	0.73
1:F:141:ASN:HD21	2:F:1432:FAD:H61A	1.34	0.73
1:B:29:SER:O	1:B:33:SER:HB2	1.90	0.72
1:C:102[A]:MET:HE3	4:C:1434:SPM:C11	2.21	0.71
1:C:73:LEU:HB3	1:C:338:VAL:HB	1.73	0.70
1:D:45:THR:HG23	6:D:2031:HOH:O	1.91	0.69
5:B:1436:PE4:H163	6:B:2204:HOH:O	1.93	0.68
1:A:379:MET:HE1	1:B:401:PHE:CA	2.25	0.67
1:B:141:ASN:ND2	2:B:1432:FAD:H61A	1.90	0.66
1:A:379:MET:HE1	1:B:401:PHE:HA	1.78	0.65
1:F:81:GLU:OE2	1:F:331:ARG:HD3	1.96	0.65
1:F:73:LEU:HB3	1:F:338:VAL:HB	1.79	0.65
1:F:70:MET:HE1	4:F:1433:SPM:N14	2.11	0.65
1:A:99:LEU:HD22	1:A:131:LEU:HD23	1.79	0.65
1:A:314:GLN:HE21	1:D:315:SER:H	1.44	0.65
1:B:70:MET:HE1	4:B:1433:SPM:HN42	1.61	0.65
1:A:73:LEU:HB3	1:A:338:VAL:HB	1.80	0.64
1:F:99:LEU:HD22	1:F:131:LEU:HD23	1.78	0.64
1:B:73:LEU:HB3	1:B:338:VAL:HB	1.79	0.64
1:A:379:MET:CE	1:B:401:PHE:HA	2.28	0.64
1:B:296:LEU:O	1:B:300:LYS:HG3	1.98	0.63
1:F:151:GLN:HG3	6:F:2073:HOH:O	1.99	0.63
1:E:35:GLN:HE21	1:E:40:SER:HB3	1.63	0.63
1:F:96:ALA:HB1	1:F:171:SER:HB2	1.79	0.63
1:D:141:ASN:ND2	2:D:1433:FAD:H61A	1.95	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:GLN:HE21	1:A:98:ALA:HB2	1.63	0.62
1:C:45:THR:CG2	6:C:2040:HOH:O	2.46	0.62
1:A:45:THR:HG23	6:A:2044:HOH:O	2.00	0.62
1:F:95:VAL:HG13	4:F:1433:SPM:C8	2.29	0.61
1:A:326:ARG:HB3	1:A:365:VAL:HG13	1.81	0.61
1:F:38:GLN:HG3	1:F:232:PRO:O	1.99	0.61
1:C:27:LYS:HE2	6:C:2009:HOH:O	2.00	0.61
1:C:102[A]:MET:HE3	4:C:1434:SPM:H112	1.83	0.60
1:D:99:LEU:HD22	1:D:131:LEU:HD23	1.83	0.60
1:C:38:GLN:HG3	1:C:232:PRO:O	2.02	0.60
1:A:71:GLU:HB2	1:A:75:HIS:CD2	2.37	0.60
1:D:73:LEU:HB3	1:D:338:VAL:HB	1.82	0.60
1:D:70:MET:HE1	4:D:1434:SPM:N14	2.16	0.60
1:B:96:ALA:HB1	1:B:171:SER:HB2	1.83	0.59
5:F:1435:PE4:C11	6:F:2204:HOH:O	2.49	0.59
1:D:96:ALA:HB1	1:D:171:SER:HB2	1.85	0.59
5:B:1436:PE4:C11	6:B:2206:HOH:O	2.51	0.59
1:C:102[A]:MET:HE3	4:C:1434:SPM:H111	1.83	0.59
1:C:141:ASN:ND2	2:C:1433:FAD:H61A	1.94	0.59
1:C:96:ALA:HB1	1:C:171:SER:HB2	1.84	0.59
1:B:315:SER:H	1:C:314:GLN:HE21	1.51	0.58
1:F:110:PRO:HA	1:F:113:GLN:HE21	1.67	0.58
1:B:222:LYS:HD2	6:B:2103:HOH:O	2.03	0.58
1:B:314:GLN:HE21	1:C:315:SER:H	1.50	0.58
1:B:351:LYS:NZ	5:B:1436:PE4:H122	2.17	0.58
1:F:35:GLN:HE21	1:F:40:SER:HB3	1.69	0.58
1:C:99:LEU:HD22	1:C:131:LEU:HD23	1.85	0.58
2:A:1432:FAD:O5B	1:B:304:ARG:HG2	2.04	0.58
1:A:379:MET:HE3	2:B:1432:FAD:C9	2.34	0.58
2:B:1432:FAD:O2'	4:B:1433:SPM:N1	2.35	0.57
5:B:1436:PE4:C12	6:B:2206:HOH:O	2.51	0.57
1:C:326:ARG:HB3	1:C:365:VAL:HG13	1.85	0.57
1:A:45:THR:CG2	6:A:2044:HOH:O	2.51	0.57
1:B:351:LYS:NZ	5:B:1436:PE4:H131	2.19	0.57
1:E:96:ALA:HB1	1:E:171:SER:HB2	1.86	0.57
1:B:299:ALA:HA	1:B:310:ILE:HG22	1.85	0.57
5:F:1435:PE4:H111	6:F:2204:HOH:O	2.04	0.57
5:B:1436:PE4:H52	6:B:2207:HOH:O	2.04	0.57
1:B:310:ILE:HG23	1:B:316:VAL:HG11	1.85	0.57
1:A:379:MET:CE	2:B:1432:FAD:H2'	2.36	0.56
1:E:326:ARG:NE	6:E:2137:HOH:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ALA:HA	1:A:310:ILE:HG22	1.88	0.56
1:C:38:GLN:NE2	1:C:41:ARG:HH21	2.04	0.55
1:A:10:GLN:CG	1:A:75:HIS:CE1	2.88	0.55
1:B:45:THR:HG23	6:B:2046:HOH:O	2.06	0.55
1:A:322:ASP:O	1:A:326:ARG:HG3	2.07	0.55
1:B:95:VAL:HG13	4:B:1433:SPM:H62	1.89	0.55
1:E:141:ASN:ND2	2:E:1432:FAD:H61A	2.04	0.55
1:E:98:ALA:O	1:E:102[A]:MET:HG3	2.06	0.55
1:C:102[A]:MET:CE	4:C:1434:SPM:H112	2.38	0.54
1:C:352:LEU:O	1:C:356:MET:HG2	2.07	0.54
1:A:81:GLU:OE2	1:A:331:ARG:HD3	2.07	0.54
1:E:313:HIS:HD2	6:E:2128:HOH:O	1.90	0.54
1:A:310:ILE:HG23	1:A:316:VAL:HG11	1.88	0.54
1:A:315:SER:H	1:D:314:GLN:HE21	1.56	0.54
1:C:371:ILE:HG21	3:C:1437:GOL:H2	1.90	0.54
1:F:299:ALA:HA	1:F:310:ILE:HG22	1.89	0.54
1:C:102[B]:MET:HE3	1:C:106:LEU:HG	1.89	0.54
1:F:95:VAL:HG13	4:F:1433:SPM:H82	1.88	0.54
1:A:96:ALA:HB1	1:A:171:SER:HB2	1.90	0.54
1:B:326:ARG:HB3	1:B:365:VAL:HG13	1.89	0.54
1:F:326:ARG:HB3	1:F:365:VAL:HG13	1.88	0.54
1:E:61:GLN:HE21	1:E:98:ALA:HB2	1.73	0.53
1:E:361:TYR:O	1:E:365:VAL:HB	2.09	0.53
1:B:326:ARG:NH1	6:B:2151:HOH:O	2.40	0.53
1:A:379:MET:HE2	2:B:1432:FAD:H2'	1.90	0.53
1:A:38:GLN:NE2	1:A:234:LEU:H	2.06	0.53
3:F:1434:GOL:C2	6:F:2201:HOH:O	2.56	0.53
1:E:326:ARG:HB3	1:E:365:VAL:HG13	1.91	0.53
1:A:326:ARG:HD3	1:A:365:VAL:HG22	1.90	0.53
1:F:310:ILE:HG23	1:F:316:VAL:HG11	1.91	0.53
1:B:351:LYS:HZ2	5:B:1436:PE4:H131	1.74	0.52
1:F:141:ASN:ND2	2:F:1432:FAD:H61A	2.06	0.52
1:B:304:ARG:HB2	1:B:310:ILE:HD13	1.90	0.52
1:E:99:LEU:HD22	1:E:131:LEU:HD23	1.92	0.52
5:B:1436:PE4:H101	5:B:1436:PE4:H41	1.92	0.52
1:C:45:THR:HG23	6:C:2040:HOH:O	2.09	0.52
1:F:99:LEU:HD23	1:F:102[A]:MET:HE3	1.92	0.52
1:A:310:ILE:HA	1:A:313:HIS:HD2	1.75	0.52
1:E:168:LEU:HD13	1:E:169:TRP:NE1	2.25	0.52
1:C:402:ASP:HA	4:C:1434:SPM:N1	2.24	0.51
1:A:38:GLN:HG3	1:A:232:PRO:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ASN:ND2	2:A:1432:FAD:H61A	2.02	0.51
1:B:309:HIS:O	1:B:312:GLU:HB2	2.11	0.51
1:C:326:ARG:HD3	1:C:365:VAL:HG22	1.91	0.51
1:B:99:LEU:HD22	1:B:131:LEU:HD23	1.92	0.51
1:B:95:VAL:HG13	4:B:1433:SPM:C6	2.40	0.51
1:B:110:PRO:HA	1:B:113:GLN:HE21	1.76	0.51
1:C:102[B]:MET:HE2	1:C:275:MET:SD	2.51	0.51
4:C:1434:SPM:C4	6:C:2164:HOH:O	2.47	0.51
5:F:1435:PE4:H62	5:F:1435:PE4:H101	1.93	0.50
1:A:304:ARG:HB2	1:A:310:ILE:HD13	1.92	0.50
1:B:45:THR:CG2	6:B:2046:HOH:O	2.58	0.50
1:D:129:ALA:HA	1:D:183:LEU:O	2.11	0.50
5:B:1436:PE4:H121	6:B:2206:HOH:O	2.11	0.50
1:C:110:PRO:HA	1:C:113:GLN:HE21	1.77	0.50
5:F:1435:PE4:C14	6:F:2203:HOH:O	2.45	0.50
1:C:35:GLN:HE21	1:C:35:GLN:HA	1.76	0.50
5:B:1436:PE4:C16	6:B:2204:HOH:O	2.57	0.49
1:E:199:ASP:HB3	1:E:202:VAL:CG1	2.42	0.49
1:B:361:TYR:O	1:B:365:VAL:HB	2.13	0.49
1:B:99:LEU:HD23	1:B:102[B]:MET:HE3	1.95	0.49
1:F:326:ARG:NH1	1:F:368:GLU:OE1	2.45	0.49
2:A:1432:FAD:H51A	1:B:304:ARG:HD3	1.94	0.49
1:C:183:LEU:HD11	1:C:212:LEU:HG	1.95	0.49
5:B:1436:PE4:H101	5:B:1436:PE4:C6	2.42	0.48
1:D:16:HIS:HE1	6:D:2020:HOH:O	1.96	0.48
1:D:45:THR:CG2	6:D:2031:HOH:O	2.57	0.48
1:F:352:LEU:HD12	1:F:356:MET:HE3	1.96	0.48
1:B:314:GLN:HE22	1:C:313:HIS:HB3	1.78	0.48
1:F:300:LYS:O	1:F:309:HIS:ND1	2.47	0.48
1:B:35:GLN:HE21	1:B:40:SER:HB3	1.78	0.47
1:F:21:ALA:HA	1:F:25:LEU:HB2	1.96	0.47
1:F:38:GLN:HE22	1:F:238:ILE:HA	1.78	0.47
1:C:42:PHE:O	1:C:45:THR:HB	2.14	0.47
1:F:95:VAL:CG1	4:F:1433:SPM:C6	2.92	0.47
1:A:171:SER:HA	1:A:241:SER:O	2.14	0.47
1:A:379:MET:HE1	1:B:401:PHE:HB2	1.96	0.47
1:B:168:LEU:C	1:B:170:PRO:HD3	2.40	0.47
5:B:1436:PE4:H101	5:B:1436:PE4:H62	1.96	0.47
1:D:29:SER:O	1:D:33[B]:SER:HB3	2.15	0.47
1:D:199:ASP:HB3	1:D:202:VAL:HG13	1.97	0.47
1:F:296:LEU:O	1:F:300:LYS:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:361:TYR:O	1:D:365:VAL:HB	2.15	0.47
1:B:168:LEU:C	1:B:170:PRO:CD	2.88	0.46
1:F:407:GLY:O	1:F:411:ARG:HG2	2.16	0.46
1:D:202:VAL:HG22	6:D:2068:HOH:O	2.14	0.46
1:A:84:PHE:CZ	1:A:283:MET:HE3	2.51	0.46
1:B:50:ARG:HD2	1:B:126:GLU:OE1	2.15	0.46
1:E:45:THR:HG23	6:E:2036:HOH:O	2.14	0.46
1:C:129:ALA:HA	1:C:183:LEU:O	2.16	0.46
1:C:349:LYS:HD3	6:C:2151:HOH:O	2.15	0.46
1:D:406:ILE:N	1:D:406:ILE:HD12	2.31	0.46
1:E:45:THR:CG2	6:E:2036:HOH:O	2.64	0.46
1:A:199:ASP:HB3	1:A:202:VAL:CG1	2.46	0.46
1:C:401:PHE:C	1:C:401:PHE:CD2	2.93	0.46
1:D:16:HIS:CD2	3:D:1437:GOL:H11	2.51	0.46
1:D:53:VAL:HG22	1:D:58:ILE:CG1	2.46	0.45
5:F:1435:PE4:H122	5:F:1435:PE4:H102	1.43	0.45
1:A:183:LEU:HD11	1:A:212:LEU:HG	1.99	0.45
1:D:169:TRP:N	1:D:170:PRO:HD2	2.31	0.45
1:D:22[A]:ASN:OD1	6:D:2006:HOH:O	2.21	0.45
1:E:322:ASP:O	1:E:326:ARG:HG3	2.16	0.45
1:D:118:LYS:HB3	1:D:119:PRO:HD3	1.98	0.45
5:F:1435:PE4:H121	5:F:1435:PE4:H141	1.37	0.45
1:B:84:PHE:CE1	1:B:283:MET:HG2	2.51	0.45
1:D:401:PHE:CD2	1:D:401:PHE:C	2.94	0.45
1:E:21:ALA:HA	1:E:25:LEU:HB2	1.99	0.45
1:F:151:GLN:CG	6:F:2073:HOH:O	2.59	0.45
1:F:320:LEU:HD23	6:F:2167:HOH:O	2.15	0.45
1:A:42:PHE:O	1:A:45:THR:HB	2.16	0.45
1:E:304:ARG:CD	2:F:1432:FAD:H51A	2.47	0.45
1:A:304:ARG:HG2	2:B:1432:FAD:O5B	2.17	0.45
1:F:310:ILE:HA	1:F:313:HIS:HD2	1.82	0.45
1:B:61:GLN:HE21	1:B:98:ALA:HB2	1.81	0.44
1:B:255:GLU:CD	6:B:2122:HOH:O	2.61	0.44
5:F:1435:PE4:H101	5:F:1435:PE4:C6	2.47	0.44
6:A:2191:HOH:O	1:B:310:ILE:HG12	2.17	0.44
2:C:1433:FAD:O2P	2:C:1433:FAD:H52A	2.17	0.44
1:A:314:GLN:NE2	1:D:315:SER:H	2.14	0.44
1:B:314:GLN:NE2	1:C:315:SER:H	2.15	0.44
1:B:315:SER:H	1:C:314:GLN:NE2	2.14	0.44
1:C:92:ILE:HG21	1:C:240:THR:HG22	1.99	0.44
1:E:368:GLU:CD	6:E:2151:HOH:O	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:GLU:OE2	1:B:331:ARG:HD3	2.17	0.44
1:E:153:THR:HA	1:E:189:ARG:O	2.18	0.44
1:B:401:PHE:C	1:B:401:PHE:CD2	2.95	0.44
1:D:364:ASP:OD1	3:D:1436:GOL:O2	2.35	0.44
1:A:401:PHE:C	1:A:401:PHE:CD2	2.96	0.44
1:F:379:MET:HE3	1:F:379:MET:HA	2.00	0.43
2:A:1432:FAD:C8A	1:B:310:ILE:HD11	2.49	0.43
1:B:169:TRP:N	1:B:170:PRO:CD	2.80	0.43
1:D:326:ARG:HB3	1:D:365:VAL:HG13	2.00	0.43
1:A:379:MET:HE1	1:B:401:PHE:HB3	1.98	0.43
1:F:128:LEU:HD11	1:F:176:TRP:CE2	2.53	0.43
1:D:198:GLN:HE22	1:D:204:PRO:HB3	1.84	0.43
1:B:349:LYS:HZ3	1:B:421:ASP:CG	2.27	0.43
5:B:1436:PE4:C10	6:B:2206:HOH:O	2.66	0.43
1:C:335:TRP:O	1:C:339:THR:HB	2.19	0.43
1:D:296:LEU:O	1:D:300:LYS:HG2	2.19	0.43
1:E:98:ALA:O	1:E:102[B]:MET:HG2	2.19	0.43
1:F:168:LEU:C	1:F:170:PRO:CD	2.92	0.43
2:C:1433:FAD:H9	2:C:1433:FAD:H1'2	1.82	0.43
1:A:352:LEU:O	1:A:356:MET:HG2	2.19	0.43
1:E:110:PRO:HA	1:E:113:GLN:HE21	1.83	0.43
1:E:237:HIS:HD2	6:E:2034:HOH:O	2.02	0.43
3:F:1434:GOL:C3	6:F:2201:HOH:O	2.66	0.43
1:A:98:ALA:O	1:A:102[B]:MET:HG3	2.19	0.42
1:A:314:GLN:HE22	1:D:313:HIS:HB3	1.84	0.42
1:B:21:ALA:HA	1:B:25:LEU:HB2	2.01	0.42
1:B:134:SER:HA	1:B:139:THR:HG21	2.01	0.42
1:D:35:GLN:HE21	1:D:40:SER:HB3	1.84	0.42
2:F:1432:FAD:HM73	2:F:1432:FAD:HM81	1.90	0.42
3:F:1434:GOL:H2	6:F:2201:HOH:O	2.19	0.42
1:A:315:SER:H	1:D:314:GLN:NE2	2.15	0.42
1:D:359:LYS:HD2	1:D:409:ARG:HG3	2.00	0.42
1:A:304:ARG:HG2	2:B:1432:FAD:C5B	2.50	0.42
1:B:45:THR:HG21	6:B:2113:HOH:O	2.19	0.42
1:C:61:GLN:HE21	1:C:98:ALA:HB2	1.84	0.42
1:C:118:LYS:HB3	1:C:119:PRO:HD3	2.01	0.42
1:F:95:VAL:CG1	4:F:1433:SPM:H62	2.50	0.42
1:C:168:LEU:O	1:C:169:TRP:HB2	2.19	0.42
1:F:73:LEU:HD21	1:F:275:MET:HE1	2.01	0.42
1:F:102[A]:MET:HE2	4:F:1433:SPM:H111	2.01	0.42
1:B:198:GLN:NE2	6:B:2087:HOH:O	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1436:PE4:H91	5:B:1436:PE4:H71	1.36	0.42
1:C:45:THR:HG21	6:C:2039:HOH:O	2.19	0.42
1:E:319:LYS:NZ	3:E:1435:GOL:O2	2.53	0.42
1:C:38:GLN:NE2	1:C:234:LEU:H	2.18	0.42
1:C:58:ILE:N	1:C:58:ILE:HD12	2.34	0.42
1:F:46:ARG:HB3	1:F:47:PRO:HD3	2.01	0.42
1:B:178:TYR:CE2	1:B:228:ILE:HG21	2.55	0.41
1:E:304:ARG:HD2	2:F:1432:FAD:H51A	2.02	0.41
1:B:118:LYS:HB3	1:B:119:PRO:HD3	2.02	0.41
1:B:183:LEU:HD11	1:B:212:LEU:HG	2.01	0.41
5:B:1436:PE4:H62	5:B:1436:PE4:C10	2.50	0.41
1:C:95:VAL:HB	4:C:1434:SPM:H82	2.01	0.41
1:D:352:LEU:O	1:D:356:MET:HG2	2.20	0.41
1:A:379:MET:HE2	2:B:1432:FAD:H4'	2.02	0.41
1:F:102[A]:MET:HE2	4:F:1433:SPM:C11	2.51	0.41
5:F:1435:PE4:H62	5:F:1435:PE4:H41	1.47	0.41
1:C:28:ALA:HA	1:C:48:PHE:CZ	2.56	0.41
1:B:28:ALA:HA	1:B:48:PHE:CZ	2.55	0.41
1:B:352:LEU:O	1:B:356:MET:HG2	2.21	0.41
1:C:352:LEU:HD12	1:C:356:MET:HE3	2.03	0.41
1:C:361:TYR:O	1:C:365:VAL:HB	2.21	0.41
1:F:430:GLY:O	1:F:431:SER:C	2.64	0.41
1:A:361:TYR:O	1:A:365:VAL:HB	2.21	0.41
1:B:53:VAL:HG22	1:B:58:ILE:HG13	2.02	0.41
1:B:340:THR:O	1:B:351:LYS:HE2	2.21	0.41
1:C:341:LEU:HD23	1:C:351:LYS:HB3	2.03	0.41
1:F:95:VAL:CG1	4:F:1433:SPM:H61	2.50	0.41
1:F:322:ASP:O	1:F:326:ARG:HG3	2.21	0.41
1:A:314:GLN:HB2	1:D:314:GLN:HB2	2.03	0.41
1:E:183:LEU:HD11	1:E:212:LEU:HG	2.03	0.40
1:A:310:ILE:HD11	2:B:1432:FAD:C8A	2.52	0.40
1:F:323:CYS:SG	6:F:2167:HOH:O	2.62	0.40
1:C:38:GLN:HE21	1:C:41:ARG:HH21	1.68	0.40
1:E:99:LEU:HA	1:E:102[B]:MET:HG3	2.03	0.40
1:B:279:LEU:HD13	4:B:1433:SPM:H112	2.03	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	429/439 (98%)	423 (99%)	4 (1%)	2 (0%)	24	17
1	B	429/439 (98%)	421 (98%)	5 (1%)	3 (1%)	18	10
1	C	429/439 (98%)	423 (99%)	4 (1%)	2 (0%)	24	17
1	D	431/439 (98%)	425 (99%)	5 (1%)	1 (0%)	43	38
1	E	429/439 (98%)	423 (99%)	4 (1%)	2 (0%)	24	17
1	F	429/439 (98%)	422 (98%)	6 (1%)	1 (0%)	43	38
All	All	2576/2634 (98%)	2537 (98%)	28 (1%)	11 (0%)	30	23

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	TRP
1	B	169	TRP
1	B	430	GLY
1	C	169	TRP
1	D	169	TRP
1	E	169	TRP
1	F	169	TRP
1	A	403	GLY
1	B	403	GLY
1	C	403	GLY
1	E	403	GLY

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	356/364 (98%)	329 (92%)	27 (8%)	12	6
1	B	356/364 (98%)	328 (92%)	28 (8%)	11	5
1	C	356/364 (98%)	329 (92%)	27 (8%)	12	6
1	D	358/364 (98%)	335 (94%)	23 (6%)	16	9
1	E	356/364 (98%)	333 (94%)	23 (6%)	15	8
1	F	356/364 (98%)	330 (93%)	26 (7%)	13	6
All	All	2138/2184 (98%)	1984 (93%)	154 (7%)	13	7

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	25	LEU
1	A	45	THR
1	A	50	ARG
1	A	66	LEU
1	A	73	LEU
1	A	83	LEU
1	A	99	LEU
1	A	102[A]	MET
1	A	102[B]	MET
1	A	112	LEU
1	A	118	LYS
1	A	124	GLU
1	A	131	LEU
1	A	164	SER
1	A	168	LEU
1	A	202	VAL
1	A	212	LEU
1	A	223	LYS
1	A	280	VAL
1	A	304	ARG
1	A	310	ILE
1	A	332	LEU
1	A	349	LYS
1	A	365	VAL
1	A	401	PHE
1	A	411	ARG
1	B	2	VAL
1	B	25	LEU
1	B	45	THR

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Mol	Chain	Res	Type
1	B	66	LEU
1	B	73	LEU
1	B	83	LEU
1	B	95	VAL
1	B	99	LEU
1	B	102[A]	MET
1	B	102[B]	MET
1	B	112	LEU
1	B	131	LEU
1	B	145	LYS
1	B	168	LEU
1	B	192	ASP
1	B	212	LEU
1	B	227	GLN
1	B	255	GLU
1	B	280	VAL
1	B	304	ARG
1	B	310	ILE
1	B	312	GLU
1	B	332	LEU
1	B	365	VAL
1	B	387	SER
1	B	401	PHE
1	B	411	ARG
1	B	431	SER
1	C	2	VAL
1	C	25	LEU
1	C	27	LYS
1	C	34	THR
1	C	36	LYS
1	C	45	THR
1	C	66	LEU
1	C	73	LEU
1	C	83	LEU
1	C	97	THR
1	C	99	LEU
1	C	112	LEU
1	C	118	LYS
1	C	131	LEU
1	C	164	SER
1	C	168	LEU
1	C	192	ASP

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Mol	Chain	Res	Type
1	C	202	VAL
1	C	212	LEU
1	C	280	VAL
1	C	332	LEU
1	C	339	THR
1	C	349	LYS
1	C	365	VAL
1	C	401	PHE
1	C	411	ARG
1	C	420	GLU
1	D	2	VAL
1	D	3	ASP
1	D	25	LEU
1	D	45	THR
1	D	50	ARG
1	D	66	LEU
1	D	83	LEU
1	D	99	LEU
1	D	112	LEU
1	D	131	LEU
1	D	160	GLU
1	D	168	LEU
1	D	192	ASP
1	D	202	VAL
1	D	212	LEU
1	D	280	VAL
1	D	300	LYS
1	D	312	GLU
1	D	332	LEU
1	D	349	LYS
1	D	365	VAL
1	D	401	PHE
1	D	411	ARG
1	E	2	VAL
1	E	25	LEU
1	E	45	THR
1	E	50	ARG
1	E	66	LEU
1	E	73	LEU
1	E	83	LEU
1	E	99	LEU
1	E	112	LEU

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Mol	Chain	Res	Type
1	E	124	GLU
1	E	131	LEU
1	E	164	SER
1	E	168	LEU
1	E	202	VAL
1	E	212	LEU
1	E	280	VAL
1	E	312	GLU
1	E	332	LEU
1	E	349	LYS
1	E	365	VAL
1	E	401	PHE
1	E	411	ARG
1	E	431	SER
1	F	2	VAL
1	F	11	LEU
1	F	25	LEU
1	F	50	ARG
1	F	59	LYS
1	F	66	LEU
1	F	73	LEU
1	F	83	LEU
1	F	95	VAL
1	F	99	LEU
1	F	112	LEU
1	F	124	GLU
1	F	168	LEU
1	F	192	ASP
1	F	202	VAL
1	F	212	LEU
1	F	222	LYS
1	F	280	VAL
1	F	300	LYS
1	F	310	ILE
1	F	312	GLU
1	F	332	LEU
1	F	365	VAL
1	F	401	PHE
1	F	409	ARG
1	F	411	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	38	GLN
1	A	43	GLN
1	A	61	GLN
1	A	75	HIS
1	A	113	GLN
1	A	137	ASN
1	A	141	ASN
1	A	159	ASN
1	A	237	HIS
1	A	256	ASN
1	A	314	GLN
1	B	16	HIS
1	B	22	ASN
1	B	35	GLN
1	B	38	GLN
1	B	43	GLN
1	B	61	GLN
1	B	113	GLN
1	B	137	ASN
1	B	141	ASN
1	B	198	GLN
1	B	227	GLN
1	B	256	ASN
1	B	266	GLN
1	B	309	HIS
1	B	314	GLN
1	C	16	HIS
1	C	18	GLN
1	C	22	ASN
1	C	35	GLN
1	C	38	GLN
1	C	43	GLN
1	C	61	GLN
1	C	113	GLN
1	C	137	ASN
1	C	141	ASN
1	C	144	GLN
1	C	309	HIS
1	C	314	GLN
1	C	357	GLN
1	D	16	HIS
1	D	18	GLN

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Mol	Chain	Res	Type
1	D	35	GLN
1	D	43	GLN
1	D	55	HIS
1	D	113	GLN
1	D	137	ASN
1	D	141	ASN
1	D	144	GLN
1	D	198	GLN
1	D	207	GLN
1	D	227	GLN
1	D	309	HIS
1	D	314	GLN
1	D	357	GLN
1	E	16	HIS
1	E	18	GLN
1	E	22	ASN
1	E	35	GLN
1	E	43	GLN
1	E	55	HIS
1	E	61	GLN
1	E	113	GLN
1	E	137	ASN
1	E	141	ASN
1	E	144	GLN
1	E	151	GLN
1	E	237	HIS
1	E	256	ASN
1	E	313	HIS
1	E	314	GLN
1	E	357	GLN
1	F	35	GLN
1	F	38	GLN
1	F	43	GLN
1	F	113	GLN
1	F	141	ASN
1	F	256	ASN
1	F	314	GLN

5.3.3 RNA ⓘ

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](#)

27 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	GOL	C	1436	-	5,5,5	0.49	0	5,5,5	0.81	0
2	FAD	F	1432	-	58,58,58	1.53	9 (15%)	85,89,89	1.98	21 (24%)
3	GOL	C	1437	-	5,5,5	0.61	0	5,5,5	1.25	1 (20%)
4	SPM	F	1433	-	13,13,13	0.40	0	12,12,12	0.86	0
4	SPM	D	1434	-	13,13,13	0.34	0	12,12,12	0.75	0
5	PE4	B	1436	-	23,23,23	0.64	0	22,22,22	0.99	2 (9%)
3	GOL	D	1432	-	5,5,5	0.45	0	5,5,5	0.54	0
3	GOL	D	1436	-	5,5,5	0.45	0	5,5,5	0.37	0
4	SPM	B	1433	-	13,13,13	0.51	0	12,12,12	1.12	1 (8%)
3	GOL	D	1437	-	5,5,5	0.47	0	5,5,5	0.53	0
2	FAD	D	1433	-	58,58,58	1.45	6 (10%)	85,89,89	1.97	20 (23%)
3	GOL	C	1435	-	5,5,5	0.38	0	5,5,5	0.32	0
3	GOL	E	1435	-	5,5,5	0.49	0	5,5,5	0.14	0
2	FAD	B	1432	-	58,58,58	1.60	9 (15%)	85,89,89	1.92	24 (28%)
3	GOL	F	1434	-	5,5,5	0.49	0	5,5,5	0.45	0
2	FAD	C	1433	-	58,58,58	1.57	8 (13%)	85,89,89	2.02	22 (25%)
2	FAD	A	1432	-	58,58,58	1.54	7 (12%)	85,89,89	1.99	24 (28%)
3	GOL	E	1433	-	5,5,5	0.34	0	5,5,5	0.47	0
3	GOL	A	1433	-	5,5,5	0.44	0	5,5,5	0.28	0
3	GOL	E	1434	-	5,5,5	0.49	0	5,5,5	0.93	0
5	PE4	F	1435	-	23,23,23	0.86	0	22,22,22	1.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	B	1434	-	5,5,5	0.42	0	5,5,5	0.30	0
3	GOL	C	1432	-	5,5,5	0.41	0	5,5,5	0.66	0
3	GOL	D	1435	-	5,5,5	0.58	0	5,5,5	0.37	0
3	GOL	B	1435	-	5,5,5	0.46	0	5,5,5	0.49	0
4	SPM	C	1434	-	13,13,13	0.32	0	12,12,12	1.14	1 (8%)
2	FAD	E	1432	-	58,58,58	1.73	11 (18%)	85,89,89	2.02	20 (23%)

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	GOL	C	1436	-	-	2/4/4/4	-
2	FAD	F	1432	-	-	10/34/50/50	0/6/6/6
3	GOL	C	1437	-	-	4/4/4/4	-
4	SPM	F	1433	-	-	4/11/11/11	-
4	SPM	D	1434	-	-	4/11/11/11	-
5	PE4	B	1436	-	-	13/21/21/21	-
3	GOL	D	1432	-	-	2/4/4/4	-
3	GOL	D	1436	-	-	2/4/4/4	-
4	SPM	B	1433	-	-	7/11/11/11	-
3	GOL	D	1437	-	-	4/4/4/4	-
2	FAD	D	1433	-	-	7/34/50/50	0/6/6/6
3	GOL	C	1435	-	-	1/4/4/4	-
3	GOL	E	1435	-	-	2/4/4/4	-
2	FAD	B	1432	-	-	12/34/50/50	0/6/6/6
3	GOL	F	1434	-	-	4/4/4/4	-
2	FAD	C	1433	-	-	7/34/50/50	0/6/6/6
2	FAD	A	1432	-	-	9/34/50/50	0/6/6/6
3	GOL	E	1433	-	-	2/4/4/4	-
3	GOL	A	1433	-	-	4/4/4/4	-
3	GOL	E	1434	-	-	2/4/4/4	-
5	PE4	F	1435	-	-	13/21/21/21	-
3	GOL	B	1434	-	-	2/4/4/4	-
3	GOL	C	1432	-	-	2/4/4/4	-
3	GOL	D	1435	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	1435	-	-	2/4/4/4	-
4	SPM	C	1434	-	-	6/11/11/11	-
2	FAD	E	1432	-	-	7/34/50/50	0/6/6/6

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1432	FAD	C4'-C3'	-6.41	1.42	1.53
2	B	1432	FAD	C4'-C3'	-5.97	1.43	1.53
2	C	1433	FAD	C4'-C3'	-5.93	1.43	1.53
2	A	1432	FAD	C4'-C3'	-5.83	1.43	1.53
2	D	1433	FAD	C4'-C3'	-5.78	1.43	1.53
2	F	1432	FAD	C4'-C3'	-5.57	1.43	1.53
2	A	1432	FAD	PA-O3P	-4.83	1.54	1.59
2	E	1432	FAD	C4X-N5	4.57	1.40	1.30
2	B	1432	FAD	C4X-N5	4.46	1.40	1.30
2	D	1433	FAD	C4X-N5	4.42	1.40	1.30
2	E	1432	FAD	P-O3P	4.29	1.64	1.59
2	C	1433	FAD	C4X-N5	4.25	1.39	1.30
2	C	1433	FAD	C5A-N7A	-3.91	1.31	1.39
2	E	1432	FAD	C10-N1	3.84	1.41	1.33
2	B	1432	FAD	C5A-N7A	-3.50	1.32	1.39
2	F	1432	FAD	PA-O3P	-3.28	1.56	1.59
2	E	1432	FAD	C5A-N7A	-3.22	1.33	1.39
2	A	1432	FAD	C4X-N5	3.10	1.37	1.30
2	D	1433	FAD	C5A-N7A	-3.06	1.33	1.39
2	F	1432	FAD	C4X-N5	3.06	1.37	1.30
2	E	1432	FAD	O4B-C1B	2.98	1.48	1.42
2	F	1432	FAD	C5A-N7A	-2.89	1.33	1.39
2	A	1432	FAD	C5A-N7A	-2.88	1.33	1.39
2	F	1432	FAD	C10-N1	2.68	1.38	1.33
2	C	1433	FAD	PA-O3P	-2.66	1.56	1.59
2	B	1432	FAD	O5'-C5'	-2.61	1.34	1.44
2	D	1433	FAD	C10-N1	2.59	1.38	1.33
2	F	1432	FAD	O3'-C3'	2.53	1.49	1.43
2	B	1432	FAD	C10-N1	2.52	1.38	1.33
2	C	1433	FAD	O3'-C3'	2.51	1.49	1.43
2	F	1432	FAD	C7M-C7	2.50	1.55	1.51
2	E	1432	FAD	O5'-C5'	-2.49	1.35	1.44
2	C	1433	FAD	O4B-C1B	2.44	1.47	1.42
2	D	1433	FAD	C8A-N9A	-2.40	1.33	1.37
2	E	1432	FAD	C4A-N9A	-2.37	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1432	FAD	C4X-C10	-2.35	1.37	1.44
2	A	1432	FAD	C7M-C7	2.33	1.55	1.51
2	A	1432	FAD	C4A-N9A	-2.22	1.33	1.37
2	B	1432	FAD	C4A-N9A	-2.18	1.33	1.37
2	C	1433	FAD	C8A-N9A	-2.17	1.33	1.37
2	D	1433	FAD	O5'-C5'	-2.15	1.36	1.44
2	B	1432	FAD	C8A-N9A	-2.13	1.33	1.37
2	E	1432	FAD	C8A-N9A	-2.11	1.34	1.37
2	B	1432	FAD	PA-O3P	2.07	1.61	1.59
2	F	1432	FAD	P-O3P	2.07	1.61	1.59
2	F	1432	FAD	C8A-N9A	-2.06	1.34	1.37
2	E	1432	FAD	P-O2P	-2.05	1.45	1.55
2	C	1433	FAD	C10-N1	2.03	1.37	1.33
2	E	1432	FAD	C2'-C3'	2.01	1.56	1.53
2	B	1432	FAD	O3'-C3'	2.01	1.47	1.43

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1432	FAD	C4'-C3'-C2'	-8.62	99.23	113.57
2	B	1432	FAD	C5'-C4'-C3'	-7.07	98.87	112.22
2	A	1432	FAD	C4'-C3'-C2'	-7.02	101.88	113.57
2	C	1433	FAD	C4'-C3'-C2'	-6.86	102.15	113.57
2	F	1432	FAD	C4'-C3'-C2'	-6.27	103.13	113.57
2	E	1432	FAD	C5'-C4'-C3'	-6.23	100.47	112.22
2	B	1432	FAD	C4'-C3'-C2'	-6.08	103.46	113.57
2	D	1433	FAD	C4'-C3'-C2'	-5.94	103.68	113.57
2	E	1432	FAD	O3'-C3'-C2'	5.61	121.67	108.93
2	C	1433	FAD	O3'-C3'-C2'	5.55	121.55	108.93
2	F	1432	FAD	O3'-C3'-C2'	5.52	121.47	108.93
2	A	1432	FAD	C5'-C4'-C3'	-5.49	101.86	112.22
2	B	1432	FAD	O3'-C3'-C2'	5.48	121.38	108.93
2	F	1432	FAD	C5'-C4'-C3'	-5.44	101.96	112.22
2	D	1433	FAD	C5'-C4'-C3'	-5.23	102.36	112.22
2	D	1433	FAD	O3'-C3'-C2'	5.21	120.78	108.93
2	D	1433	FAD	C5A-C4A-N3A	-5.18	119.58	126.72
2	A	1432	FAD	O3'-C3'-C2'	5.13	120.59	108.93
2	E	1432	FAD	C5A-C4A-N3A	-4.97	119.88	126.72
2	C	1433	FAD	C5'-C4'-C3'	-4.93	102.92	112.22
2	C	1433	FAD	C5A-C4A-N3A	-4.90	119.97	126.72
2	F	1432	FAD	C5A-C4A-N3A	-4.67	120.29	126.72
2	F	1432	FAD	N3A-C2A-N1A	-4.51	121.76	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1433	FAD	N3A-C2A-N1A	-4.39	121.94	128.58
2	B	1432	FAD	C5A-C4A-N3A	-4.30	120.79	126.72
2	A	1432	FAD	C5A-C4A-N3A	-4.20	120.93	126.72
2	A	1432	FAD	N3A-C2A-N1A	-4.19	122.24	128.58
2	F	1432	FAD	O4'-C4'-C5'	3.94	118.69	109.99
2	B	1432	FAD	N3A-C2A-N1A	-3.86	122.74	128.58
2	C	1433	FAD	N3A-C2A-N1A	-3.85	122.76	128.58
2	A	1432	FAD	O4'-C4'-C5'	3.84	118.46	109.99
2	C	1433	FAD	O5'-C5'-C4'	-3.84	99.11	109.36
2	E	1432	FAD	O5'-C5'-C4'	-3.82	99.18	109.36
2	C	1433	FAD	O4'-C4'-C5'	3.72	118.19	109.99
2	E	1432	FAD	N3A-C2A-N1A	-3.62	123.10	128.58
2	C	1433	FAD	O3'-C3'-C4'	-3.62	100.71	108.93
2	E	1432	FAD	O3'-C3'-C4'	-3.53	100.91	108.93
2	D	1433	FAD	C4A-C5A-N7A	-3.51	106.57	110.58
2	D	1433	FAD	C2A-N3A-C4A	3.41	120.16	111.83
2	A	1432	FAD	C4X-C10-N10	3.36	121.29	116.48
2	D	1433	FAD	C4X-C10-N10	3.33	121.25	116.48
2	C	1433	FAD	C5A-N7A-C8A	3.33	108.68	103.45
2	C	1433	FAD	N9A-C8A-N7A	-3.29	109.28	113.94
2	D	1433	FAD	N9A-C8A-N7A	-3.24	109.34	113.94
2	D	1433	FAD	C5A-N7A-C8A	3.23	108.53	103.45
2	F	1432	FAD	N3A-C4A-N9A	3.23	132.65	127.17
2	F	1432	FAD	O5'-C5'-C4'	-3.19	100.84	109.36
2	A	1432	FAD	O5'-C5'-C4'	-3.16	100.92	109.36
2	D	1433	FAD	N3A-C4A-N9A	3.12	132.47	127.17
2	E	1432	FAD	O4'-C4'-C5'	3.10	116.81	109.99
2	D	1433	FAD	O4'-C4'-C5'	3.09	116.81	109.99
2	E	1432	FAD	N3A-C4A-N9A	3.07	132.39	127.17
2	A	1432	FAD	C4A-C5A-N7A	-3.06	107.09	110.58
2	F	1432	FAD	C2A-N3A-C4A	3.05	119.29	111.83
2	C	1433	FAD	N3A-C4A-N9A	3.05	132.36	127.17
2	D	1433	FAD	O3'-C3'-C4'	-3.05	102.01	108.93
2	C	1433	FAD	C4A-C5A-N7A	-3.01	107.14	110.58
2	C	1433	FAD	C4-N3-C2	-3.00	120.32	125.64
2	D	1433	FAD	C10-C4X-N5	-2.99	118.70	124.81
2	F	1432	FAD	C4X-C10-N10	2.98	120.75	116.48
2	C	1433	FAD	C2A-N3A-C4A	2.98	119.12	111.83
2	A	1432	FAD	C4-N3-C2	-2.98	120.36	125.64
2	C	1433	FAD	C9A-C5X-N5	-2.97	119.31	122.45
2	F	1432	FAD	N9A-C8A-N7A	-2.94	109.76	113.94
2	B	1432	FAD	O5'-C5'-C4'	-2.93	101.55	109.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1432	FAD	N3A-C4A-N9A	2.91	132.11	127.17
2	E	1432	FAD	C2A-N3A-C4A	2.89	118.89	111.83
2	B	1432	FAD	O4'-C4'-C5'	2.85	116.28	109.99
2	F	1432	FAD	C10-C4X-N5	-2.83	119.03	124.81
2	F	1432	FAD	O2P-P-O3P	2.72	114.62	107.27
4	B	1433	SPM	C3-C4-N5	-2.69	104.86	112.07
2	F	1432	FAD	C5A-N7A-C8A	2.67	107.64	103.45
2	D	1433	FAD	O2A-PA-O3P	2.67	114.48	107.27
2	D	1433	FAD	C4-C4X-N5	2.66	121.89	118.21
2	A	1432	FAD	N9A-C8A-N7A	-2.66	110.17	113.94
2	A	1432	FAD	C9A-C5X-N5	-2.64	119.65	122.45
2	B	1432	FAD	C10-C4X-N5	-2.63	119.45	124.81
2	C	1433	FAD	O3P-PA-O1A	-2.61	102.85	110.70
2	F	1432	FAD	C4A-C5A-N7A	-2.61	107.60	110.58
2	B	1432	FAD	C4-N3-C2	-2.61	121.01	125.64
2	A	1432	FAD	C5A-N7A-C8A	2.60	107.54	103.45
2	B	1432	FAD	C4X-C10-N10	2.60	120.20	116.48
2	E	1432	FAD	N9A-C8A-N7A	-2.59	110.26	113.94
4	C	1434	SPM	C12-C11-N10	2.58	119.00	112.07
2	B	1432	FAD	O4-C4-C4X	-2.58	119.72	126.53
5	B	1436	PE4	O6-C10-C9	-2.57	98.64	110.35
2	B	1432	FAD	N9A-C8A-N7A	-2.57	110.29	113.94
2	C	1433	FAD	O4-C4-C4X	-2.56	119.78	126.53
2	C	1433	FAD	C4X-C4-N3	2.55	119.75	113.25
2	A	1432	FAD	C2A-N3A-C4A	2.54	118.04	111.83
2	A	1432	FAD	N3A-C4A-N9A	2.53	131.48	127.17
2	B	1432	FAD	C9A-C5X-N5	-2.51	119.79	122.45
2	A	1432	FAD	O4-C4-C4X	-2.51	119.90	126.53
2	A	1432	FAD	C4X-C4-N3	2.51	119.65	113.25
2	D	1433	FAD	O5'-C5'-C4'	-2.50	102.70	109.36
2	E	1432	FAD	C9A-C5X-N5	-2.49	119.81	122.45
2	D	1433	FAD	C4-N3-C2	-2.49	121.22	125.64
2	B	1432	FAD	C2A-N3A-C4A	2.48	117.88	111.83
2	A	1432	FAD	C10-C4X-N5	-2.47	119.76	124.81
2	E	1432	FAD	O2P-P-O3P	2.46	113.91	107.27
2	E	1432	FAD	C4A-C5A-N7A	-2.45	107.78	110.58
2	D	1433	FAD	O2P-P-O3P	2.43	113.84	107.27
2	C	1433	FAD	O2P-P-O3P	2.43	113.84	107.27
2	A	1432	FAD	O2-C2-N3	2.40	123.19	118.58
2	F	1432	FAD	C4-N3-C2	-2.39	121.40	125.64
2	F	1432	FAD	C9A-C5X-N5	-2.36	119.95	122.45
2	E	1432	FAD	C4X-C4-N3	2.35	119.23	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1433	FAD	C10-C4X-N5	-2.30	120.11	124.81
2	B	1432	FAD	O3'-C3'-C4'	-2.29	103.72	108.93
2	E	1432	FAD	C10-C4X-N5	-2.28	120.15	124.81
2	B	1432	FAD	O2-C2-N3	2.27	122.93	118.58
2	C	1433	FAD	O3P-P-O1P	-2.26	103.92	110.70
2	E	1432	FAD	C4X-C10-N10	2.24	119.68	116.48
2	C	1433	FAD	C4X-C10-N10	2.21	119.65	116.48
2	E	1432	FAD	C5A-N7A-C8A	2.21	106.92	103.45
2	A	1432	FAD	O2'-C2'-C3'	-2.20	104.10	109.25
2	A	1432	FAD	C2A-N1A-C6A	2.20	122.34	118.73
2	B	1432	FAD	C5A-N7A-C8A	2.20	106.90	103.45
2	B	1432	FAD	O2P-P-O3P	2.19	113.18	107.27
2	E	1432	FAD	O2P-P-O1P	2.18	122.58	112.44
2	D	1433	FAD	C4X-C4-N3	2.18	118.79	113.25
2	A	1432	FAD	O2-C2-N1	-2.18	118.19	121.80
2	B	1432	FAD	C5X-C9A-N10	2.17	119.93	117.97
2	F	1432	FAD	O3'-C3'-C4'	-2.16	104.02	108.93
2	F	1432	FAD	C4X-C4-N3	2.16	118.74	113.25
2	B	1432	FAD	C4X-C4-N3	2.14	118.69	113.25
2	B	1432	FAD	O2-C2-N1	-2.12	118.28	121.80
3	C	1437	GOL	O3-C3-C2	2.12	119.90	110.38
2	F	1432	FAD	C4-C4X-N5	2.10	121.11	118.21
2	F	1432	FAD	C4A-N9A-C8A	2.10	107.94	105.74
2	A	1432	FAD	C10-N1-C2	2.06	121.32	116.85
2	A	1432	FAD	O3P-PA-O1A	-2.03	104.58	110.70
5	B	1436	PE4	O6-C11-C12	-2.03	101.10	110.35
2	B	1432	FAD	C4A-C5A-N7A	-2.01	108.28	110.58
2	B	1432	FAD	O2A-PA-O3P	2.01	112.71	107.27
2	E	1432	FAD	C4-N3-C2	-2.00	122.09	125.64

There are no chirality outliers.

All (138) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1432	FAD	C1'-C2'-C3'-O3'
2	A	1432	FAD	C1'-C2'-C3'-C4'
2	A	1432	FAD	O2'-C2'-C3'-C4'
2	A	1432	FAD	C3'-C4'-C5'-O5'
2	A	1432	FAD	O4'-C4'-C5'-O5'
2	A	1432	FAD	C5'-O5'-P-O1P
2	B	1432	FAD	C5B-O5B-PA-O2A
2	B	1432	FAD	C1'-C2'-C3'-O3'

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Mol	Chain	Res	Type	Atoms
2	B	1432	FAD	C1'-C2'-C3'-C4'
2	B	1432	FAD	O2'-C2'-C3'-C4'
2	B	1432	FAD	C3'-C4'-C5'-O5'
2	B	1432	FAD	O4'-C4'-C5'-O5'
2	B	1432	FAD	C5'-O5'-P-O1P
2	C	1433	FAD	N10-C1'-C2'-O2'
2	C	1433	FAD	C1'-C2'-C3'-O3'
2	C	1433	FAD	C1'-C2'-C3'-C4'
2	C	1433	FAD	O2'-C2'-C3'-C4'
2	C	1433	FAD	C3'-C4'-C5'-O5'
2	C	1433	FAD	O4'-C4'-C5'-O5'
2	D	1433	FAD	C1'-C2'-C3'-O3'
2	D	1433	FAD	C1'-C2'-C3'-C4'
2	D	1433	FAD	O2'-C2'-C3'-C4'
2	D	1433	FAD	C3'-C4'-C5'-O5'
2	D	1433	FAD	O4'-C4'-C5'-O5'
2	D	1433	FAD	C5'-O5'-P-O1P
2	E	1432	FAD	N10-C1'-C2'-O2'
2	E	1432	FAD	C1'-C2'-C3'-O3'
2	E	1432	FAD	C1'-C2'-C3'-C4'
2	E	1432	FAD	O2'-C2'-C3'-C4'
2	E	1432	FAD	C3'-C4'-C5'-O5'
2	E	1432	FAD	O4'-C4'-C5'-O5'
2	F	1432	FAD	C5B-O5B-PA-O2A
2	F	1432	FAD	C5B-O5B-PA-O3P
2	F	1432	FAD	C1'-C2'-C3'-O3'
2	F	1432	FAD	C1'-C2'-C3'-C4'
2	F	1432	FAD	O2'-C2'-C3'-C4'
2	F	1432	FAD	C3'-C4'-C5'-O5'
2	F	1432	FAD	O4'-C4'-C5'-O5'
2	F	1432	FAD	C5'-O5'-P-O1P
3	A	1433	GOL	O1-C1-C2-C3
3	A	1433	GOL	C1-C2-C3-O3
3	B	1435	GOL	C1-C2-C3-O3
3	C	1436	GOL	O1-C1-C2-C3
3	D	1435	GOL	O1-C1-C2-C3
3	D	1437	GOL	C1-C2-C3-O3
3	E	1433	GOL	C1-C2-C3-O3
3	E	1435	GOL	C1-C2-C3-O3
3	E	1435	GOL	O2-C2-C3-O3
3	F	1434	GOL	C1-C2-C3-O3
5	B	1436	PE4	C6-C5-O3-C4

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Mol	Chain	Res	Type	Atoms
5	F	1435	PE4	C6-C5-O3-C4
5	F	1435	PE4	C14-C13-O7-C12
2	A	1432	FAD	O2'-C2'-C3'-O3'
2	F	1432	FAD	O2'-C2'-C3'-O3'
5	F	1435	PE4	O3-C5-C6-O4
5	B	1436	PE4	O7-C13-C14-O8
2	B	1432	FAD	O2'-C2'-C3'-O3'
2	C	1433	FAD	O2'-C2'-C3'-O3'
2	D	1433	FAD	O2'-C2'-C3'-O3'
5	F	1435	PE4	C7-C8-O5-C9
3	A	1433	GOL	O1-C1-C2-O2
3	D	1435	GOL	O2-C2-C3-O3
3	D	1437	GOL	O2-C2-C3-O3
4	B	1433	SPM	N10-C11-C12-C13
4	C	1434	SPM	C2-C3-C4-N5
5	B	1436	PE4	O3-C5-C6-O4
5	B	1436	PE4	C14-C13-O7-C12
5	B	1436	PE4	O6-C11-C12-O7
2	E	1432	FAD	O2'-C2'-C3'-O3'
5	B	1436	PE4	O2-C3-C4-O3
4	B	1433	SPM	C3-C4-N5-C6
4	D	1434	SPM	C2-C3-C4-N5
3	B	1434	GOL	O1-C1-C2-C3
3	C	1432	GOL	O1-C1-C2-C3
3	C	1437	GOL	O1-C1-C2-C3
3	C	1437	GOL	C1-C2-C3-O3
3	D	1432	GOL	C1-C2-C3-O3
3	D	1435	GOL	C1-C2-C3-O3
3	D	1436	GOL	C1-C2-C3-O3
3	D	1437	GOL	O1-C1-C2-C3
3	E	1434	GOL	O1-C1-C2-C3
4	F	1433	SPM	C8-C9-N10-C11
3	A	1433	GOL	O2-C2-C3-O3
3	B	1435	GOL	O2-C2-C3-O3
3	D	1432	GOL	O2-C2-C3-O3
3	D	1435	GOL	O1-C1-C2-O2
3	E	1433	GOL	O2-C2-C3-O3
3	E	1434	GOL	O1-C1-C2-O2
3	F	1434	GOL	O2-C2-C3-O3
5	F	1435	PE4	O6-C11-C12-O7
5	B	1436	PE4	C7-C8-O5-C9
4	D	1434	SPM	C8-C9-N10-C11

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Mol	Chain	Res	Type	Atoms
5	F	1435	PE4	C12-C11-O6-C10
4	C	1434	SPM	C8-C9-N10-C11
3	C	1432	GOL	O1-C1-C2-O2
3	C	1436	GOL	O1-C1-C2-O2
3	D	1436	GOL	O2-C2-C3-O3
5	B	1436	PE4	O1-C1-C2-O2
4	B	1433	SPM	C11-C12-C13-N14
4	D	1434	SPM	C7-C6-N5-C4
4	D	1434	SPM	C11-C12-C13-N14
5	B	1436	PE4	C5-C6-O4-C7
5	F	1435	PE4	C1-C2-O2-C3
5	F	1435	PE4	C8-C7-O4-C6
5	B	1436	PE4	C9-C10-O6-C11
5	F	1435	PE4	C11-C12-O7-C13
2	A	1432	FAD	C5B-O5B-PA-O3P
2	B	1432	FAD	C5B-O5B-PA-O3P
2	B	1432	FAD	C5'-O5'-P-O2P
2	B	1432	FAD	C5'-O5'-P-O3P
2	F	1432	FAD	C5B-O5B-PA-O1A
3	B	1434	GOL	O1-C1-C2-O2
3	F	1434	GOL	O1-C1-C2-C3
4	B	1433	SPM	C2-C3-C4-N5
4	B	1433	SPM	C8-C9-N10-C11
4	C	1434	SPM	C11-C12-C13-N14
4	F	1433	SPM	C11-C12-C13-N14
4	B	1433	SPM	N5-C6-C7-C8
5	F	1435	PE4	C5-C6-O4-C7
5	F	1435	PE4	O6-C10-C9-O5
3	C	1435	GOL	C1-C2-C3-O3
4	C	1434	SPM	C7-C6-N5-C4
3	C	1437	GOL	O1-C1-C2-O2
3	C	1437	GOL	O2-C2-C3-O3
5	B	1436	PE4	C12-C11-O6-C10
5	B	1436	PE4	C8-C7-O4-C6
4	C	1434	SPM	C3-C4-N5-C6
5	F	1435	PE4	C10-C9-O5-C8
4	F	1433	SPM	C7-C6-N5-C4
3	D	1437	GOL	O1-C1-C2-O2
3	F	1434	GOL	O1-C1-C2-O2
4	B	1433	SPM	C6-C7-C8-C9
5	F	1435	PE4	O7-C13-C14-O8
4	C	1434	SPM	N1-C2-C3-C4

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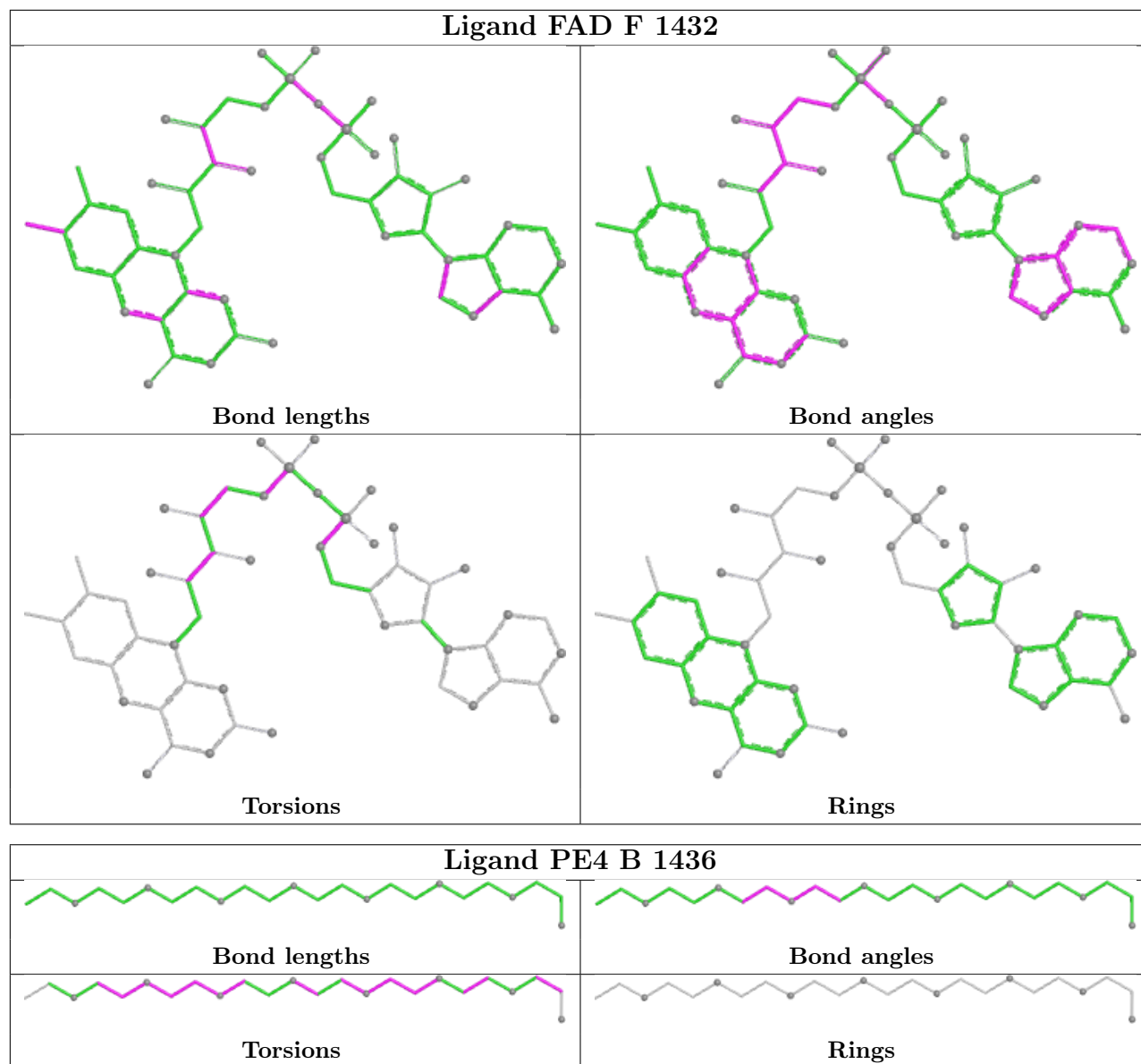
Mol	Chain	Res	Type	Atoms
4	F	1433	SPM	C7-C8-C9-N10
2	A	1432	FAD	C4'-C5'-O5'-P
5	B	1436	PE4	C11-C12-O7-C13
2	B	1432	FAD	PA-O3P-P-O2P

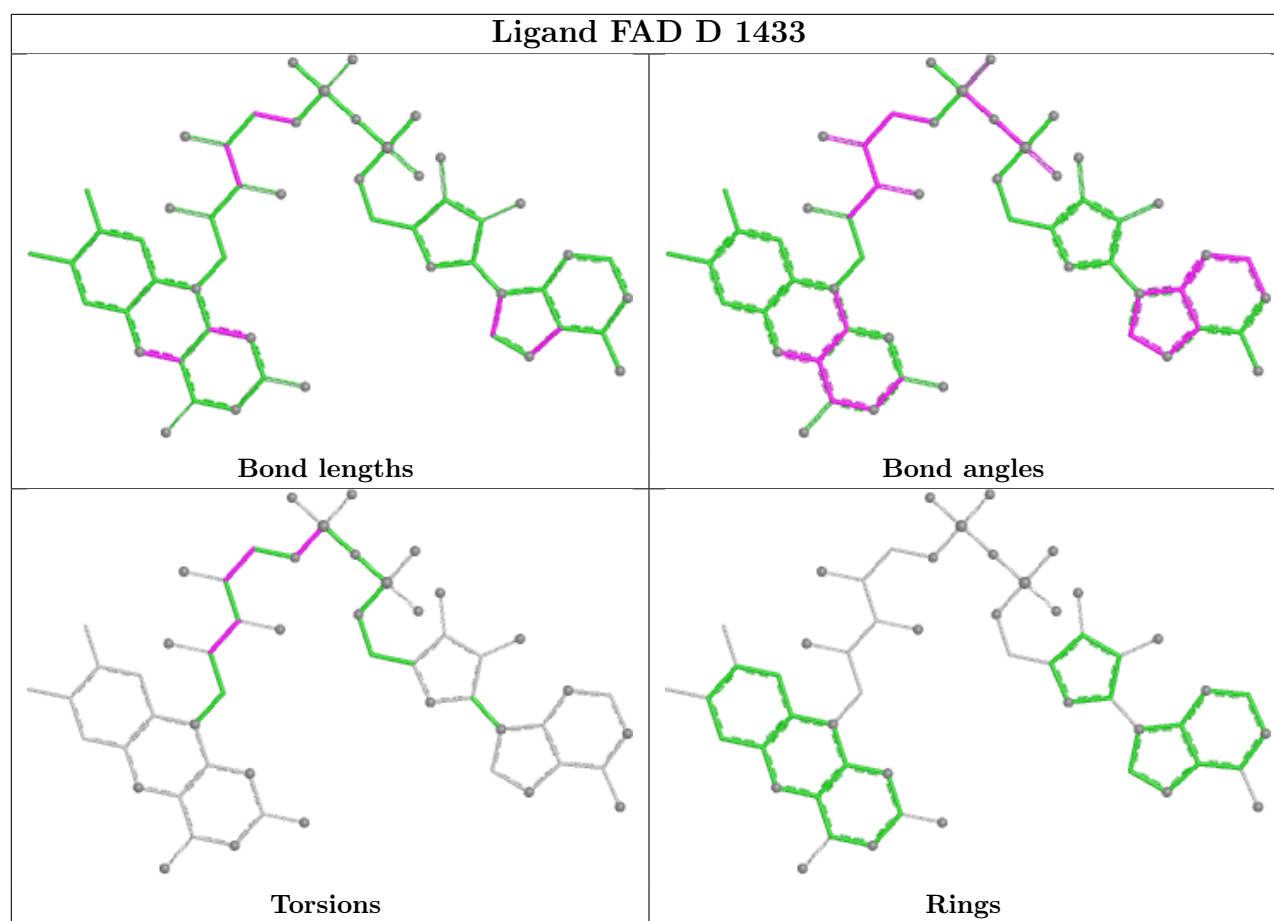
There are no ring outliers.

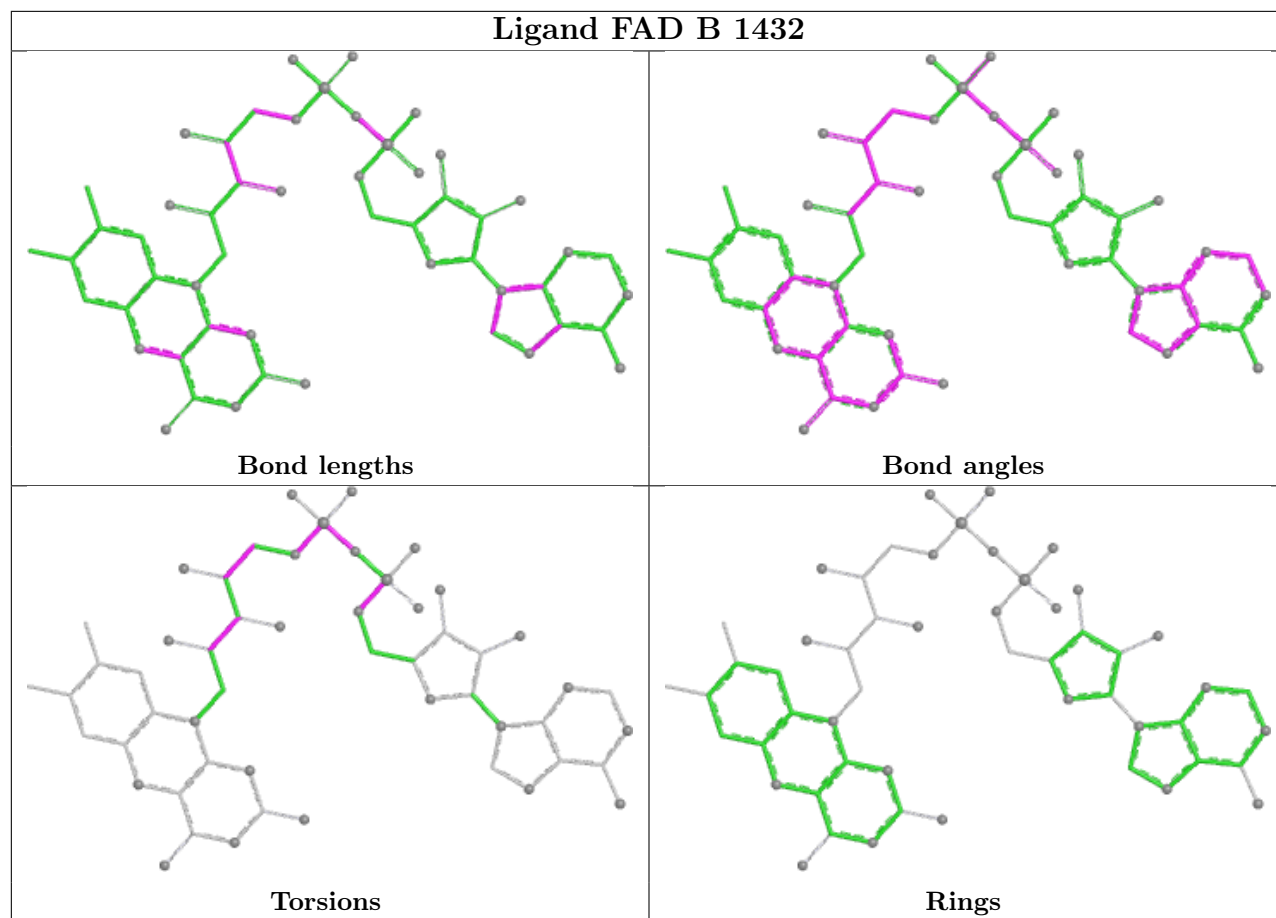
17 monomers are involved in 83 short contacts:

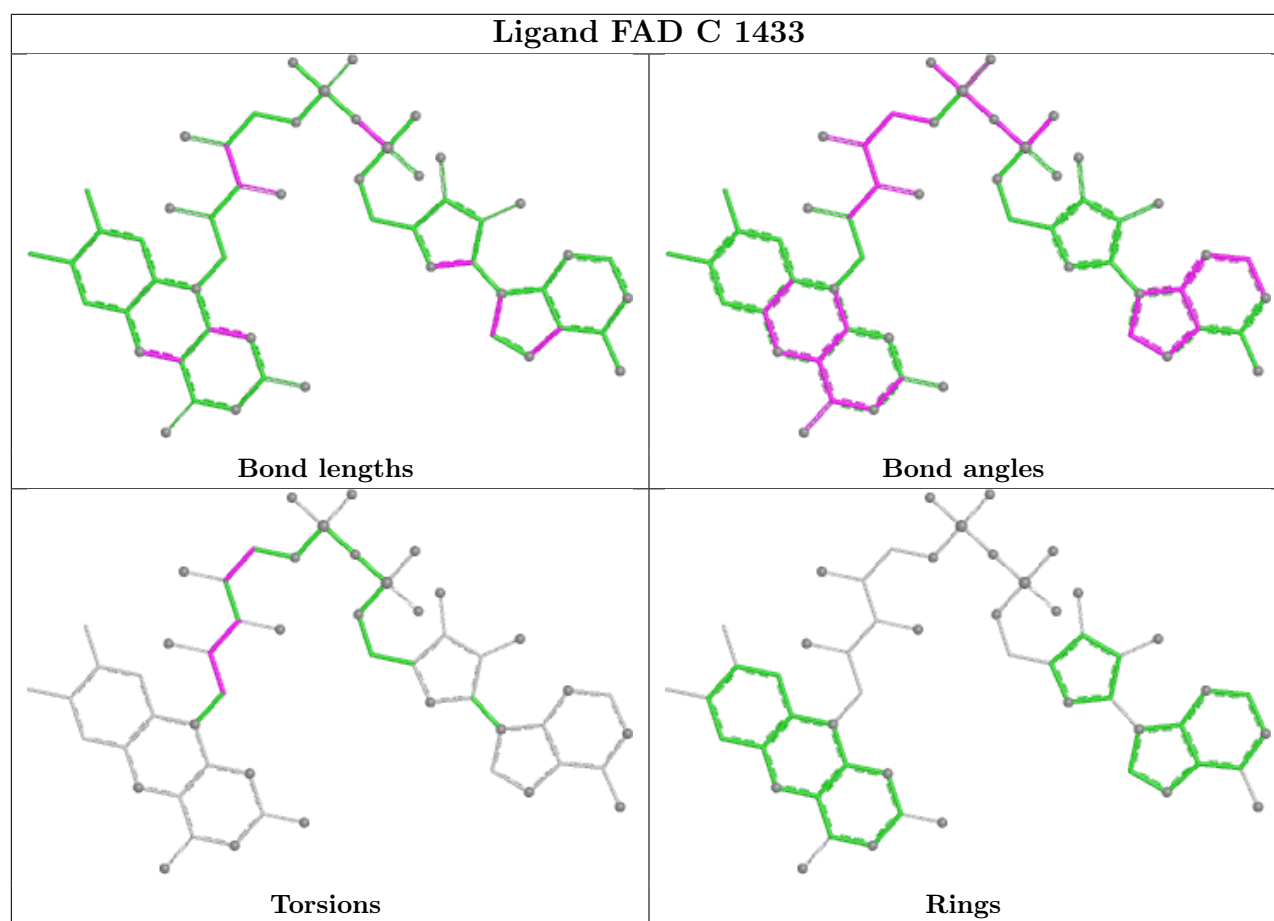
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1432	FAD	5	0
3	C	1437	GOL	1	0
4	F	1433	SPM	8	0
4	D	1434	SPM	1	0
5	B	1436	PE4	16	0
3	D	1436	GOL	1	0
4	B	1433	SPM	5	0
3	D	1437	GOL	1	0
2	D	1433	FAD	2	0
3	E	1435	GOL	1	0
2	B	1432	FAD	11	0
3	F	1434	GOL	3	0
2	C	1433	FAD	4	0
2	A	1432	FAD	5	0
5	F	1435	PE4	9	0
4	C	1434	SPM	9	0
2	E	1432	FAD	2	0

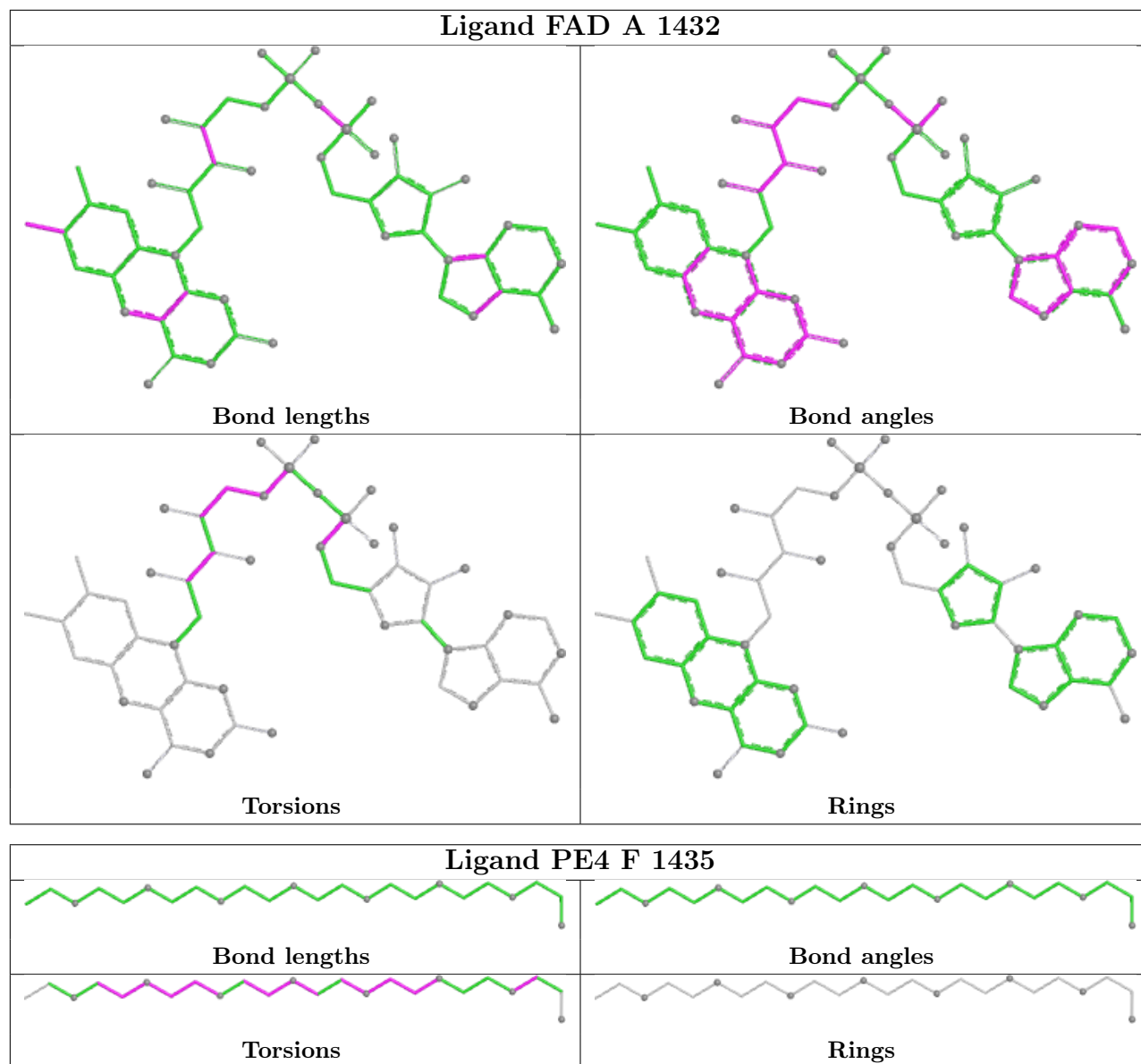
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

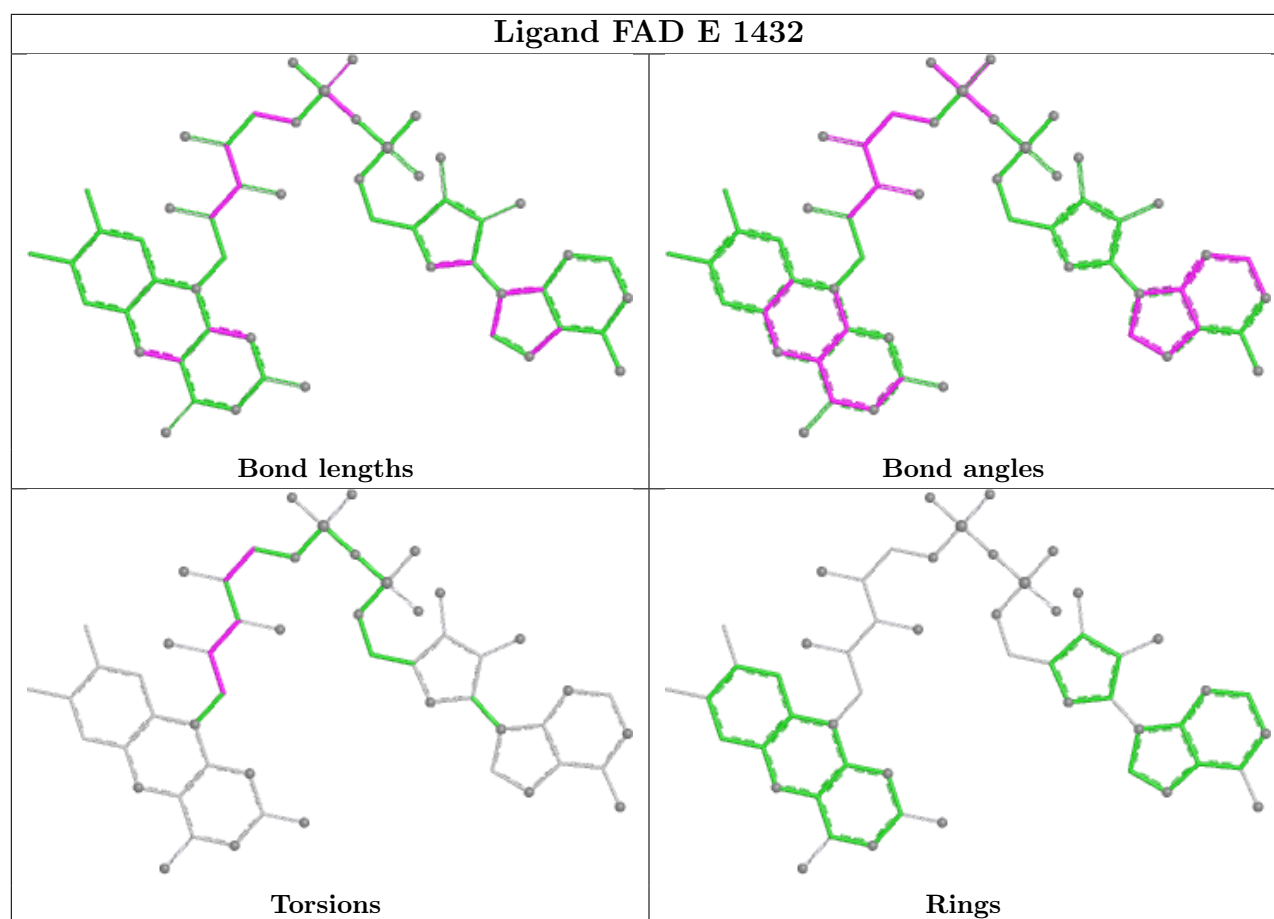












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	430/439 (97%)	0.23	10 (2%) 61 63	17, 25, 36, 45	1 (0%)
1	B	430/439 (97%)	0.27	14 (3%) 49 49	16, 24, 36, 49	1 (0%)
1	C	430/439 (97%)	0.40	18 (4%) 40 41	18, 27, 42, 54	1 (0%)
1	D	430/439 (97%)	0.40	8 (1%) 66 68	18, 27, 42, 49	3 (0%)
1	E	430/439 (97%)	0.23	7 (1%) 70 73	16, 24, 38, 46	1 (0%)
1	F	430/439 (97%)	0.27	13 (3%) 52 53	16, 25, 39, 49	1 (0%)
All	All	2580/2634 (97%)	0.30	70 (2%) 56 58	16, 25, 39, 54	8 (0%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	108	ASP	5.8
1	C	33	SER	5.2
1	B	33	SER	4.4
1	F	151	GLN	4.4
1	F	431	SER	4.2
1	C	36	LYS	3.8
1	C	347	GLU	3.7
1	E	192	ASP	3.6
1	B	431	SER	3.5
1	F	224	ASP	3.3
1	C	196	LYS	3.3
1	C	193	ASP	3.3
1	A	431	SER	3.2
1	D	196	LYS	3.0
1	E	431	SER	3.0
1	C	159	ASN	3.0
1	B	430	GLY	2.9
1	D	192	ASP	2.9
1	B	36	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	196	LYS	2.8
1	D	224	ASP	2.8
1	C	223	LYS	2.8
1	F	430	GLY	2.7
1	E	2	VAL	2.7
1	F	34	THR	2.7
1	A	421	ASP	2.6
1	C	34	THR	2.6
1	C	2	VAL	2.5
1	C	200	PRO	2.5
1	B	223	LYS	2.5
1	D	255	GLU	2.5
1	F	219	ALA	2.5
1	F	157	VAL	2.4
1	E	108	ASP	2.4
1	E	347	GLU	2.4
1	A	102[A]	MET	2.4
1	C	219	ALA	2.4
1	A	415	ARG	2.4
1	B	347	GLU	2.4
1	B	255	GLU	2.4
1	F	345	ALA	2.3
1	A	124	GLU	2.3
1	D	345	ALA	2.3
1	D	2	VAL	2.3
1	A	194	PRO	2.3
1	F	3	ASP	2.3
1	C	3	ASP	2.3
1	F	193	ASP	2.3
1	E	415	ARG	2.2
1	B	275	MET	2.2
1	A	420	GLU	2.2
1	C	415	ARG	2.2
1	B	365	VAL	2.2
1	C	328	GLU	2.2
1	F	347	GLU	2.2
1	C	254	HIS	2.2
1	C	194	PRO	2.2
1	B	2	VAL	2.1
1	D	13	ALA	2.1
1	D	30	ALA	2.1
1	A	192	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	220	ASN	2.1
1	A	2	VAL	2.1
1	A	344	GLU	2.1
1	B	102[A]	MET	2.0
1	B	423	GLU	2.0
1	C	431	SER	2.1
1	B	37	ASP	2.0
1	B	224	ASP	2.0
1	E	222	LYS	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.

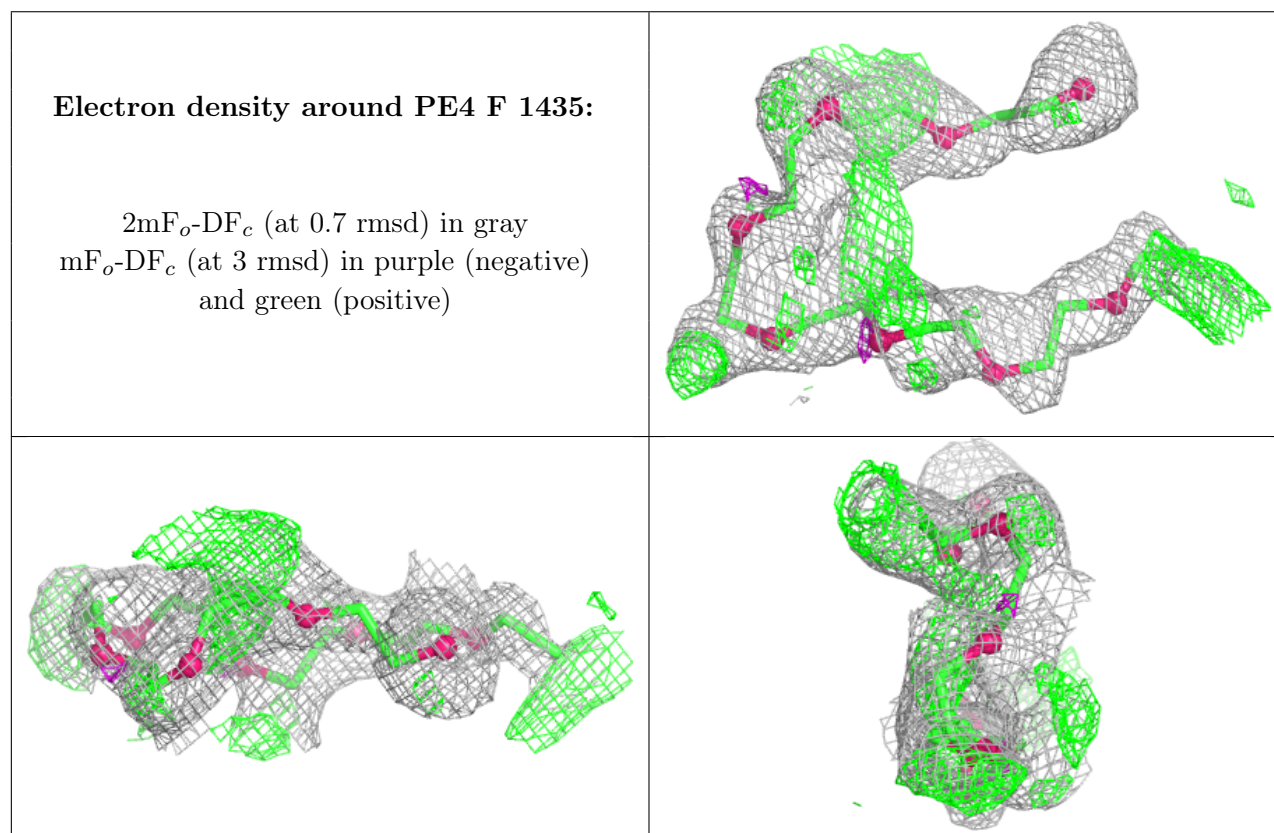
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	E	1435	6/6	0.37	0.25	58,59,59,59	0
3	GOL	A	1433	6/6	0.60	0.21	57,57,58,59	0
5	PE4	F	1435	24/24	0.63	0.26	49,53,55,57	0
3	GOL	C	1437	6/6	0.68	0.20	42,44,45,45	0
4	SPM	C	1434	14/14	0.68	0.21	45,46,47,49	0
3	GOL	D	1432	6/6	0.68	0.18	52,52,54,55	0
3	GOL	D	1436	6/6	0.69	0.18	48,49,49,50	0
5	PE4	B	1436	24/24	0.72	0.24	43,47,56,60	0
3	GOL	F	1434	6/6	0.72	0.19	47,51,53,54	0
3	GOL	B	1435	6/6	0.73	0.17	53,55,55,55	0
3	GOL	B	1434	6/6	0.75	0.17	45,46,48,48	0
3	GOL	C	1432	6/6	0.78	0.16	52,54,54,55	0
3	GOL	C	1435	6/6	0.79	0.15	48,49,50,50	0
3	GOL	D	1435	6/6	0.79	0.16	45,46,48,49	0

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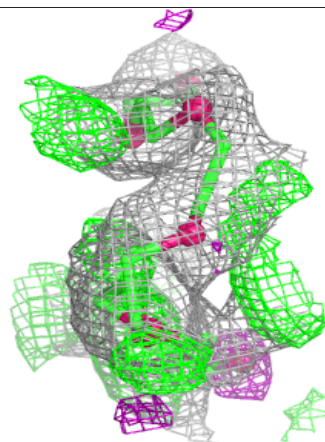
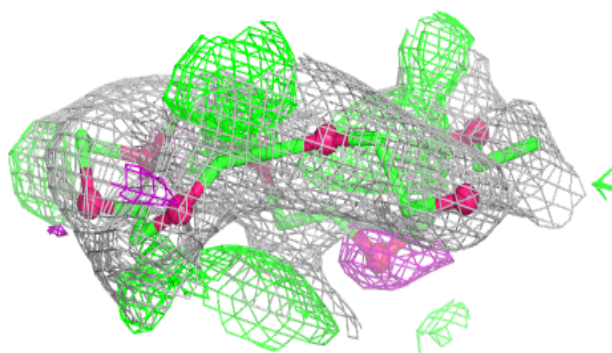
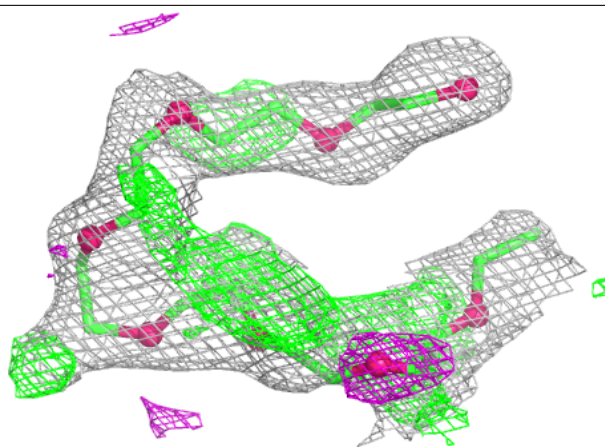
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SPM	F	1433	14/14	0.80	0.17	33,43,48,49	0
3	GOL	E	1434	6/6	0.81	0.15	45,48,49,50	0
3	GOL	D	1437	6/6	0.81	0.15	43,45,46,47	0
4	SPM	D	1434	14/14	0.81	0.19	40,52,56,56	0
4	SPM	B	1433	14/14	0.83	0.15	34,42,50,51	0
3	GOL	C	1436	6/6	0.85	0.12	39,41,42,42	0
3	GOL	E	1433	6/6	0.87	0.12	46,47,48,48	0
2	FAD	C	1433	53/53	0.96	0.06	15,19,23,25	0
2	FAD	D	1433	53/53	0.96	0.07	16,21,23,26	0
2	FAD	F	1432	53/53	0.96	0.07	13,17,22,24	0
2	FAD	B	1432	53/53	0.96	0.06	15,19,22,24	0
2	FAD	A	1432	53/53	0.97	0.06	16,20,22,22	0
2	FAD	E	1432	53/53	0.97	0.06	15,18,21,22	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.

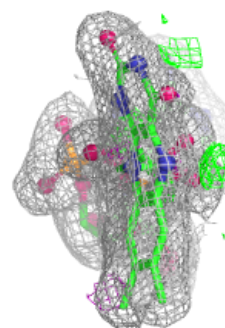
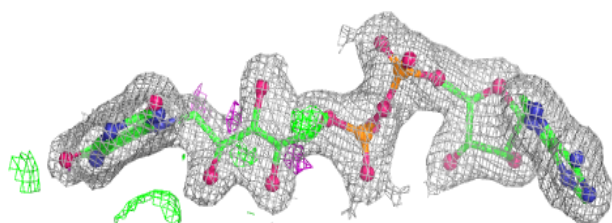
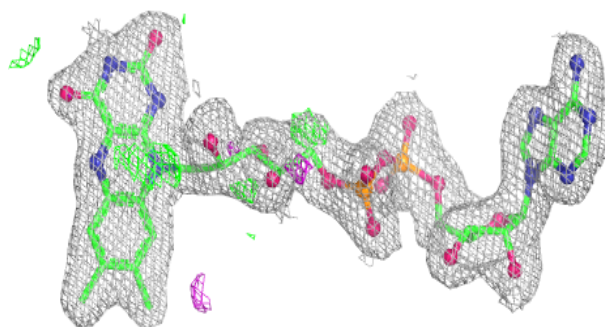


Electron density around PE4 B 1436:

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

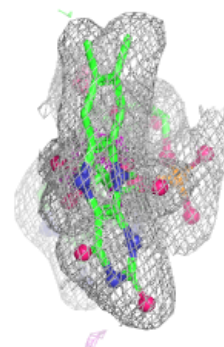
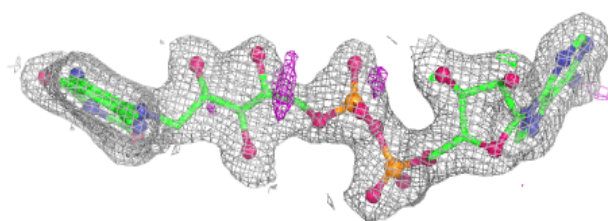
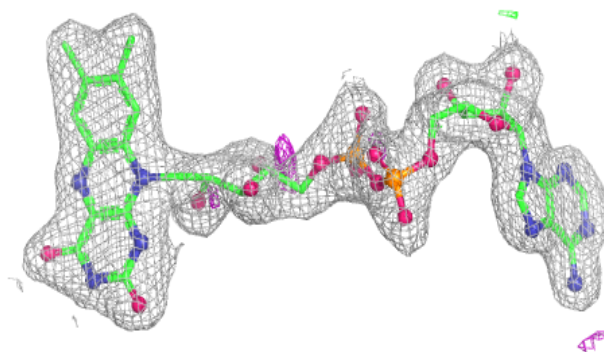
**Electron density around FAD C 1433:**

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

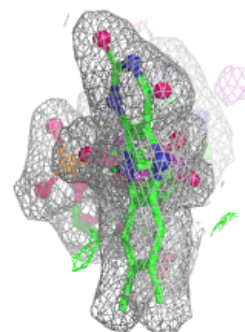
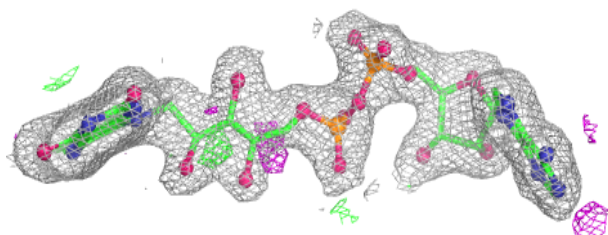
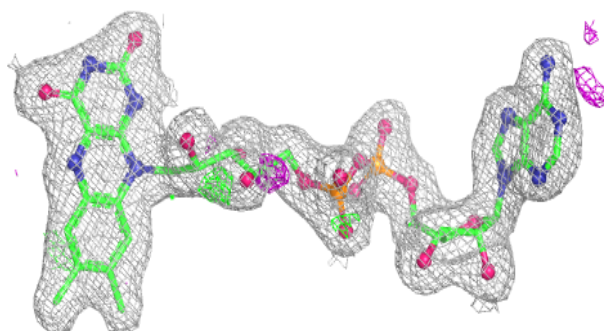


Electron density around FAD D 1433:

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

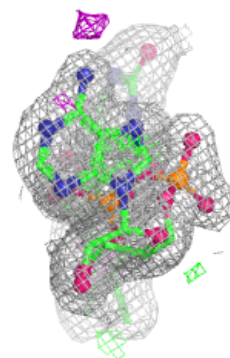
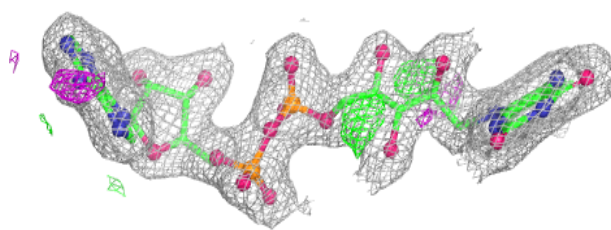
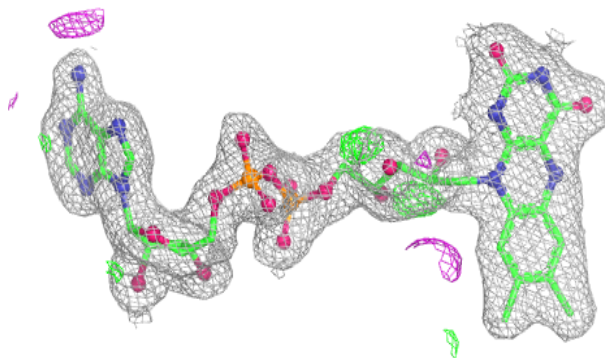
**Electron density around FAD F 1432:**

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

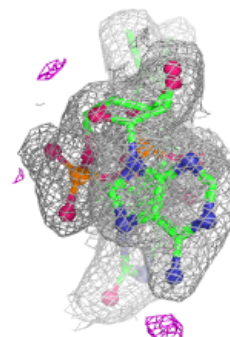
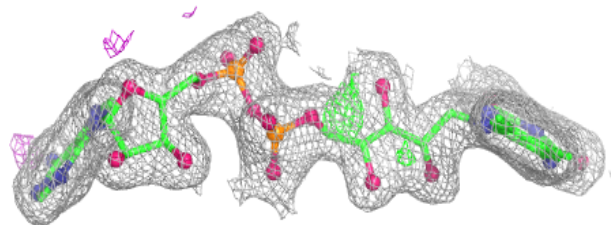
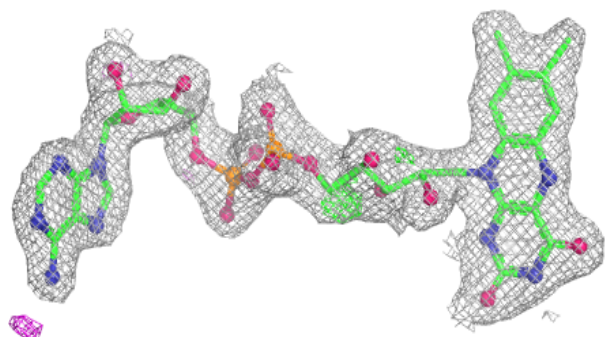


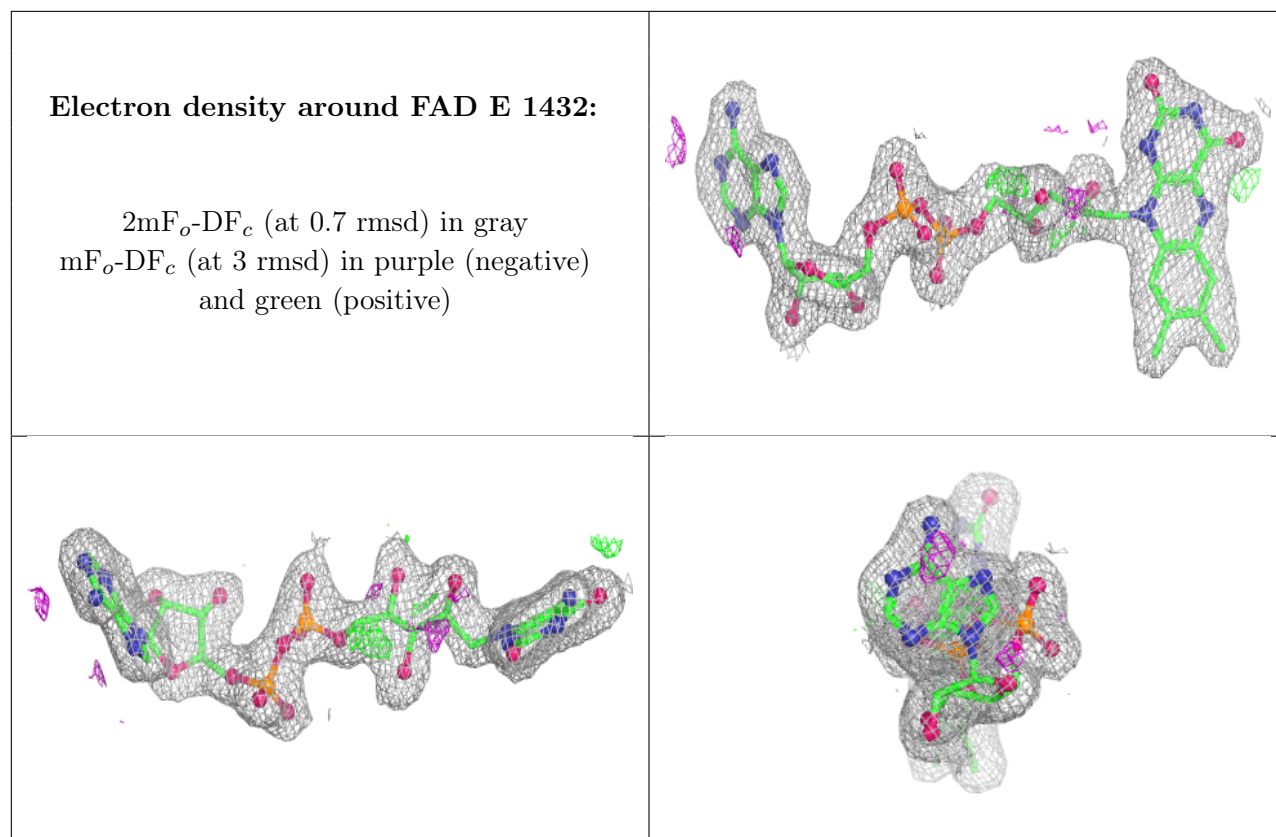
Electron density around FAD B 1432:

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

**Electron density around FAD A 1432:**

$2mF_o-DF_c$ (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.