



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:04 PM UTC

PDB ID : 2GVC / pdb_00002gvc
Title : Crystal structure of flavin-containing monooxygenase (FMO) from *S. pombe* and substrate (methimazole) complex
Authors : Eswaramoorthy, S.; Swaminathan, S.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2006-05-02
Resolution : 2.22 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

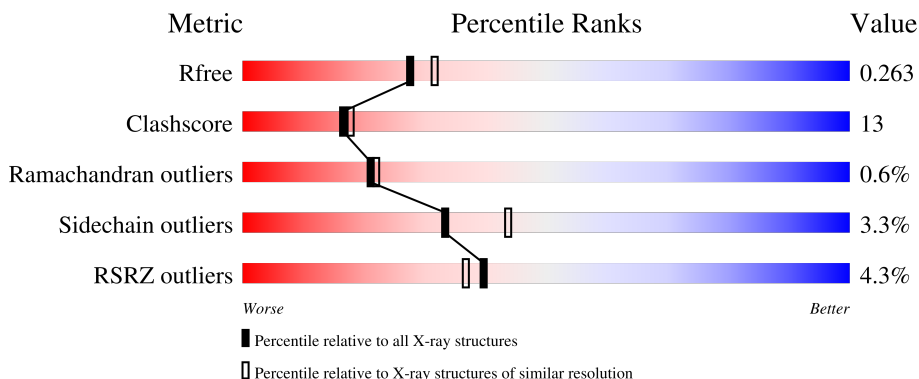
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	447	6% 70% 26% ..
1	B	447	3% 75% 21% ..
1	D	447	4% 72% 24% ..
1	E	447	3% 74% 23% ..

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	MMZ	A	501	-	X	-	-
4	MMZ	B	501	-	X	-	-
4	MMZ	D	501	-	X	-	-
4	MMZ	E	501	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14753 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.

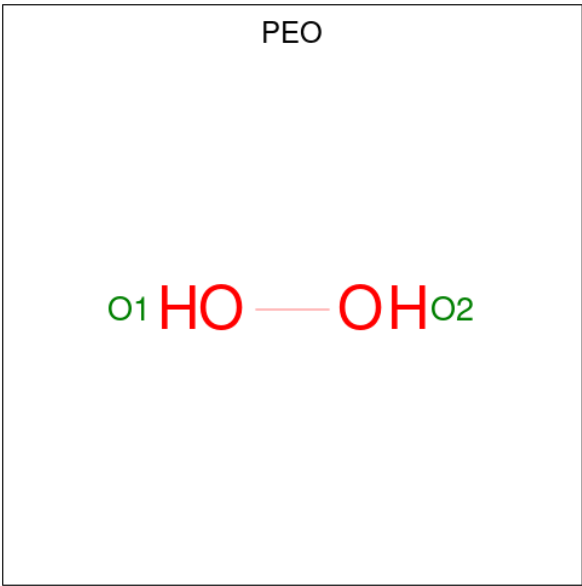
- Molecule 1 is a protein called monooxygenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	Se	0	0	0
			3486	2259	578	641	4	4			
1	B	442	Total	C	N	O	S	Se	0	0	0
			3486	2259	578	641	4	4			
1	D	442	Total	C	N	O	S	Se	0	0	0
			3486	2259	578	641	4	4			
1	E	442	Total	C	N	O	S	Se	0	0	0
			3486	2259	578	641	4	4			

There are 20 discrepancies between the modelled and reference sequences:

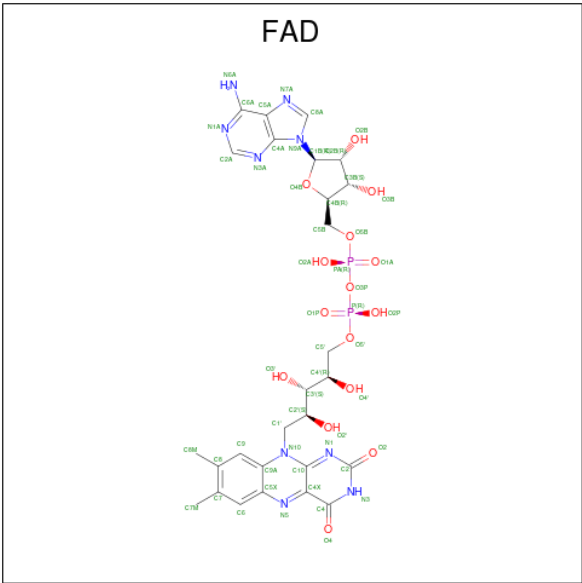
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q9HFE4
A	97	MSE	MET	modified residue	UNP Q9HFE4
A	377	MSE	MET	modified residue	UNP Q9HFE4
A	386	MSE	MET	modified residue	UNP Q9HFE4
A	433	MSE	MET	modified residue	UNP Q9HFE4
B	1	MSE	MET	modified residue	UNP Q9HFE4
B	97	MSE	MET	modified residue	UNP Q9HFE4
B	377	MSE	MET	modified residue	UNP Q9HFE4
B	386	MSE	MET	modified residue	UNP Q9HFE4
B	433	MSE	MET	modified residue	UNP Q9HFE4
D	1	MSE	MET	modified residue	UNP Q9HFE4
D	97	MSE	MET	modified residue	UNP Q9HFE4
D	377	MSE	MET	modified residue	UNP Q9HFE4
D	386	MSE	MET	modified residue	UNP Q9HFE4
D	433	MSE	MET	modified residue	UNP Q9HFE4
E	1	MSE	MET	modified residue	UNP Q9HFE4
E	97	MSE	MET	modified residue	UNP Q9HFE4
E	377	MSE	MET	modified residue	UNP Q9HFE4
E	386	MSE	MET	modified residue	UNP Q9HFE4
E	433	MSE	MET	modified residue	UNP Q9HFE4

- Molecule 2 is HYDROGEN PEROXIDE (CCD ID: PEO) (formula: H₂O₂).



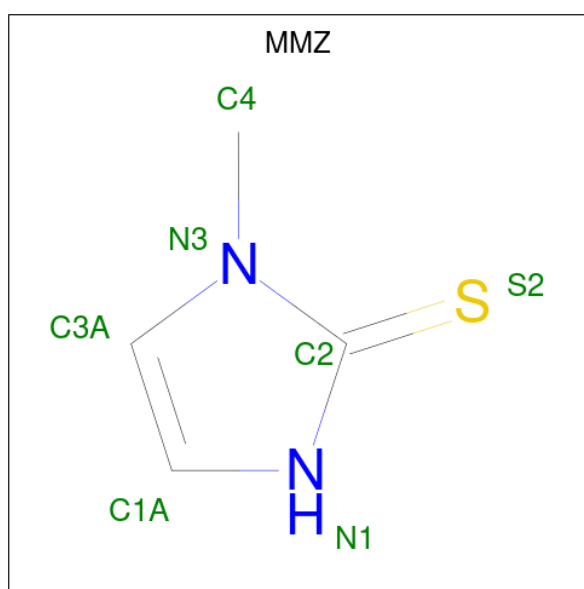
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O 2 2	0	0
2	B	1	Total O 2 2	0	0
2	D	1	Total O 2 2	0	0
2	E	1	Total O 2 2	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 4 is 1-METHYL-1,3-DIHYDRO-2H-IMIDAZOLE-2-THIONE (CCD ID: MMZ) (formula: C₄H₆N₂S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	S	0	0
			7	4	2	1		
4	B	1	Total	C	N	S	0	0
			7	4	2	1		
4	D	1	Total	C	N	S	0	0
			7	4	2	1		
4	E	1	Total	C	N	S	0	0
			7	4	2	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

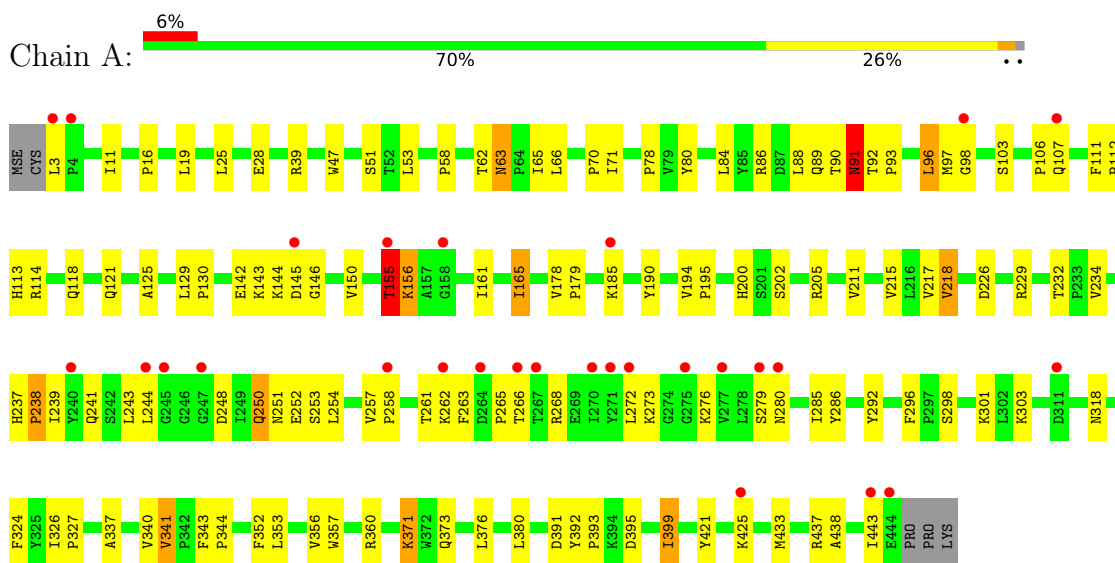
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	146	Total	O	0	0
			146	146		
6	B	114	Total	O	0	0
			114	114		
6	D	135	Total	O	0	0
			135	135		
6	E	142	Total	O	0	0
			142	142		

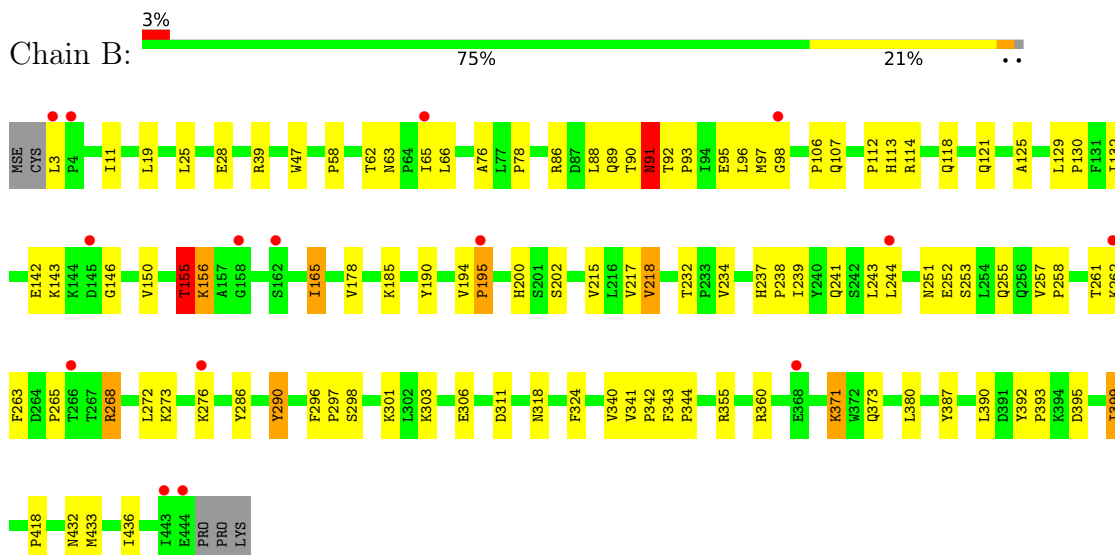
3 Residue-property plots [i](#)

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.

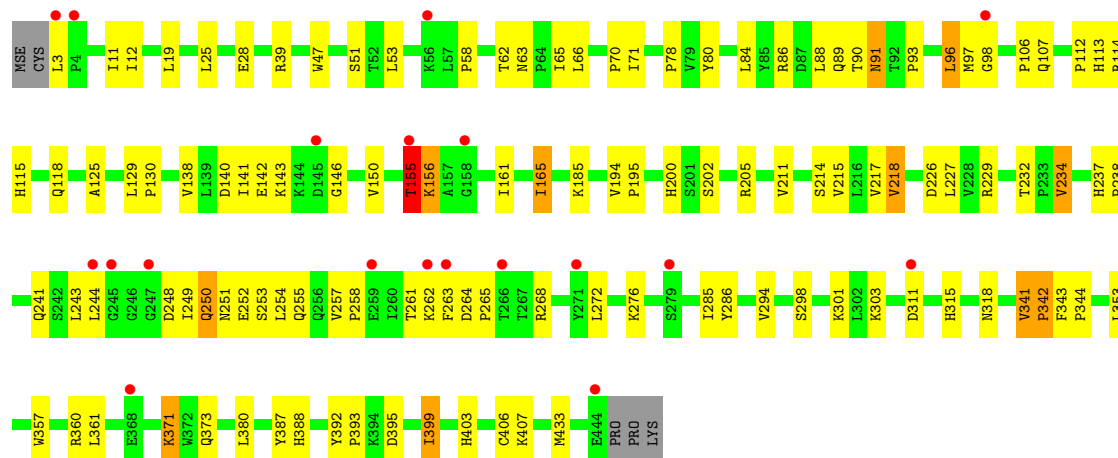
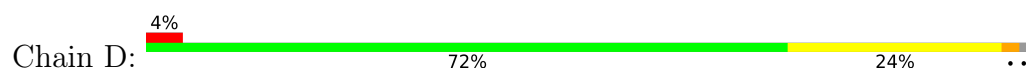
- Molecule 1: monooxygenase



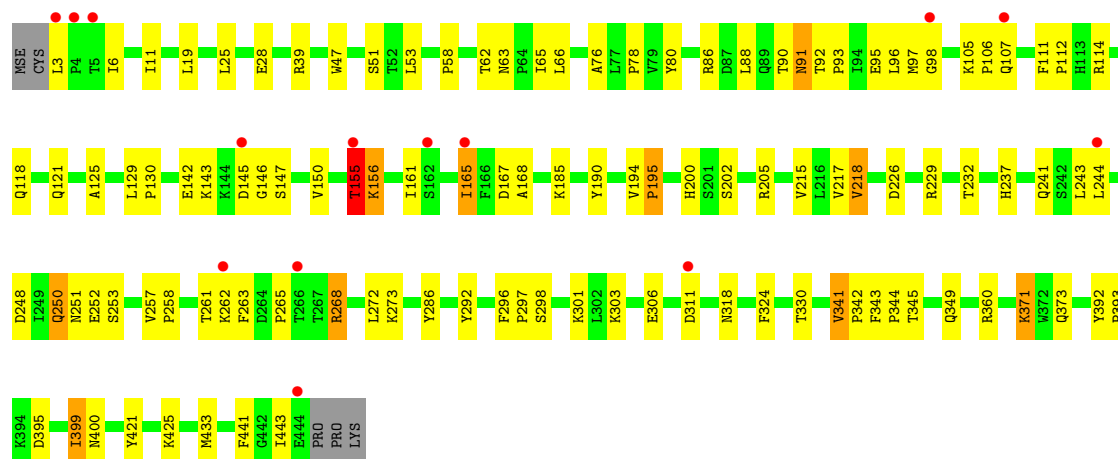
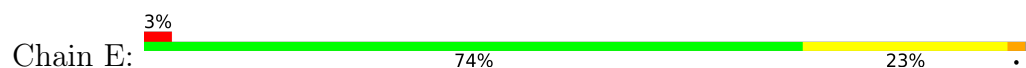
- Molecule 1: monooxygenase



- Molecule 1: monooxygenase



• Molecule 1: monooxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	72.70Å 84.45Å 113.51Å 107.73° 90.76° 106.50°	Depositor
Resolution (Å)	50.00 – 2.22 50.00 – 2.22	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.22) 86.8 (50.00-2.22)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 2.22Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.265 0.229 , 0.263	Depositor DCC
R_{free} test set	4516 reflections (4.03%)	wwPDB-VP
Wilson B-factor (Å ²)	21.2	Xtrriage
Anisotropy	0.119	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14753	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 73.87 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6986e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, FAD, MMZ, PEO

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	0.46	0/3583	0.97	19/4880 (0.4%)
1	B	0.46	0/3583	0.97	14/4880 (0.3%)
1	D	0.45	0/3583	0.93	11/4880 (0.2%)
1	E	0.45	0/3583	0.97	17/4880 (0.3%)
All	All	0.46	0/14332	0.96	61/19520 (0.3%)

There are no bond length outliers.

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	341	VAL	CA-C-N	8.31	130.23	119.84
1	E	341	VAL	C-N-CA	8.31	130.23	119.84
1	E	194	VAL	CA-C-N	8.12	129.99	119.84
1	E	194	VAL	C-N-CA	8.12	129.99	119.84
1	B	194	VAL	CA-C-N	7.99	129.82	119.84
1	B	194	VAL	C-N-CA	7.99	129.82	119.84
1	B	341	VAL	CA-C-N	7.65	129.40	119.84
1	B	341	VAL	C-N-CA	7.65	129.40	119.84
1	A	341	VAL	CA-C-N	7.60	129.34	119.84
1	A	341	VAL	C-N-CA	7.60	129.34	119.84
1	E	155	THR	N-CA-C	-7.44	98.80	109.96
1	A	86	ARG	N-CA-C	7.43	120.03	111.11
1	D	155	THR	N-CA-C	-7.27	98.19	109.76
1	D	341	VAL	CA-C-N	7.25	128.90	119.84
1	D	341	VAL	C-N-CA	7.25	128.90	119.84
1	B	215	VAL	N-CA-C	7.12	118.85	108.53
1	A	215	VAL	N-CA-C	7.10	118.70	108.48
1	D	86	ARG	N-CA-C	6.98	119.54	111.02
1	A	194	VAL	CA-C-N	6.76	128.29	119.84
1	A	194	VAL	C-N-CA	6.76	128.29	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	155	THR	N-CA-C	-6.69	99.93	109.96
1	D	234	VAL	N-CA-C	6.67	117.72	112.12
1	B	234	VAL	N-CA-C	6.63	116.86	111.62
1	B	324	PHE	N-CA-C	6.40	119.14	108.96
1	B	86	ARG	N-CA-C	6.37	118.79	111.02
1	A	234	VAL	N-CA-C	6.19	117.32	112.12
1	B	296	PHE	CA-C-N	6.09	127.45	119.84
1	B	296	PHE	C-N-CA	6.09	127.45	119.84
1	A	51	SER	N-CA-C	-5.99	105.82	113.01
1	B	132	ILE	N-CA-C	5.91	116.44	108.17
1	D	294	VAL	CA-C-N	5.90	127.22	119.84
1	D	294	VAL	C-N-CA	5.90	127.22	119.84
1	A	292	TYR	N-CA-C	-5.80	102.32	110.50
1	E	296	PHE	CA-C-N	5.77	127.06	119.84
1	E	296	PHE	C-N-CA	5.77	127.06	119.84
1	A	155	THR	N-CA-C	-5.74	101.35	109.96
1	E	292	TYR	N-CA-C	-5.71	102.84	110.55
1	B	91	ASN	N-CA-C	-5.69	105.54	112.88
1	D	51	SER	N-CA-C	-5.57	105.75	112.54
1	A	63	ASN	CA-C-N	5.55	125.64	119.87
1	A	63	ASN	C-N-CA	5.55	125.64	119.87
1	E	215	VAL	N-CA-C	5.53	117.37	108.85
1	E	330	THR	N-CA-C	-5.51	106.54	113.20
1	E	324	PHE	N-CA-C	5.49	118.48	109.76
1	E	111	PHE	CA-C-N	5.47	125.44	120.03
1	E	111	PHE	C-N-CA	5.47	125.44	120.03
1	A	324	PHE	N-CA-C	5.44	118.41	109.76
1	B	418	PRO	N-CA-C	5.36	119.91	111.38
1	D	194	VAL	CA-C-N	5.34	126.51	119.84
1	D	194	VAL	C-N-CA	5.34	126.51	119.84
1	A	341	VAL	N-CA-C	-5.33	97.37	108.88
1	E	145	ASP	CB-CA-C	-5.28	110.50	116.63
1	E	86	ARG	N-CA-C	5.27	117.45	111.02
1	A	285	ILE	N-CA-C	5.24	114.29	106.85
1	E	147	SER	N-CA-C	5.21	117.33	109.41
1	A	91	ASN	N-CA-C	-5.18	105.64	112.94
1	A	266	THR	N-CA-C	5.16	116.91	111.28
1	D	215	VAL	N-CA-C	5.16	116.79	108.85
1	E	51	SER	N-CA-C	-5.12	106.86	113.01
1	A	296	PHE	CA-C-N	5.10	126.21	119.84
1	A	296	PHE	C-N-CA	5.10	126.21	119.84

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	3486	0	3483	99	0
1	B	3486	0	3483	85	0
1	D	3486	0	3483	97	0
1	E	3486	0	3483	89	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
3	A	53	0	31	2	0
3	B	53	0	31	1	0
3	D	53	0	31	2	0
3	E	53	0	31	1	0
4	A	7	0	6	0	0
4	B	7	0	6	0	0
4	D	7	0	6	0	0
4	E	7	0	6	0	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
5	D	6	0	8	0	0
5	E	6	0	8	0	0
6	A	146	0	0	4	0
6	B	114	0	0	3	0
6	D	135	0	0	4	0
6	E	142	0	0	3	0
All	All	14753	0	14112	365	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 13.

All (365) 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:B:155:THR:HG21	6:B:615:HOH:O	1.57	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:185:LYS:HG2	1:E:262:LYS:HZ2	1.24	1.00
1:B:114:ARG:HH11	1:B:118:GLN:HE22	1.05	1.00
1:A:114:ARG:HH11	1:A:118:GLN:HE22	1.13	0.95
1:D:155:THR:HG21	6:D:634:HOH:O	1.64	0.95
1:E:114:ARG:HH11	1:E:118:GLN:HE22	1.16	0.93
1:A:155:THR:HG21	6:A:645:HOH:O	1.75	0.86
1:D:39:ARG:HD2	6:D:521:HOH:O	1.74	0.86
1:D:218:VAL:HG13	1:D:286:TYR:HA	1.58	0.86
1:D:93:PRO:HD2	1:D:433:MSE:HE2	1.58	0.85
1:E:155:THR:HG21	6:E:637:HOH:O	1.75	0.85
1:E:39:ARG:HD2	6:E:521:HOH:O	1.77	0.85
1:E:251:ASN:HD22	1:E:253:SER:H	1.22	0.84
1:E:218:VAL:HG13	1:E:286:TYR:HA	1.59	0.84
1:D:63:ASN:OD1	1:D:65:ILE:HG22	1.78	0.83
1:E:261:THR:HG22	1:E:262:LYS:HG3	1.60	0.83
1:D:114:ARG:HH11	1:D:118:GLN:HE22	1.22	0.82
1:E:395:ASP:O	1:E:399:ILE:HG23	1.79	0.82
1:B:39:ARG:HD2	6:B:523:HOH:O	1.81	0.81
1:D:47:TRP:O	1:D:118:GLN:HG2	1.81	0.80
1:B:218:VAL:HG13	1:B:286:TYR:HA	1.62	0.79
1:B:251:ASN:HD22	1:B:253:SER:H	1.33	0.77
1:A:218:VAL:HG13	1:A:286:TYR:HA	1.68	0.76
1:B:63:ASN:OD1	1:B:65:ILE:HG22	1.86	0.76
1:B:93:PRO:HD2	1:B:433:MSE:HE2	1.67	0.76
1:E:251:ASN:ND2	1:E:253:SER:H	1.83	0.76
1:A:3:LEU:HD22	6:A:565:HOH:O	1.86	0.74
1:A:39:ARG:HD2	6:A:545:HOH:O	1.86	0.74
1:A:47:TRP:O	1:A:118:GLN:HG2	1.87	0.74
1:A:142:GLU:HB3	1:A:298:SER:CB	2.18	0.74
1:B:114:ARG:HH11	1:B:118:GLN:NE2	1.82	0.74
1:B:114:ARG:NH1	1:B:118:GLN:HE22	1.82	0.74
1:E:91:ASN:C	1:E:91:ASN:HD22	1.94	0.74
1:B:155:THR:O	1:B:156:LYS:HB2	1.88	0.73
1:D:142:GLU:HB3	1:D:298:SER:CB	2.17	0.73
1:D:263:PHE:O	1:D:265:PRO:HD3	1.89	0.73
1:E:93:PRO:HD2	1:E:433:MSE:HE2	1.71	0.72
1:B:261:THR:HG22	1:B:262:LYS:HG3	1.71	0.71
1:A:106:PRO:HG2	1:B:106:PRO:HG2	1.71	0.71
1:D:3:LEU:HD13	1:D:146:GLY:O	1.91	0.71
1:E:185:LYS:HG2	1:E:262:LYS:NZ	2.04	0.71
1:A:28:GLU:OE1	1:A:360:ARG:HD3	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:ASN:ND2	1:B:253:SER:H	1.88	0.70
1:E:47:TRP:O	1:E:118:GLN:HG2	1.92	0.70
1:A:155:THR:O	1:A:156:LYS:CB	2.39	0.69
1:D:261:THR:HG22	1:D:262:LYS:HG3	1.74	0.69
1:E:318:ASN:H	1:E:373:GLN:HE22	1.40	0.69
1:A:97:MSE:HE1	1:A:112:PRO:HD2	1.75	0.69
1:A:318:ASN:H	1:A:373:GLN:HE22	1.40	0.69
1:E:155:THR:O	1:E:156:LYS:HB2	1.91	0.69
1:A:155:THR:O	1:A:156:LYS:HB2	1.91	0.68
1:E:114:ARG:HH11	1:E:118:GLN:NE2	1.89	0.68
1:D:155:THR:O	1:D:156:LYS:CB	2.41	0.68
1:D:155:THR:O	1:D:156:LYS:HB2	1.93	0.68
1:A:395:ASP:O	1:A:399:ILE:HG23	1.93	0.68
1:E:244:LEU:HD12	1:E:244:LEU:H	1.58	0.68
1:D:395:ASP:O	1:D:399:ILE:HG23	1.94	0.68
1:B:3:LEU:HD13	1:B:146:GLY:O	1.93	0.68
1:B:200:HIS:HD2	1:B:202:SER:OG	1.77	0.67
1:A:98:GLY:HA2	1:A:343:PHE:HD2	1.60	0.67
1:A:251:ASN:HD22	1:A:253:SER:H	1.43	0.67
1:A:232:THR:O	1:A:237:HIS:HE1	1.78	0.66
1:B:318:ASN:HA	1:B:373:GLN:HE22	1.60	0.66
1:D:251:ASN:O	1:D:255:GLN:NE2	2.27	0.66
1:A:261:THR:HG22	1:A:262:LYS:HG3	1.78	0.66
1:B:165:ILE:HD13	1:B:165:ILE:H	1.61	0.66
1:D:238:PRO:HB3	1:D:252:GLU:O	1.96	0.66
1:B:395:ASP:O	1:B:399:ILE:HG23	1.95	0.66
1:D:106:PRO:HG2	1:E:106:PRO:HG2	1.76	0.66
1:E:3:LEU:HD13	1:E:146:GLY:O	1.95	0.66
1:B:155:THR:O	1:B:156:LYS:CB	2.44	0.66
1:D:232:THR:O	1:D:237:HIS:HE1	1.80	0.65
1:B:241:GLN:HG2	1:B:243:LEU:HD22	1.77	0.65
1:E:155:THR:O	1:E:156:LYS:CB	2.45	0.64
1:B:106:PRO:O	1:B:107:GLN:HB2	1.96	0.64
1:D:241:GLN:HG2	1:D:243:LEU:HD22	1.79	0.63
1:B:232:THR:O	1:B:237:HIS:HE1	1.82	0.63
1:E:341:VAL:O	1:E:344:PRO:HD2	1.97	0.63
1:B:241:GLN:HG2	1:B:243:LEU:CD2	2.29	0.63
1:D:241:GLN:HG2	1:D:243:LEU:CD2	2.29	0.62
1:E:63:ASN:OD1	1:E:65:ILE:HG22	1.99	0.62
1:E:244:LEU:HD12	1:E:244:LEU:N	2.14	0.62
1:D:93:PRO:CD	1:D:433:MSE:HE2	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:LEU:HD13	1:A:146:GLY:O	1.99	0.61
1:A:91:ASN:C	1:A:91:ASN:HD22	2.08	0.61
1:D:244:LEU:HD12	1:D:244:LEU:H	1.64	0.61
1:E:165:ILE:HD13	1:E:165:ILE:H	1.64	0.61
1:D:91:ASN:C	1:D:91:ASN:HD22	2.09	0.61
1:D:185:LYS:HB3	1:D:262:LYS:HG2	1.82	0.61
1:D:318:ASN:H	1:D:373:GLN:HE22	1.47	0.61
1:B:343:PHE:HB2	1:B:344:PRO:HD3	1.82	0.60
1:B:142:GLU:HB3	1:B:298:SER:CB	2.31	0.60
1:E:142:GLU:HB3	1:E:298:SER:CB	2.30	0.60
1:D:97:MSE:HE1	1:D:112:PRO:HD2	1.83	0.60
1:E:106:PRO:O	1:E:107:GLN:HB2	2.02	0.60
1:A:392:TYR:CD1	1:A:393:PRO:HA	2.37	0.60
1:B:263:PHE:O	1:B:265:PRO:HD3	2.01	0.59
1:D:84:LEU:HD22	1:D:88:LEU:HD13	1.83	0.59
1:A:185:LYS:HG2	1:A:262:LYS:NZ	2.17	0.59
1:E:232:THR:O	1:E:237:HIS:HE1	1.85	0.59
1:A:337:ALA:HB1	1:A:340:VAL:HG11	1.85	0.59
1:D:53:LEU:HD11	1:E:76:ALA:HB2	1.84	0.59
1:D:257:VAL:HB	1:D:258:PRO:HD2	1.85	0.59
1:B:93:PRO:CD	1:B:433:MSE:HE2	2.31	0.59
1:A:244:LEU:HD12	1:A:244:LEU:H	1.67	0.59
1:A:93:PRO:HD2	1:A:433:MSE:HE2	1.83	0.59
1:A:185:LYS:HB3	1:A:262:LYS:HG2	1.85	0.59
1:B:19:LEU:HD13	1:B:125:ALA:HB2	1.85	0.58
1:D:343:PHE:HB2	1:D:344:PRO:HD3	1.85	0.58
1:B:98:GLY:HA2	1:B:343:PHE:HD2	1.68	0.58
1:B:392:TYR:CD1	1:B:393:PRO:HA	2.38	0.58
1:E:97:MSE:HE1	1:E:112:PRO:HD2	1.85	0.58
1:E:190:TYR:O	1:E:268:ARG:NH2	2.37	0.58
1:E:244:LEU:H	1:E:244:LEU:CD1	2.17	0.58
1:D:19:LEU:HD13	1:D:125:ALA:HB2	1.86	0.57
1:D:392:TYR:CD1	1:D:393:PRO:HA	2.39	0.57
1:A:343:PHE:HB2	1:A:344:PRO:HD3	1.85	0.57
1:A:251:ASN:ND2	1:A:253:SER:H	2.02	0.57
1:A:62:THR:O	1:A:62:THR:HG22	2.04	0.56
1:A:258:PRO:HG2	1:A:272:LEU:HB3	1.87	0.56
1:E:88:LEU:C	1:E:88:LEU:HD23	2.30	0.56
1:A:71:ILE:N	1:A:71:ILE:HD12	2.21	0.56
1:A:341:VAL:O	1:A:344:PRO:HD2	2.06	0.56
1:D:244:LEU:HD12	1:D:244:LEU:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:PRO:O	1:D:107:GLN:HB2	2.04	0.56
1:D:272:LEU:HD12	1:D:276:LYS:HG3	1.88	0.56
1:A:257:VAL:HB	1:A:258:PRO:HD2	1.87	0.56
1:D:28:GLU:OE1	1:D:360:ARG:HD3	2.05	0.56
1:E:98:GLY:HA2	1:E:343:PHE:HD2	1.70	0.56
1:E:318:ASN:N	1:E:373:GLN:HE22	2.04	0.56
1:B:47:TRP:O	1:B:118:GLN:HG2	2.05	0.56
1:A:165:ILE:HD13	1:A:165:ILE:H	1.70	0.55
1:A:263:PHE:O	1:A:265:PRO:HD3	2.07	0.55
1:A:92:THR:O	1:A:97:MSE:HE2	2.05	0.55
1:A:96:LEU:HD23	1:A:433:MSE:CE	2.36	0.55
1:A:244:LEU:HD12	1:A:244:LEU:N	2.20	0.55
1:B:91:ASN:C	1:B:91:ASN:HD22	2.13	0.55
1:D:251:ASN:HD22	1:D:253:SER:H	1.53	0.55
1:B:244:LEU:HD12	1:B:244:LEU:N	2.22	0.55
1:E:91:ASN:C	1:E:91:ASN:ND2	2.64	0.55
1:E:114:ARG:NH1	1:E:118:GLN:HE22	1.94	0.55
1:E:19:LEU:HD12	1:E:121:GLN:HE22	1.72	0.55
1:B:185:LYS:HB3	1:B:262:LYS:HG2	1.89	0.54
1:E:392:TYR:CD1	1:E:393:PRO:HA	2.41	0.54
1:B:78:PRO:HD2	1:B:155:THR:CG2	2.37	0.54
1:A:84:LEU:HD22	1:A:88:LEU:HD13	1.89	0.54
1:B:93:PRO:HB2	1:B:95:GLU:OE1	2.07	0.54
1:E:200:HIS:CD2	1:E:202:SER:H	2.25	0.54
1:A:190:TYR:O	1:A:268:ARG:NH2	2.40	0.53
1:D:399:ILE:HD12	1:D:399:ILE:C	2.32	0.53
1:B:97:MSE:HE1	1:B:112:PRO:HD2	1.89	0.53
1:D:62:THR:O	1:D:62:THR:HG22	2.08	0.53
1:B:258:PRO:HG2	1:B:272:LEU:HB3	1.90	0.53
1:A:226:ASP:OD1	1:A:229:ARG:NH2	2.41	0.53
1:E:371:LYS:NZ	1:E:371:LYS:HB3	2.24	0.53
1:D:58:PRO:HG3	1:D:66:LEU:CD2	2.39	0.52
1:D:88:LEU:HD23	1:D:88:LEU:C	2.34	0.52
1:E:301:LYS:O	1:E:303:LYS:HG3	2.09	0.52
1:A:318:ASN:N	1:A:373:GLN:HE22	2.06	0.52
1:B:318:ASN:H	1:B:373:GLN:HE22	1.55	0.52
1:E:226:ASP:OD1	1:E:229:ARG:NH2	2.42	0.52
1:A:399:ILE:C	1:A:399:ILE:HD12	2.34	0.52
1:D:343:PHE:CD1	1:D:343:PHE:N	2.78	0.52
1:A:142:GLU:HB3	1:A:298:SER:HB3	1.92	0.52
1:A:185:LYS:HG2	1:A:262:LYS:HZ3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:GLN:HB3	1:E:105:LYS:HD2	1.90	0.52
1:B:238:PRO:HB3	1:B:252:GLU:O	2.10	0.52
1:B:272:LEU:HD12	1:B:276:LYS:HG3	1.92	0.52
1:D:341:VAL:O	1:D:344:PRO:HD2	2.10	0.52
1:E:241:GLN:HG2	1:E:243:LEU:HD22	1.92	0.52
1:A:217:VAL:O	1:A:241:GLN:HA	2.09	0.51
1:D:244:LEU:H	1:D:244:LEU:CD1	2.23	0.51
1:B:306:GLU:OE1	1:B:306:GLU:N	2.33	0.51
1:E:19:LEU:HD13	1:E:125:ALA:HB2	1.91	0.51
1:B:19:LEU:HD12	1:B:121:GLN:HE22	1.75	0.51
1:A:244:LEU:H	1:A:244:LEU:CD1	2.23	0.51
1:D:78:PRO:HD2	1:D:155:THR:CG2	2.40	0.51
1:A:399:ILE:HD11	1:A:421:TYR:HA	1.93	0.51
1:E:62:THR:HG22	1:E:62:THR:O	2.09	0.51
1:D:200:HIS:HD2	1:D:202:SER:OG	1.94	0.51
1:A:238:PRO:HB3	1:A:252:GLU:O	2.11	0.50
1:E:91:ASN:ND2	1:E:92:THR:HG23	2.25	0.50
1:E:318:ASN:HA	1:E:373:GLN:HE22	1.76	0.50
1:E:78:PRO:HD2	1:E:155:THR:CG2	2.41	0.50
1:B:165:ILE:HG12	6:B:555:HOH:O	2.10	0.50
1:E:343:PHE:HB2	1:E:344:PRO:HD3	1.93	0.50
1:B:165:ILE:H	1:B:165:ILE:CD1	2.24	0.50
1:D:89:GLN:HG2	1:D:113:HIS:HA	1.94	0.50
1:A:106:PRO:O	1:A:107:GLN:HB2	2.11	0.50
1:A:376:LEU:O	1:A:380:LEU:HG	2.12	0.50
1:D:342:PRO:HG2	3:D:500:FAD:N1	2.27	0.50
1:A:90:THR:HA	3:A:500:FAD:O4	2.11	0.50
1:D:78:PRO:HG2	1:D:155:THR:HG23	1.94	0.50
1:E:39:ARG:HD3	1:E:80:TYR:CE1	2.47	0.50
1:E:441:PHE:O	1:E:443:ILE:HG23	2.12	0.50
1:A:53:LEU:HD11	1:B:76:ALA:HB2	1.93	0.50
1:B:301:LYS:O	1:B:303:LYS:HG3	2.12	0.50
1:B:432:ASN:O	1:B:436:ILE:HG13	2.12	0.50
1:D:165:ILE:H	1:D:165:ILE:HD13	1.77	0.49
1:A:200:HIS:CD2	1:A:202:SER:H	2.31	0.49
1:E:11:ILE:HD11	1:E:25:LEU:HD12	1.94	0.49
1:A:111:PHE:CE2	1:A:437:ARG:HA	2.48	0.49
1:B:62:THR:HG22	1:B:62:THR:O	2.10	0.49
1:B:340:VAL:O	1:B:342:PRO:HD3	2.12	0.49
1:D:142:GLU:HB3	1:D:298:SER:HB3	1.94	0.49
1:E:93:PRO:HB2	1:E:95:GLU:OE1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:HIS:CD2	1:B:202:SER:H	2.30	0.49
1:A:239:ILE:O	1:A:254:LEU:HD12	2.12	0.49
1:A:241:GLN:HG2	1:A:243:LEU:HD22	1.95	0.49
1:B:318:ASN:CA	1:B:373:GLN:HE22	2.24	0.49
1:D:257:VAL:HB	1:D:272:LEU:HD13	1.94	0.49
1:A:11:ILE:HD11	1:A:25:LEU:HD12	1.95	0.49
1:B:257:VAL:HB	1:B:258:PRO:HD2	1.95	0.49
1:B:190:TYR:O	1:B:268:ARG:NH2	2.45	0.49
1:D:226:ASP:OD1	1:D:229:ARG:NH2	2.46	0.49
1:B:88:LEU:C	1:B:88:LEU:HD23	2.38	0.48
1:A:53:LEU:HD21	1:A:205:ARG:HG3	1.95	0.48
1:B:318:ASN:N	1:B:373:GLN:HE22	2.11	0.48
1:B:343:PHE:CD1	1:B:343:PHE:N	2.82	0.48
1:D:165:ILE:HD13	6:D:637:HOH:O	2.12	0.48
1:B:244:LEU:HD12	1:B:244:LEU:H	1.76	0.48
1:E:93:PRO:CD	1:E:433:MSE:HE2	2.41	0.48
1:D:39:ARG:HB2	1:D:80:TYR:CE2	2.48	0.48
1:E:6:ILE:HG23	1:E:167:ASP:HB2	1.95	0.48
1:D:11:ILE:HD11	1:D:25:LEU:HD12	1.95	0.48
1:E:165:ILE:H	1:E:165:ILE:CD1	2.27	0.48
1:E:306:GLU:OE1	1:E:306:GLU:N	2.36	0.48
1:B:258:PRO:HG3	1:B:273:LYS:O	2.14	0.48
1:D:249:ILE:HG21	1:D:254:LEU:HD23	1.96	0.48
1:D:251:ASN:ND2	1:D:253:SER:H	2.12	0.47
1:E:343:PHE:CD1	1:E:343:PHE:N	2.82	0.47
1:A:371:LYS:NZ	1:A:371:LYS:HB3	2.29	0.47
1:B:185:LYS:HG2	1:B:262:LYS:NZ	2.29	0.47
1:B:290:TYR:N	1:B:290:TYR:CD1	2.82	0.47
1:D:361:LEU:HD11	1:D:406:CYS:HA	1.96	0.47
1:B:19:LEU:CD1	1:B:125:ALA:HB2	2.44	0.47
1:B:258:PRO:O	1:B:272:LEU:HD22	2.14	0.47
1:B:390:LEU:O	1:B:395:ASP:HB3	2.14	0.47
1:E:58:PRO:HG3	1:E:66:LEU:CD2	2.44	0.47
1:A:257:VAL:HB	1:A:272:LEU:HD13	1.96	0.47
1:D:343:PHE:N	1:D:343:PHE:HD1	2.12	0.47
1:A:248:ASP:C	1:A:250:GLN:HE21	2.22	0.47
1:D:39:ARG:HD3	1:D:80:TYR:CE1	2.50	0.47
1:A:63:ASN:OD1	1:A:65:ILE:HG22	2.15	0.46
1:B:217:VAL:O	1:B:241:GLN:HA	2.15	0.46
1:A:39:ARG:HB2	1:A:80:TYR:CE2	2.50	0.46
1:B:11:ILE:HD11	1:B:25:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:ARG:HG3	1:B:355:ARG:HH11	1.80	0.46
1:B:380:LEU:HD11	1:B:387:TYR:HA	1.96	0.46
1:B:371:LYS:NZ	1:B:371:LYS:HB3	2.30	0.46
1:A:258:PRO:HG3	1:A:273:LYS:O	2.15	0.46
1:D:211:VAL:HG23	1:D:211:VAL:O	2.15	0.46
1:A:114:ARG:HB2	1:A:118:GLN:HE21	1.81	0.46
1:D:19:LEU:CD1	1:D:125:ALA:HB2	2.45	0.46
1:A:144:LYS:O	1:A:145:ASP:HB2	2.15	0.46
1:E:78:PRO:HG2	1:E:155:THR:HG23	1.97	0.46
1:E:263:PHE:O	1:E:265:PRO:HD3	2.15	0.46
1:A:318:ASN:HA	1:A:373:GLN:HE22	1.81	0.46
1:B:89:GLN:HG2	1:B:113:HIS:HA	1.98	0.45
1:B:178:VAL:O	1:B:290:TYR:HB3	2.17	0.45
1:B:244:LEU:H	1:B:244:LEU:CD1	2.29	0.45
1:A:200:HIS:HD2	1:A:202:SER:OG	2.00	0.45
1:A:88:LEU:HD11	3:A:500:FAD:H6	1.99	0.45
1:D:214:SER:HA	6:D:545:HOH:O	2.15	0.45
1:E:90:THR:HA	3:E:500:FAD:O4	2.16	0.45
1:A:301:LYS:O	1:A:303:LYS:HG3	2.17	0.45
1:A:343:PHE:N	1:A:343:PHE:CD1	2.85	0.45
1:E:6:ILE:HD13	1:E:168:ALA:HB2	1.98	0.45
1:A:279:SER:O	1:A:280:ASN:HB2	2.16	0.45
1:B:92:THR:O	1:B:97:MSE:HE2	2.17	0.45
1:E:28:GLU:OE1	1:E:360:ARG:HD3	2.17	0.45
1:E:78:PRO:HD2	1:E:155:THR:HG22	1.99	0.45
1:A:272:LEU:HD12	1:A:276:LYS:HG3	1.98	0.44
1:D:217:VAL:O	1:D:241:GLN:HA	2.17	0.44
1:D:90:THR:HA	3:D:500:FAD:O4	2.17	0.44
1:D:315:HIS:HB2	1:D:388:HIS:CD2	2.52	0.44
1:A:326:ILE:HB	1:A:327:PRO:HD3	2.00	0.44
1:D:53:LEU:HD21	1:D:205:ARG:HG3	1.99	0.44
1:E:425:LYS:HB2	1:E:425:LYS:HE3	1.79	0.44
1:E:371:LYS:HB3	1:E:371:LYS:HZ3	1.82	0.44
1:A:226:ASP:OD1	1:A:437:ARG:NH2	2.51	0.44
1:D:98:GLY:HA2	1:D:343:PHE:HD2	1.81	0.44
1:E:399:ILE:HG13	1:E:400:ASN:N	2.32	0.44
1:D:237:HIS:HD2	1:D:252:GLU:OE2	2.01	0.44
1:E:217:VAL:O	1:E:241:GLN:HA	2.17	0.44
1:A:89:GLN:HG2	1:A:113:HIS:HA	2.00	0.44
1:A:391:ASP:O	1:A:392:TYR:C	2.60	0.44
1:D:237:HIS:CD2	1:D:252:GLU:OE2	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39:ARG:HD3	1:E:80:TYR:CD1	2.52	0.43
1:E:161:ILE:HD12	1:E:161:ILE:N	2.32	0.43
1:B:306:GLU:H	1:B:306:GLU:CD	2.20	0.43
1:D:318:ASN:N	1:D:373:GLN:HE22	2.15	0.43
1:E:318:ASN:H	1:E:373:GLN:NE2	2.13	0.43
1:A:71:ILE:N	1:A:71:ILE:CD1	2.81	0.43
1:A:352:PHE:O	1:A:356:VAL:HG23	2.18	0.43
1:B:28:GLU:OE1	1:B:360:ARG:HD3	2.18	0.43
1:B:257:VAL:HB	1:B:272:LEU:HD13	1.99	0.43
1:A:78:PRO:HG2	1:A:155:THR:HG23	1.99	0.43
1:A:90:THR:HG23	1:A:112:PRO:O	2.18	0.43
1:E:268:ARG:NH1	6:E:537:HOH:O	2.52	0.43
1:A:103:SER:HB2	6:A:559:HOH:O	2.19	0.43
1:D:96:LEU:HD23	1:D:433:MSE:CE	2.49	0.43
1:B:58:PRO:HG3	1:B:66:LEU:CD2	2.49	0.43
1:E:244:LEU:N	1:E:244:LEU:CD1	2.80	0.43
1:D:71:ILE:N	1:D:71:ILE:HD12	2.34	0.42
1:D:200:HIS:CD2	1:D:202:SER:H	2.37	0.42
1:E:399:ILE:C	1:E:399:ILE:HD12	2.43	0.42
1:B:129:LEU:N	1:B:130:PRO:HD2	2.34	0.42
1:D:403:HIS:O	1:D:407:LYS:HG2	2.20	0.42
1:D:113:HIS:CE1	1:D:114:ARG:HG2	2.54	0.42
1:E:318:ASN:CA	1:E:373:GLN:HE22	2.31	0.42
1:A:58:PRO:HG3	1:A:66:LEU:CD2	2.50	0.42
1:B:98:GLY:HA2	1:B:343:PHE:CD2	2.53	0.42
1:E:200:HIS:HD2	1:E:202:SER:H	1.65	0.42
1:D:161:ILE:N	1:D:161:ILE:HD12	2.34	0.42
1:D:264:ASP:O	1:D:268:ARG:N	2.51	0.42
1:A:70:PRO:HB3	1:A:80:TYR:CE1	2.54	0.42
1:A:353:LEU:HD11	1:A:357:TRP:CE2	2.55	0.42
1:D:114:ARG:O	1:D:115:HIS:C	2.62	0.42
1:E:258:PRO:HG2	1:E:272:LEU:HB3	2.01	0.42
1:A:19:LEU:HD13	1:A:125:ALA:HB2	2.02	0.42
1:E:248:ASP:C	1:E:250:GLN:HE21	2.28	0.42
1:D:12:ILE:HD12	1:D:138:VAL:HG21	2.01	0.42
1:B:343:PHE:N	1:B:343:PHE:HD1	2.18	0.41
1:D:371:LYS:NZ	1:D:371:LYS:HB3	2.35	0.41
1:D:392:TYR:HA	1:D:395:ASP:OD1	2.20	0.41
1:A:16:PRO:HG3	1:A:121:GLN:CD	2.44	0.41
1:D:380:LEU:HD11	1:D:387:TYR:HA	2.01	0.41
1:E:53:LEU:HD21	1:E:205:ARG:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:LYS:HE3	1:A:425:LYS:HB2	1.67	0.41
1:B:399:ILE:HD12	1:B:399:ILE:C	2.45	0.41
1:D:58:PRO:HG3	1:D:66:LEU:HD21	2.01	0.41
1:D:114:ARG:HG3	1:D:118:GLN:NE2	2.35	0.41
1:A:96:LEU:HD23	1:A:433:MSE:HE3	2.02	0.41
1:A:129:LEU:N	1:A:130:PRO:HD2	2.35	0.41
1:A:218:VAL:O	1:A:218:VAL:HG22	2.19	0.41
1:E:114:ARG:O	1:E:118:GLN:HG3	2.19	0.41
1:E:257:VAL:HB	1:E:272:LEU:HD13	2.02	0.41
1:A:88:LEU:C	1:A:88:LEU:HD23	2.45	0.41
1:A:91:ASN:C	1:A:91:ASN:ND2	2.74	0.41
1:A:178:VAL:HA	1:A:179:PRO:HD3	1.95	0.41
1:D:140:ASP:C	1:D:141:ILE:HG13	2.46	0.41
1:B:62:THR:O	1:B:62:THR:CG2	2.68	0.41
1:D:257:VAL:CG2	1:D:272:LEU:HD13	2.50	0.41
1:E:258:PRO:HG3	1:E:273:LYS:O	2.20	0.41
1:E:345:THR:O	1:E:349:GLN:HG3	2.21	0.41
1:D:353:LEU:HD11	1:D:357:TRP:CE2	2.55	0.41
1:A:161:ILE:N	1:A:161:ILE:HD12	2.36	0.41
1:A:438:ALA:HA	1:A:443:ILE:HG12	2.02	0.41
1:B:90:THR:HA	3:B:500:FAD:O4	2.20	0.41
1:D:129:LEU:N	1:D:130:PRO:HD2	2.36	0.41
1:E:252:GLU:C	1:E:252:GLU:CD	2.89	0.41
1:E:399:ILE:HD11	1:E:421:TYR:HA	2.02	0.41
1:B:232:THR:HA	1:B:239:ILE:HD11	2.02	0.41
1:D:227:LEU:HD21	1:D:285:ILE:HG21	2.02	0.41
1:D:248:ASP:C	1:D:250:GLN:HE21	2.29	0.41
1:E:129:LEU:N	1:E:130:PRO:HD2	2.36	0.40
1:A:62:THR:O	1:A:62:THR:CG2	2.68	0.40
1:A:211:VAL:O	1:A:211:VAL:HG23	2.20	0.40
1:D:70:PRO:HB3	1:D:80:TYR:CE1	2.56	0.40
1:D:211:VAL:HA	1:D:234:VAL:O	2.22	0.40
1:E:200:HIS:HD2	1:E:202:SER:OG	2.03	0.40
1:D:301:LYS:O	1:D:303:LYS:HG3	2.21	0.40
1:B:251:ASN:O	1:B:255:GLN:NE2	2.43	0.40
1:D:78:PRO:CG	1:D:155:THR:HG23	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	440/447 (98%)	417 (95%)	22 (5%)	1 (0%)	43	50
1	B	440/447 (98%)	419 (95%)	18 (4%)	3 (1%)	18	18
1	D	440/447 (98%)	419 (95%)	19 (4%)	2 (0%)	24	26
1	E	440/447 (98%)	421 (96%)	15 (3%)	4 (1%)	14	13
All	All	1760/1788 (98%)	1676 (95%)	74 (4%)	10 (1%)	21	22

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	LYS
1	B	156	LYS
1	D	156	LYS
1	E	156	LYS
1	E	195	PRO
1	D	342	PRO
1	E	342	PRO
1	B	195	PRO
1	B	297	PRO
1	E	297	PRO

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	384/385 (100%)	372 (97%)	12 (3%)	35	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	384/385 (100%)	371 (97%)	13 (3%)	32	42
1	D	384/385 (100%)	372 (97%)	12 (3%)	35	46
1	E	384/385 (100%)	371 (97%)	13 (3%)	32	42
All	All	1536/1540 (100%)	1486 (97%)	50 (3%)	33	44

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	96	LEU
1	A	143	LYS
1	A	150	VAL
1	A	155	THR
1	A	165	ILE
1	A	195	PRO
1	A	218	VAL
1	A	238	PRO
1	A	250	GLN
1	A	371	LYS
1	A	399	ILE
1	B	91	ASN
1	B	96	LEU
1	B	143	LYS
1	B	150	VAL
1	B	155	THR
1	B	165	ILE
1	B	195	PRO
1	B	218	VAL
1	B	268	ARG
1	B	290	TYR
1	B	311	ASP
1	B	371	LYS
1	B	399	ILE
1	D	91	ASN
1	D	96	LEU
1	D	143	LYS
1	D	150	VAL
1	D	155	THR
1	D	165	ILE
1	D	195	PRO
1	D	218	VAL

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Mol	Chain	Res	Type
1	D	250	GLN
1	D	311	ASP
1	D	371	LYS
1	D	399	ILE
1	E	91	ASN
1	E	96	LEU
1	E	143	LYS
1	E	150	VAL
1	E	155	THR
1	E	165	ILE
1	E	195	PRO
1	E	218	VAL
1	E	250	GLN
1	E	268	ARG
1	E	311	ASP
1	E	371	LYS
1	E	399	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	89	GLN
1	A	91	ASN
1	A	118	GLN
1	A	121	GLN
1	A	200	HIS
1	A	237	HIS
1	A	250	GLN
1	A	251	ASN
1	A	373	GLN
1	B	33	GLN
1	B	48	ASN
1	B	55	ASN
1	B	91	ASN
1	B	118	GLN
1	B	121	GLN
1	B	200	HIS
1	B	237	HIS
1	B	250	GLN
1	B	251	ASN
1	B	373	GLN

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Mol	Chain	Res	Type
1	D	48	ASN
1	D	91	ASN
1	D	118	GLN
1	D	121	GLN
1	D	200	HIS
1	D	237	HIS
1	D	251	ASN
1	D	369	GLN
1	D	373	GLN
1	D	384	ASN
1	E	48	ASN
1	E	91	ASN
1	E	118	GLN
1	E	121	GLN
1	E	200	HIS
1	E	237	HIS
1	E	250	GLN
1	E	251	ASN
1	E	369	GLN
1	E	373	GLN
1	E	403	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PEO	B	503	-	1,1,1	0.38	0	-		
5	GOL	A	502	-	5,5,5	0.28	0	5,5,5	0.61	0
5	GOL	B	502	-	5,5,5	0.38	0	5,5,5	0.73	0
2	PEO	A	503	-	1,1,1	0.52	0	-		
4	MMZ	B	501	-	7,7,7	2.31	2 (28%)	9,9,9	7.02	5 (55%)
3	FAD	A	500	-	58,58,58	2.20	13 (22%)	85,89,89	1.66	14 (16%)
2	PEO	E	503	-	1,1,1	0.48	0	-		
2	PEO	D	503	-	1,1,1	0.35	0	-		
3	FAD	E	500	-	58,58,58	2.15	14 (24%)	85,89,89	1.67	14 (16%)
4	MMZ	A	501	-	7,7,7	1.79	3 (42%)	9,9,9	8.97	6 (66%)
4	MMZ	D	501	-	7,7,7	2.26	2 (28%)	9,9,9	8.51	6 (66%)
4	MMZ	E	501	-	7,7,7	1.96	3 (42%)	9,9,9	8.15	6 (66%)
5	GOL	D	502	-	5,5,5	0.36	0	5,5,5	0.66	0
5	GOL	E	502	-	5,5,5	0.23	0	5,5,5	0.64	0
3	FAD	B	500	-	58,58,58	2.28	16 (27%)	85,89,89	1.67	13 (15%)
3	FAD	D	500	-	58,58,58	2.25	16 (27%)	85,89,89	1.68	14 (16%)

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
5	GOL	A	502	-	-	0/4/4/4	-
5	GOL	B	502	-	-	0/4/4/4	-
4	MMZ	B	501	-	-	-	0/1/1/1
3	FAD	A	500	-	-	12/34/50/50	0/6/6/6
3	FAD	E	500	-	-	11/34/50/50	0/6/6/6
5	GOL	D	502	-	-	0/4/4/4	-
5	GOL	E	502	-	-	0/4/4/4	-
4	MMZ	A	501	-	-	-	0/1/1/1
4	MMZ	D	501	-	-	-	0/1/1/1
4	MMZ	E	501	-	-	-	0/1/1/1
3	FAD	B	500	-	-	11/34/50/50	0/6/6/6
3	FAD	D	500	-	-	11/34/50/50	0/6/6/6

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	500	FAD	C4X-N5	6.26	1.44	1.30
3	A	500	FAD	C4X-N5	6.18	1.44	1.30
3	B	500	FAD	C4X-N5	6.14	1.44	1.30
3	E	500	FAD	C4X-N5	6.02	1.43	1.30
3	D	500	FAD	C4A-N3A	5.72	1.45	1.34
3	B	500	FAD	C4A-N3A	5.68	1.45	1.34
3	D	500	FAD	P-O5'	5.66	1.81	1.59
3	A	500	FAD	C4A-N3A	5.42	1.44	1.34
3	A	500	FAD	P-O5'	5.34	1.80	1.59
3	B	500	FAD	C9A-N10	5.33	1.50	1.41
3	E	500	FAD	P-O5'	5.29	1.80	1.59
3	B	500	FAD	P-O5'	5.25	1.80	1.59
3	E	500	FAD	C4A-N3A	5.18	1.44	1.34
3	E	500	FAD	C9A-N10	5.03	1.49	1.41
3	D	500	FAD	C9A-N10	5.00	1.49	1.41
3	D	500	FAD	C9A-C5X	4.67	1.48	1.41
3	A	500	FAD	C9A-N10	4.55	1.49	1.41
3	E	500	FAD	C9A-C5X	4.50	1.48	1.41
3	B	500	FAD	C2A-N3A	4.48	1.41	1.33
3	D	500	FAD	C2A-N3A	4.37	1.41	1.33
3	B	500	FAD	C9A-C5X	4.33	1.48	1.41
3	A	500	FAD	C9A-C5X	4.26	1.48	1.41
3	E	500	FAD	C2A-N3A	4.17	1.41	1.33
3	A	500	FAD	C2A-N3A	4.16	1.41	1.33
3	B	500	FAD	C5A-C4A	-4.15	1.31	1.39
3	A	500	FAD	C5A-C4A	-4.11	1.31	1.39
3	E	500	FAD	C5A-C4A	-3.94	1.32	1.39
4	B	501	MMZ	C3A-N3	3.89	1.45	1.37
4	D	501	MMZ	C2-S2	3.75	1.74	1.67
4	B	501	MMZ	C2-S2	3.75	1.74	1.67
3	D	500	FAD	C5A-C4A	-3.74	1.32	1.39
3	A	500	FAD	C1'-C2'	-3.72	1.47	1.52
3	D	500	FAD	C1'-C2'	-3.71	1.47	1.52
3	A	500	FAD	C5'-C4'	-3.61	1.46	1.51
3	B	500	FAD	C1'-C2'	-3.59	1.47	1.52
4	E	501	MMZ	C3A-N3	3.58	1.44	1.37
3	E	500	FAD	C1'-C2'	-3.35	1.48	1.52
3	B	500	FAD	C5'-C4'	-3.31	1.47	1.51
3	D	500	FAD	C5'-C4'	-3.28	1.47	1.51
4	D	501	MMZ	C3A-N3	3.11	1.43	1.37
4	A	501	MMZ	C3A-N3	3.08	1.43	1.37
3	B	500	FAD	PA-O3P	-3.02	1.56	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	500	FAD	C8A-N9A	2.91	1.42	1.37
3	D	500	FAD	C8A-N9A	2.86	1.42	1.37
3	D	500	FAD	C10-N1	2.75	1.38	1.33
3	E	500	FAD	C6-C7	2.66	1.43	1.39
3	E	500	FAD	C5'-C4'	-2.61	1.48	1.51
3	D	500	FAD	C6-C7	2.60	1.43	1.39
3	A	500	FAD	C2B-C3B	-2.59	1.46	1.53
3	B	500	FAD	C2B-C3B	-2.58	1.46	1.53
3	E	500	FAD	C8A-N9A	2.58	1.41	1.37
3	B	500	FAD	C10-N1	2.55	1.38	1.33
3	E	500	FAD	C2B-C3B	-2.50	1.46	1.53
3	E	500	FAD	C10-N1	2.43	1.38	1.33
3	A	500	FAD	C8A-N9A	2.41	1.41	1.37
3	A	500	FAD	C10-N1	2.37	1.38	1.33
3	A	500	FAD	C6-C7	2.36	1.42	1.39
3	B	500	FAD	C9-C9A	2.34	1.43	1.39
3	B	500	FAD	C6-C7	2.33	1.42	1.39
3	D	500	FAD	C2B-C3B	-2.32	1.47	1.53
4	A	501	MMZ	C1A-C3A	2.30	1.41	1.34
3	B	500	FAD	C2'-C3'	-2.26	1.49	1.53
3	D	500	FAD	C4A-N9A	2.24	1.42	1.37
4	A	501	MMZ	C2-S2	2.19	1.71	1.67
4	E	501	MMZ	C1A-C3A	2.17	1.41	1.34
4	E	501	MMZ	C2-S2	2.17	1.71	1.67
3	E	500	FAD	PA-O3P	-2.16	1.57	1.59
3	D	500	FAD	C4-N3	2.07	1.42	1.38
3	D	500	FAD	C2'-C3'	-2.03	1.49	1.53

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	501	MMZ	C4-N3-C2	21.00	133.04	124.81
4	A	501	MMZ	C4-N3-C2	19.79	132.57	124.81
4	E	501	MMZ	C4-N3-C2	16.57	131.31	124.81
4	A	501	MMZ	N1-C2-N3	16.07	109.82	105.43
4	E	501	MMZ	N1-C2-N3	16.07	109.82	105.43
4	B	501	MMZ	C4-N3-C2	15.99	131.08	124.81
4	B	501	MMZ	N1-C2-N3	12.18	108.76	105.43
4	D	501	MMZ	N1-C2-N3	11.68	108.62	105.43
4	D	501	MMZ	C1A-N1-C2	-5.91	108.27	110.78
4	E	501	MMZ	C1A-N1-C2	-5.87	108.28	110.78
3	D	500	FAD	C4A-N9A-C8A	-5.63	99.83	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	MMZ	C1A-N1-C2	-5.57	108.41	110.78
3	E	500	FAD	C4A-N9A-C8A	-5.40	100.06	105.74
3	A	500	FAD	C4A-N9A-C8A	-5.39	100.08	105.74
3	B	500	FAD	C4A-N9A-C8A	-5.31	100.17	105.74
3	B	500	FAD	C5A-C4A-N9A	5.14	111.41	105.81
3	D	500	FAD	C5A-C4A-N9A	5.10	111.37	105.81
3	A	500	FAD	C5A-C4A-N9A	5.09	111.36	105.81
3	E	500	FAD	C5A-C4A-N9A	5.08	111.35	105.81
3	E	500	FAD	N3A-C4A-N9A	-4.60	119.35	127.17
3	B	500	FAD	N3A-C4A-N9A	-4.56	119.42	127.17
3	A	500	FAD	N3A-C4A-N9A	-4.46	119.58	127.17
3	D	500	FAD	N3A-C4A-N9A	-4.43	119.63	127.17
4	A	501	MMZ	C3A-N3-C2	-4.33	108.35	109.60
4	B	501	MMZ	C1A-N1-C2	-4.26	108.97	110.78
3	D	500	FAD	P-O5'-C5'	4.22	145.50	121.35
4	D	501	MMZ	C4-N3-C3A	-4.14	118.22	125.11
3	B	500	FAD	C5X-C9A-N10	-4.07	114.29	117.97
3	E	500	FAD	P-O5'-C5'	3.95	143.97	121.35
3	A	500	FAD	P-O5'-C5'	3.93	143.90	121.35
3	E	500	FAD	C5X-C9A-N10	-3.83	114.51	117.97
3	A	500	FAD	C5X-C9A-N10	-3.79	114.54	117.97
3	B	500	FAD	P-O5'-C5'	3.79	143.07	121.35
3	D	500	FAD	C5X-C9A-N10	-3.65	114.67	117.97
4	A	501	MMZ	C4-N3-C3A	-3.63	119.07	125.11
3	E	500	FAD	C2'-C1'-N10	3.34	125.99	110.20
3	D	500	FAD	O3'-C3'-C4'	-3.34	101.34	108.93
4	B	501	MMZ	C4-N3-C3A	-3.25	119.70	125.11
3	B	500	FAD	C9-C9A-N10	3.25	126.22	121.85
4	E	501	MMZ	C3A-N3-C2	-3.23	108.67	109.60
3	E	500	FAD	O3'-C3'-C4'	-3.20	101.65	108.93
4	D	501	MMZ	C3A-N3-C2	-3.20	108.68	109.60
3	A	500	FAD	O3'-C3'-C4'	-3.19	101.68	108.93
3	B	500	FAD	O3'-C3'-C4'	-3.19	101.68	108.93
3	D	500	FAD	C2'-C1'-N10	3.16	125.12	110.20
4	A	501	MMZ	S2-C2-N1	-3.12	123.12	127.26
3	B	500	FAD	C2'-C1'-N10	3.11	124.92	110.20
3	E	500	FAD	O5'-P-O1P	3.09	121.19	108.94
4	E	501	MMZ	C4-N3-C3A	-3.06	120.01	125.11
3	A	500	FAD	O5'-P-O1P	3.04	120.98	108.94
3	B	500	FAD	C4'-C3'-C2'	3.03	118.62	113.57
3	B	500	FAD	O5'-P-O1P	3.03	120.95	108.94
3	D	500	FAD	O5'-P-O1P	2.99	120.79	108.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	500	FAD	C4'-C3'-C2'	2.97	118.51	113.57
3	B	500	FAD	O2B-C2B-C3B	2.88	121.06	111.82
3	E	500	FAD	C9-C9A-N10	2.88	125.72	121.85
3	A	500	FAD	C2'-C1'-N10	2.86	123.70	110.20
3	D	500	FAD	C9-C9A-N10	2.84	125.67	121.85
4	D	501	MMZ	S2-C2-N1	-2.83	123.50	127.26
3	A	500	FAD	C9-C9A-N10	2.82	125.64	121.85
3	E	500	FAD	O2B-C2B-C3B	2.73	120.58	111.82
3	D	500	FAD	C4'-C3'-C2'	2.71	118.08	113.57
3	B	500	FAD	N3A-C2A-N1A	-2.68	124.53	128.58
3	A	500	FAD	O2B-C2B-C3B	2.58	120.08	111.82
3	D	500	FAD	N3A-C2A-N1A	-2.56	124.70	128.58
3	A	500	FAD	N3A-C2A-N1A	-2.55	124.72	128.58
4	E	501	MMZ	S2-C2-N1	-2.55	123.87	127.26
3	A	500	FAD	C4'-C3'-C2'	2.49	117.71	113.57
3	E	500	FAD	N3A-C2A-N1A	-2.40	124.95	128.58
3	D	500	FAD	O2B-C2B-C3B	2.38	119.46	111.82
3	A	500	FAD	C4X-C10-N10	2.24	119.69	116.48
4	B	501	MMZ	S2-C2-N1	-2.23	124.29	127.26
3	D	500	FAD	C4X-C10-N10	2.20	119.64	116.48
3	D	500	FAD	C8M-C8-C9	-2.19	115.72	119.57
3	E	500	FAD	C4X-C10-N10	2.17	119.59	116.48
3	A	500	FAD	C8M-C8-C9	-2.10	115.88	119.57
3	B	500	FAD	C4X-C10-N10	2.05	119.42	116.48
3	E	500	FAD	C8M-C8-C9	-2.01	116.02	119.57

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	500	FAD	N10-C1'-C2'-O2'
3	A	500	FAD	N10-C1'-C2'-C3'
3	A	500	FAD	O4'-C4'-C5'-O5'
3	A	500	FAD	C5'-O5'-P-O1P
3	A	500	FAD	C5'-O5'-P-O2P
3	A	500	FAD	C5'-O5'-P-O3P
3	B	500	FAD	N10-C1'-C2'-O2'
3	B	500	FAD	N10-C1'-C2'-C3'
3	B	500	FAD	C5'-O5'-P-O2P
3	B	500	FAD	C5'-O5'-P-O3P
3	D	500	FAD	N10-C1'-C2'-O2'
3	D	500	FAD	N10-C1'-C2'-C3'

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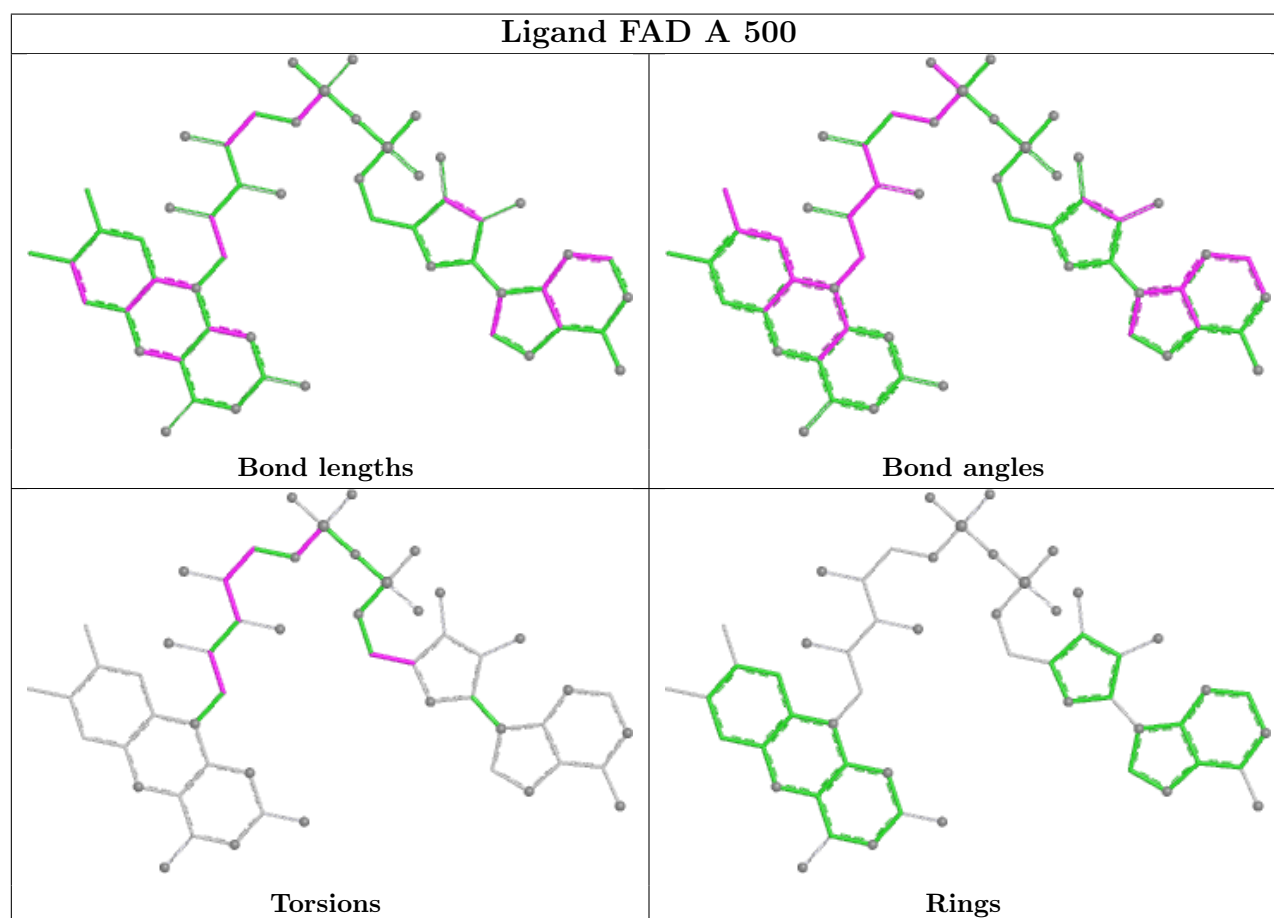
Mol	Chain	Res	Type	Atoms
3	D	500	FAD	O4'-C4'-C5'-O5'
3	D	500	FAD	C5'-O5'-P-O1P
3	D	500	FAD	C5'-O5'-P-O2P
3	D	500	FAD	C5'-O5'-P-O3P
3	E	500	FAD	N10-C1'-C2'-O2'
3	E	500	FAD	N10-C1'-C2'-C3'
3	E	500	FAD	O4'-C4'-C5'-O5'
3	E	500	FAD	C5'-O5'-P-O1P
3	E	500	FAD	C5'-O5'-P-O2P
3	E	500	FAD	C5'-O5'-P-O3P
3	D	500	FAD	O3'-C3'-C4'-O4'
3	D	500	FAD	C2'-C3'-C4'-O4'
3	A	500	FAD	O3'-C3'-C4'-C5'
3	D	500	FAD	O3'-C3'-C4'-C5'
3	A	500	FAD	C2'-C3'-C4'-C5'
3	D	500	FAD	C2'-C3'-C4'-C5'
3	A	500	FAD	C2'-C3'-C4'-O4'
3	A	500	FAD	O3'-C3'-C4'-O4'
3	E	500	FAD	O3'-C3'-C4'-C5'
3	A	500	FAD	C3'-C4'-C5'-O5'
3	D	500	FAD	C3'-C4'-C5'-O5'
3	B	500	FAD	O3'-C3'-C4'-C5'
3	E	500	FAD	O3'-C3'-C4'-O4'
3	E	500	FAD	C2'-C3'-C4'-C5'
3	B	500	FAD	O3'-C3'-C4'-O4'
3	B	500	FAD	O4'-C4'-C5'-O5'
3	B	500	FAD	C2'-C3'-C4'-C5'
3	E	500	FAD	C2'-C3'-C4'-O4'
3	B	500	FAD	C5'-O5'-P-O1P
3	B	500	FAD	C2'-C3'-C4'-O4'
3	E	500	FAD	C3'-C4'-C5'-O5'
3	A	500	FAD	O4B-C4B-C5B-O5B
3	B	500	FAD	O4B-C4B-C5B-O5B

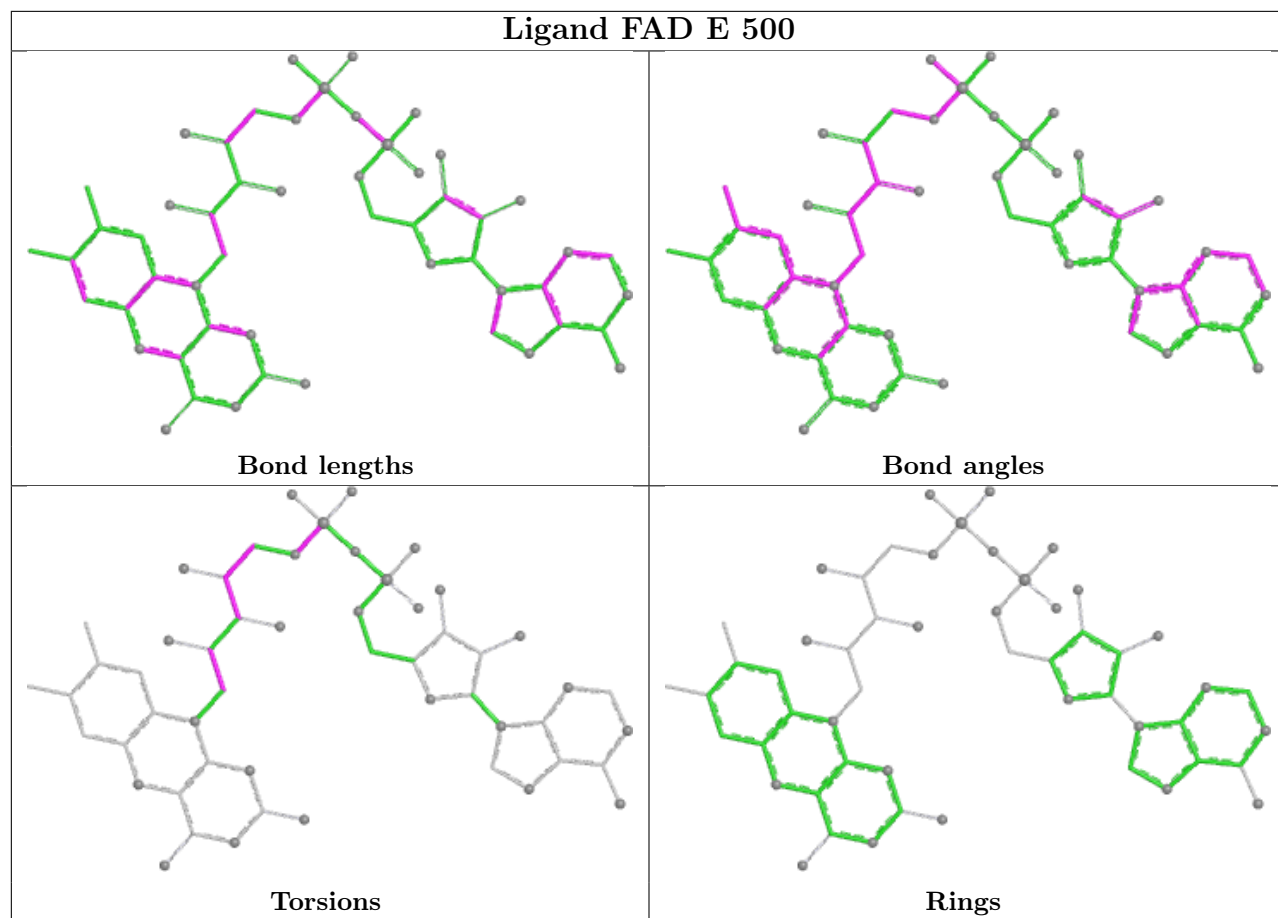
There are no ring outliers.

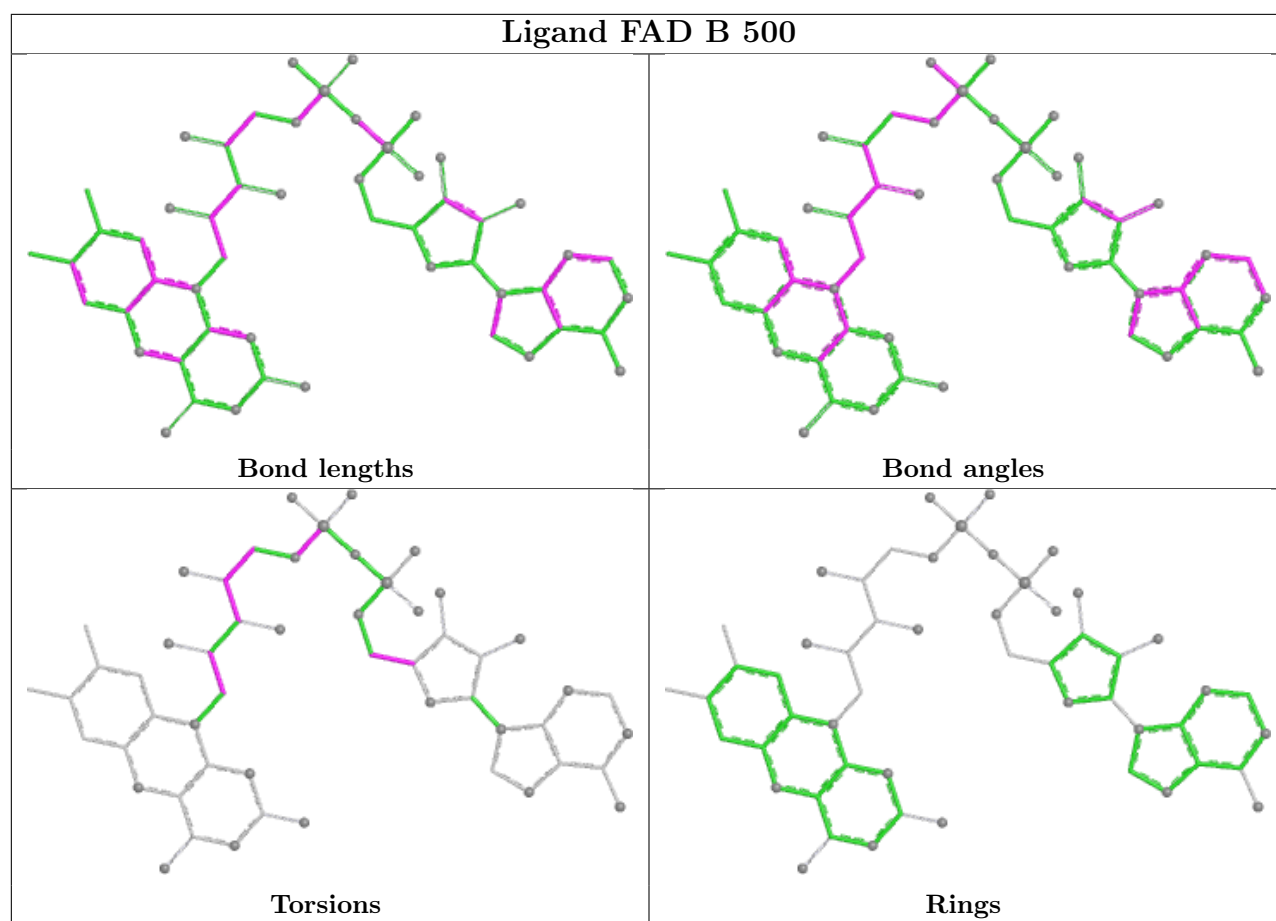
4 monomers are involved in 6 short contacts:

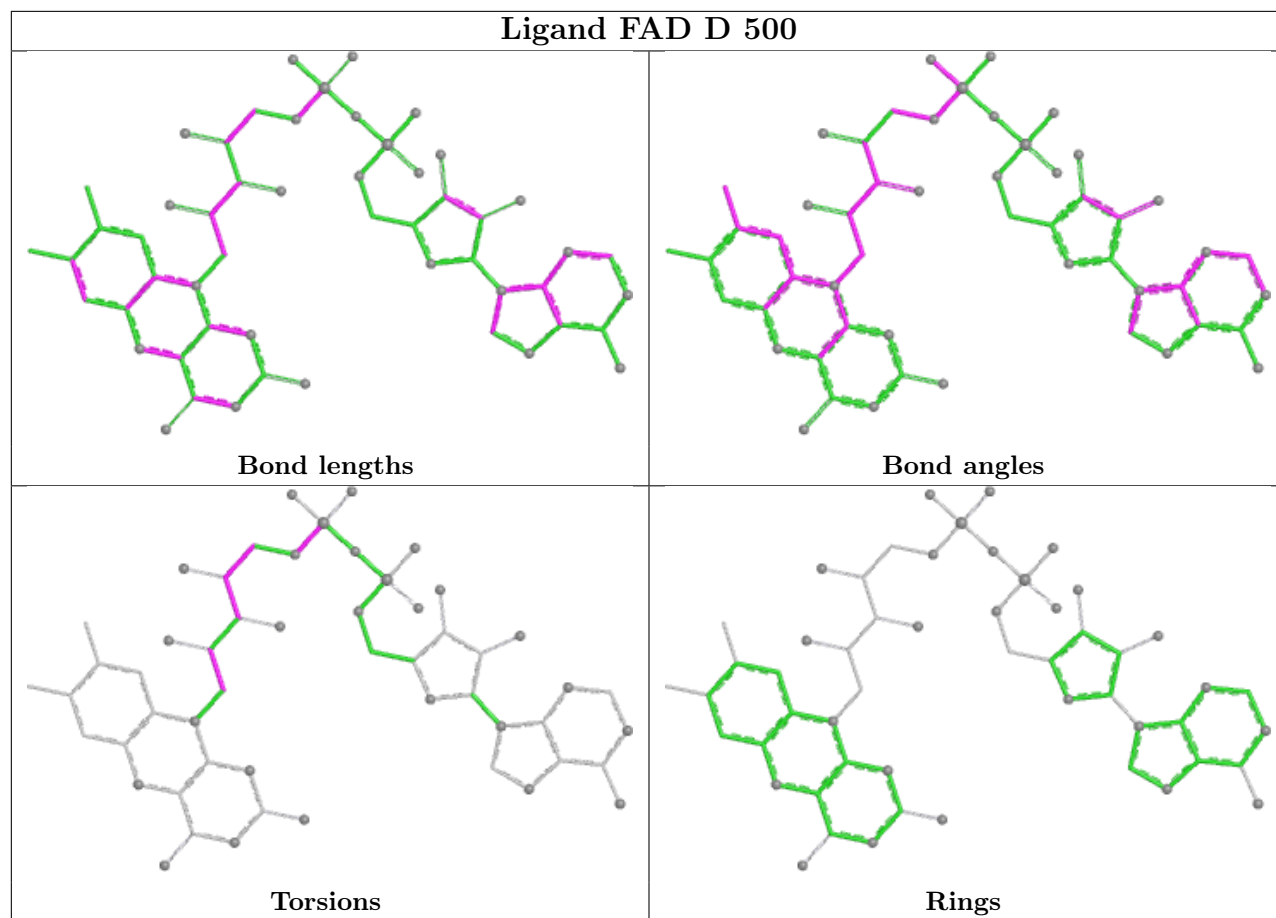
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	FAD	2	0
3	E	500	FAD	1	0
3	B	500	FAD	1	0
3	D	500	FAD	2	0

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	438/447 (97%)	0.34	28 (6%) 25 22	9, 26, 41, 50	0
1	B	438/447 (97%)	0.33	15 (3%) 48 45	11, 27, 41, 50	0
1	D	438/447 (97%)	0.27	19 (4%) 40 37	11, 26, 40, 50	0
1	E	438/447 (97%)	0.26	14 (3%) 50 47	10, 26, 40, 50	0
All	All	1752/1788 (97%)	0.30	76 (4%) 40 37	9, 26, 41, 50	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	444	GLU	6.1
1	A	3	LEU	5.9
1	B	3	LEU	5.7
1	D	3	LEU	5.5
1	E	3	LEU	5.3
1	E	4	PRO	5.1
1	D	244	LEU	5.0
1	B	4	PRO	4.8
1	D	4	PRO	4.7
1	A	4	PRO	4.7
1	B	266	THR	4.7
1	A	444	GLU	4.6
1	E	244	LEU	4.0
1	B	444	GLU	4.0
1	D	266	THR	3.9
1	B	244	LEU	3.9
1	A	244	LEU	3.8
1	E	311	ASP	3.7
1	D	444	GLU	3.7
1	D	271	TYR	3.5
1	B	162	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	98	GLY	3.3
1	A	272	LEU	3.3
1	A	155	THR	3.3
1	B	262	LYS	3.3
1	D	262	LYS	3.3
1	D	145	ASP	3.2
1	A	311	ASP	3.1
1	B	98	GLY	3.1
1	E	98	GLY	3.0
1	D	155	THR	2.9
1	A	277	VAL	2.9
1	A	271	TYR	2.9
1	A	98	GLY	2.8
1	E	5	THR	2.8
1	B	443	ILE	2.7
1	A	262	LYS	2.7
1	E	262	LYS	2.7
1	E	145	ASP	2.6
1	A	443	ILE	2.6
1	A	279	SER	2.6
1	D	311	ASP	2.5
1	B	145	ASP	2.5
1	A	266	THR	2.5
1	A	145	ASP	2.5
1	A	425	LYS	2.4
1	A	185	LYS	2.3
1	D	158	GLY	2.3
1	A	270	ILE	2.3
1	A	275	GLY	2.3
1	A	267	THR	2.3
1	E	162	SER	2.3
1	D	247	GLY	2.3
1	D	279	SER	2.3
1	D	368	GLU	2.3
1	A	247	GLY	2.2
1	D	245	GLY	2.2
1	B	195	PRO	2.2
1	A	107	GLN	2.2
1	E	107	GLN	2.2
1	B	158	GLY	2.2
1	D	56	LYS	2.2
1	E	155	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	240	TYR	2.1
1	A	258	PRO	2.1
1	D	259	GLU	2.1
1	B	65	ILE	2.1
1	B	276	LYS	2.1
1	A	280	ASN	2.1
1	E	165	ILE	2.1
1	A	158	GLY	2.1
1	A	245	GLY	2.1
1	E	266	THR	2.0
1	D	263	PHE	2.0
1	B	368	GLU	2.0
1	A	264	ASP	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	MMZ	E	501	7/7	0.71	0.23	48,50,51,52	0
4	MMZ	A	501	7/7	0.72	0.23	48,50,51,52	0
2	PEO	E	503	2/2	0.77	0.19	43,43,43,43	0
2	PEO	D	503	2/2	0.78	0.20	43,43,43,44	0
4	MMZ	B	501	7/7	0.79	0.20	49,50,52,53	0
4	MMZ	D	501	7/7	0.80	0.20	48,50,52,52	0
2	PEO	A	503	2/2	0.81	0.20	45,45,45,46	0
2	PEO	B	503	2/2	0.87	0.14	41,41,41,43	0
5	GOL	B	502	6/6	0.93	0.08	15,16,17,18	0
5	GOL	A	502	6/6	0.95	0.07	18,18,19,20	0

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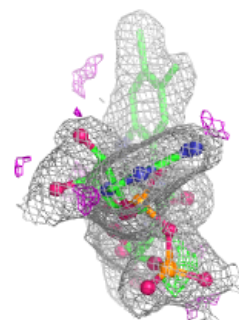
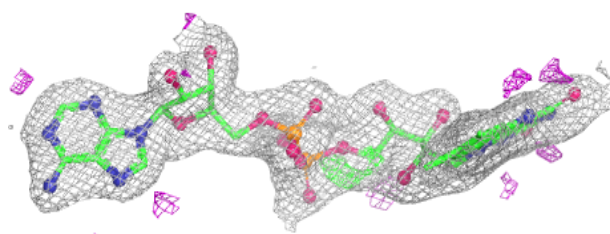
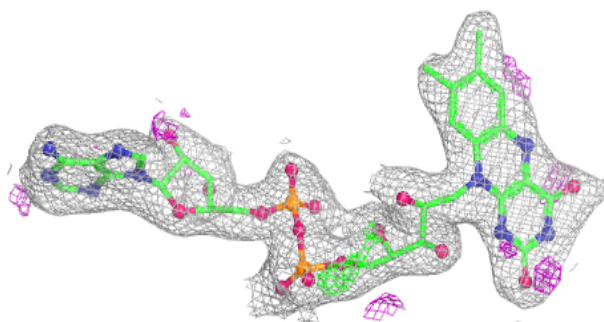
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	E	502	6/6	0.95	0.07	15,16,17,20	0
3	FAD	E	500	53/53	0.96	0.07	10,18,22,23	0
3	FAD	A	500	53/53	0.96	0.07	12,19,21,22	0
3	FAD	B	500	53/53	0.96	0.08	11,19,23,24	0
5	GOL	D	502	6/6	0.96	0.06	15,15,17,18	0
3	FAD	D	500	53/53	0.96	0.07	11,18,22,22	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.

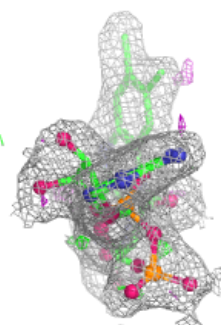
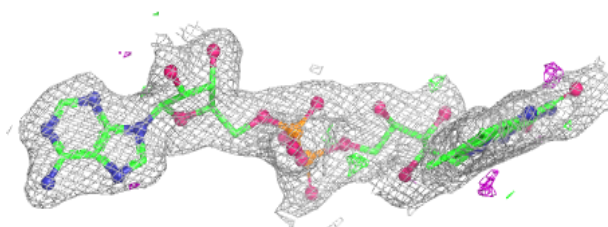
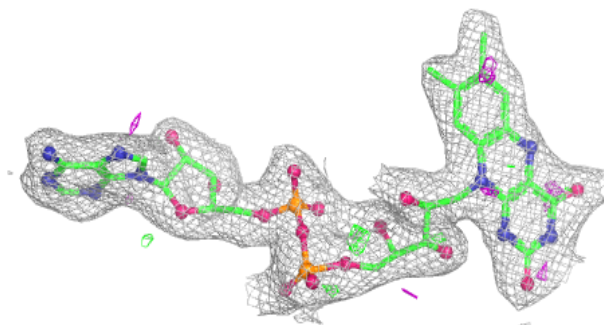
Electron density around FAD E 500:

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

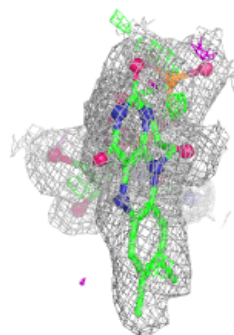
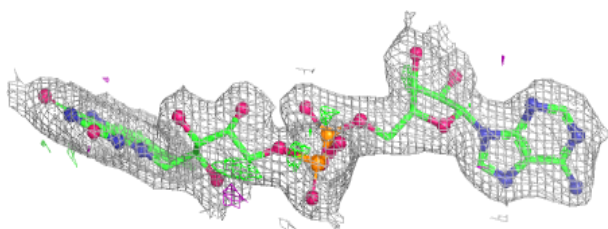
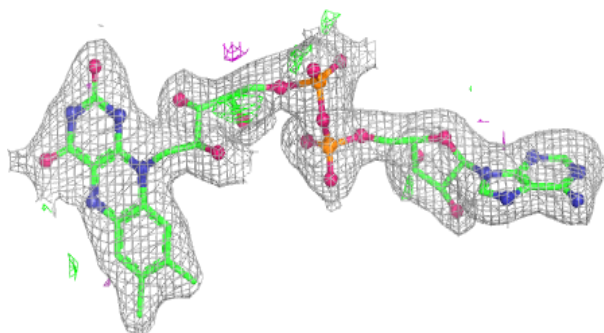


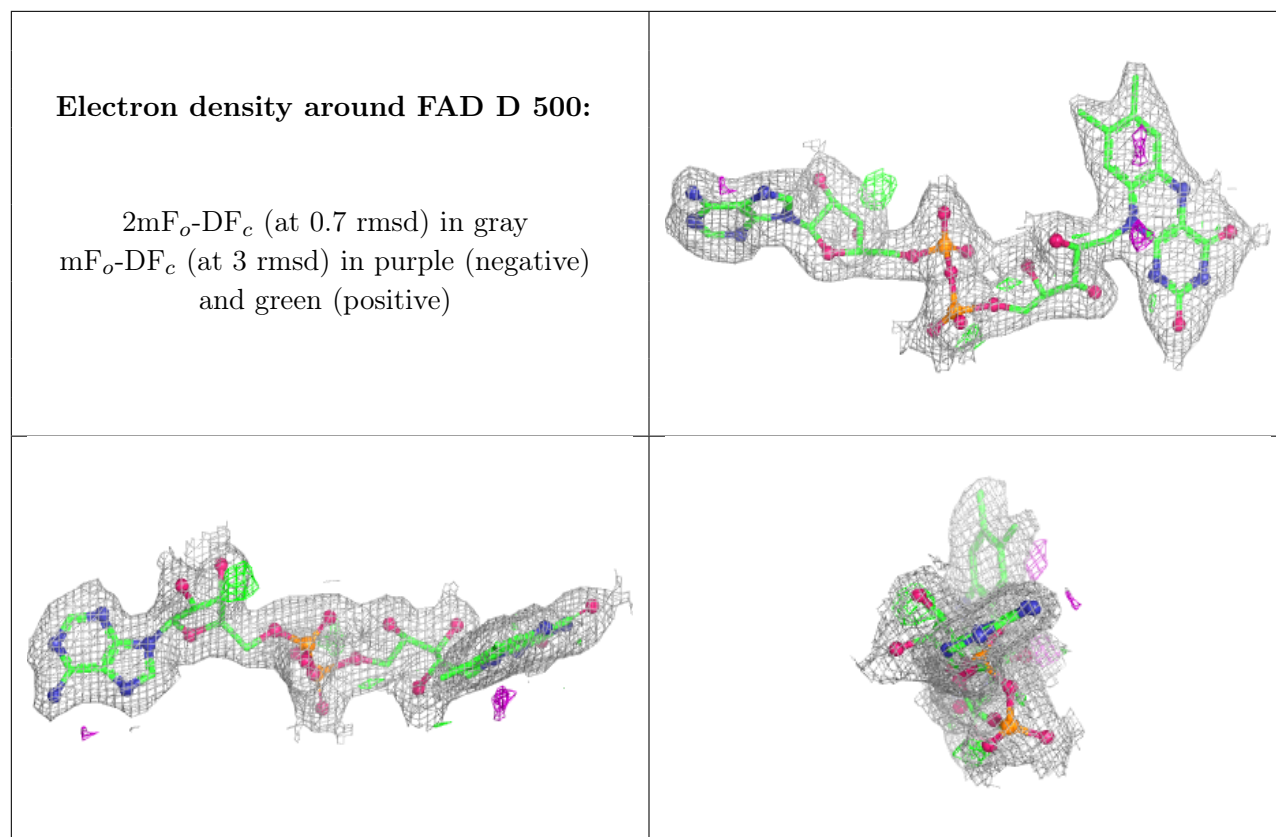
Electron density around FAD A 500:

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

**Electron density around FAD B 500:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.