



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:17 PM UTC

PDB ID : 2VVL / pdb_00002vvl
Title : The structure of MAO-N-D3, a variant of monoamine oxidase from *Aspergillus niger*.
Authors : Atkin, K.E.; Hart, S.; Turkenburg, J.P.; Brzozowski, A.M.; Grogan, G.J.
Deposited on : 2008-06-10
Resolution : 2.45 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

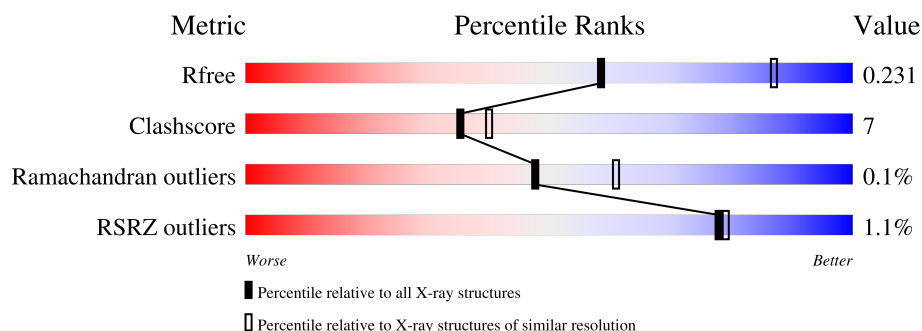
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	495	
1	B	495	
1	C	495	
1	D	495	
1	E	495	
1	F	495	

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Mol	Chain	Length	Quality of chain
1	H	495	% 78%17% . .
2	G	495	2% 79%16% . .

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
3	FAD	A	600	X	-	-	-
3	FAD	B	600	X	-	-	-
3	FAD	C	600	X	-	-	-
3	FAD	D	600	X	-	-	-
3	FAD	E	600	X	-	-	-
3	FAD	F	600	X	-	-	-
3	FAD	G	600	X	-	-	-
3	FAD	H	600	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 31496 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 MONOAMINE OXIDASE N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	478	Total	C	N	O	S	29	1	0
			3782	2390	669	700	23			
1	B	476	Total	C	N	O	S	40	1	0
			3770	2382	667	698	23			
1	C	477	Total	C	N	O	S	43	1	0
			3778	2387	668	701	22			
1	D	478	Total	C	N	O	S	55	0	0
			3778	2387	666	702	23			
1	E	477	Total	C	N	O	S	50	1	0
			3777	2387	668	699	23			
1	F	478	Total	C	N	O	S	53	1	0
			3782	2389	669	702	22			
1	H	478	Total	C	N	O	S	60	1	0
			3785	2393	669	700	23			

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	246	MET	ILE	engineered mutation	UNP P46882
A	336	SER	ASN	engineered mutation	UNP P46882
B	246	MET	ILE	engineered mutation	UNP P46882
B	336	SER	ASN	engineered mutation	UNP P46882
C	246	MET	ILE	engineered mutation	UNP P46882
C	336	SER	ASN	engineered mutation	UNP P46882
D	246	MET	ILE	engineered mutation	UNP P46882
D	336	SER	ASN	engineered mutation	UNP P46882
E	246	MET	ILE	engineered mutation	UNP P46882
E	336	SER	ASN	engineered mutation	UNP P46882
F	246	MET	ILE	engineered mutation	UNP P46882
F	336	SER	ASN	engineered mutation	UNP P46882
H	246	MET	ILE	engineered mutation	UNP P46882
H	336	SER	ASN	engineered mutation	UNP P46882
A	300	VAL	ALA	conflict	UNP P46882

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Chain	Residue	Modelled	Actual	Comment	Reference
A	304	VAL	LEU	conflict	UNP P46882
A	450	GLY	ARG	conflict	UNP P46882
B	300	VAL	ALA	conflict	UNP P46882
B	304	VAL	LEU	conflict	UNP P46882
B	450	GLY	ARG	conflict	UNP P46882
C	300	VAL	ALA	conflict	UNP P46882
C	304	VAL	LEU	conflict	UNP P46882
C	450	GLY	ARG	conflict	UNP P46882
D	300	VAL	ALA	conflict	UNP P46882
D	304	VAL	LEU	conflict	UNP P46882
D	450	GLY	ARG	conflict	UNP P46882
E	300	VAL	ALA	conflict	UNP P46882
E	304	VAL	LEU	conflict	UNP P46882
E	450	GLY	ARG	conflict	UNP P46882
F	300	VAL	ALA	conflict	UNP P46882
F	304	VAL	LEU	conflict	UNP P46882
F	450	GLY	ARG	conflict	UNP P46882
H	300	VAL	ALA	conflict	UNP P46882
H	304	VAL	LEU	conflict	UNP P46882
H	450	GLY	ARG	conflict	UNP P46882

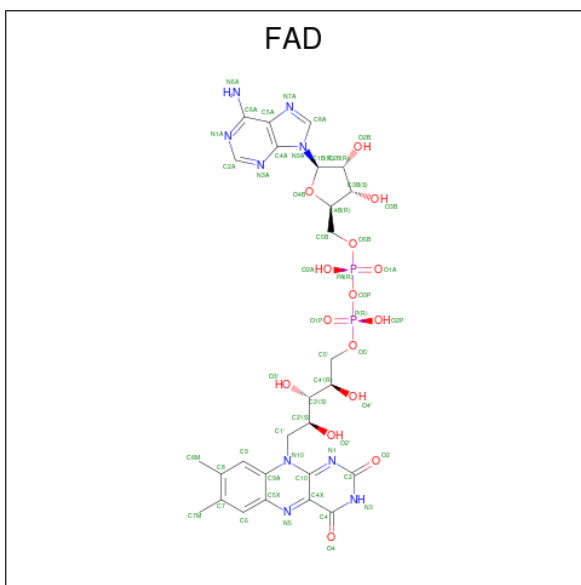
- Molecule 2 is a protein called MONOAMINE OXIDASE N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	478	Total	C	N	O	S	46	1	0
			3785	2392	669	701	23			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	246	MET	ILE	engineered mutation	UNP P46882
G	336	SER	ASN	engineered mutation	UNP P46882
G	20	THR	PRO	conflict	UNP P46882
G	300	VAL	ALA	conflict	UNP P46882
G	304	VAL	LEU	conflict	UNP P46882
G	450	GLY	ARG	conflict	UNP P46882

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	118	Total	O	0	0
			118	118		
5	B	134	Total	O	0	0
			134	134		
5	C	95	Total	O	0	0
			95	95		
5	D	102	Total	O	0	0
			102	102		
5	E	122	Total	O	0	0
			122	122		

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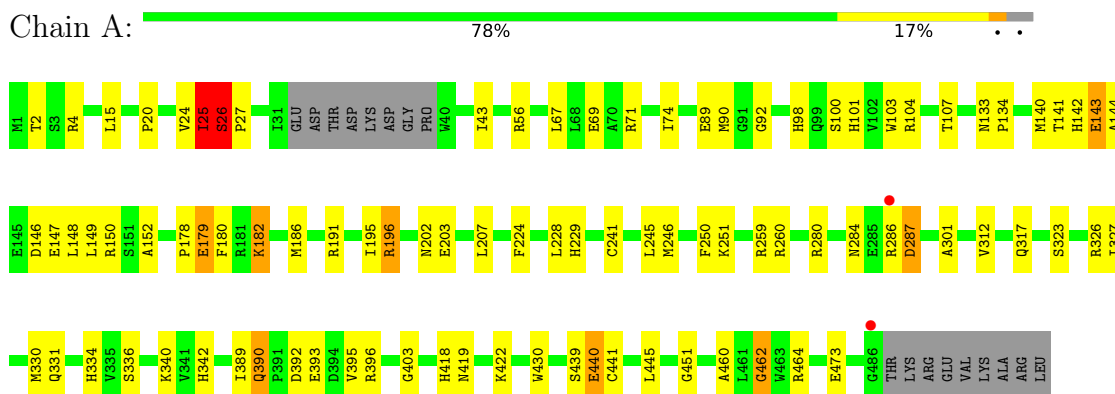
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	103	Total 103	O 103	0	0
5	G	53	Total 53	O 53	0	0
5	H	80	Total 80	O 80	0	0

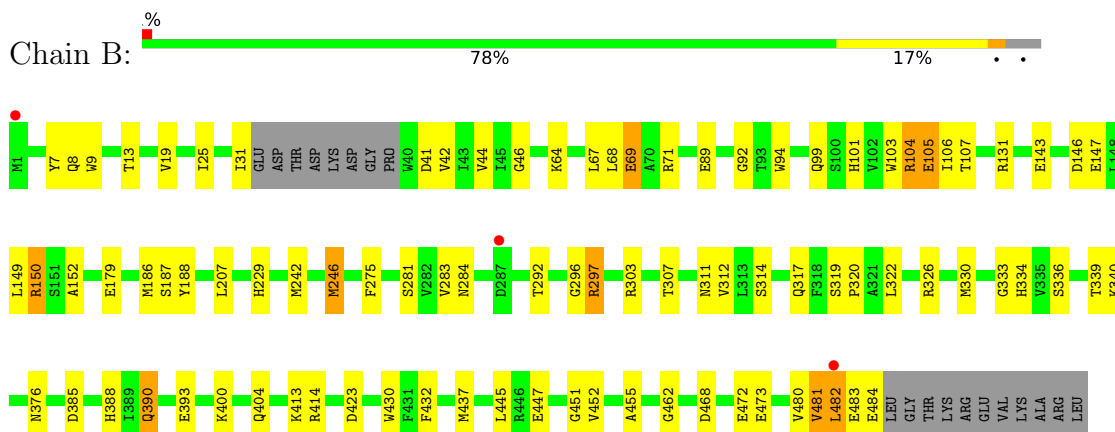
3 Residue-property plots

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.

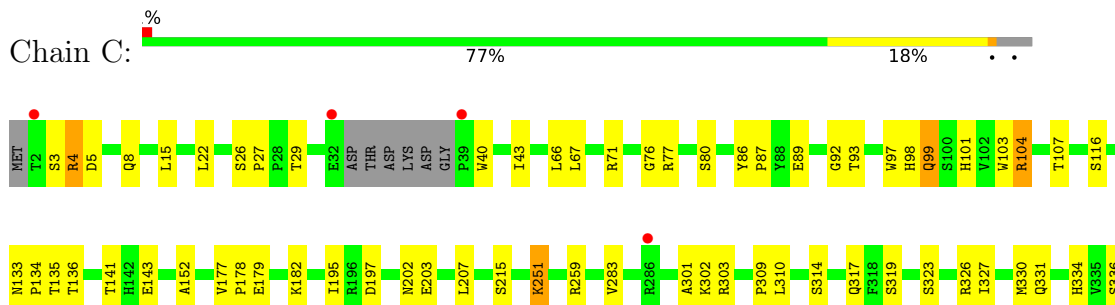
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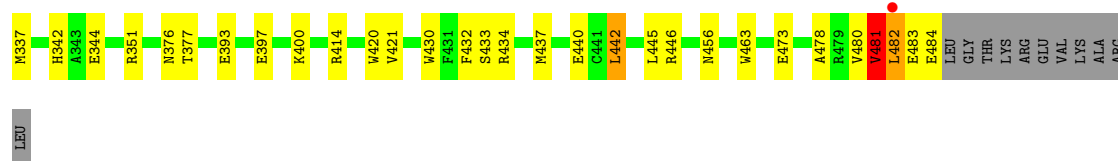


• Molecule 1: MONOAMINE OXIDASE N

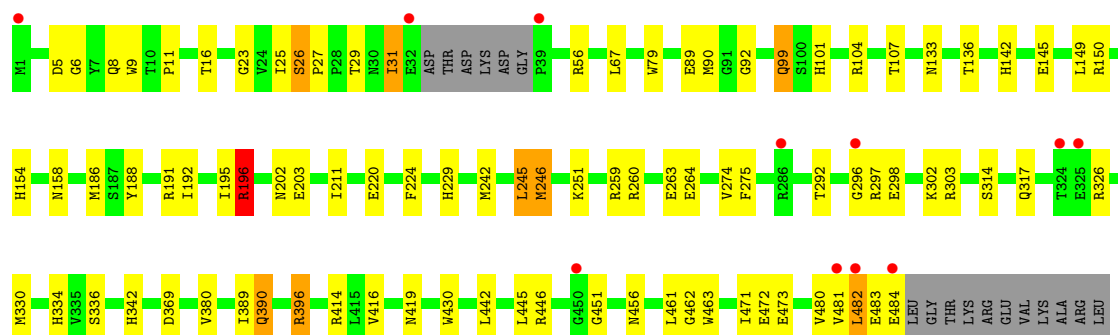
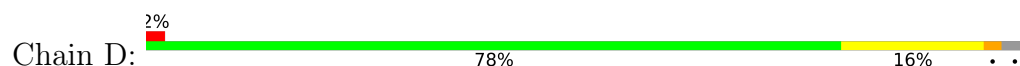


• Molecule 1: MONOAMINE OXIDASE N

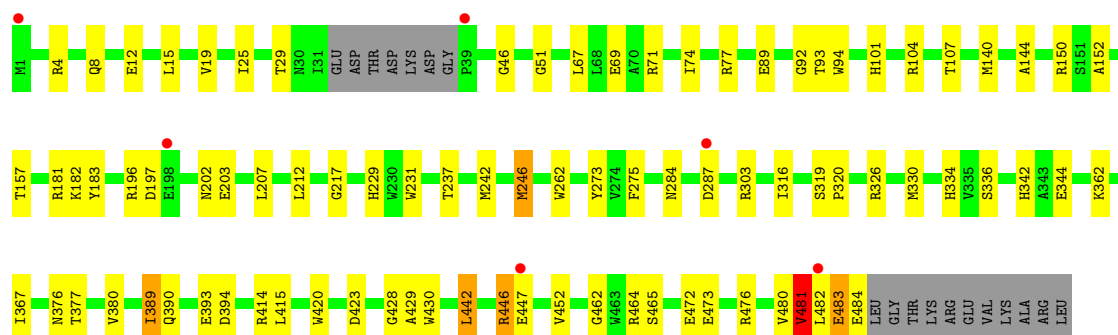
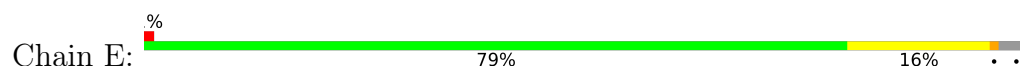




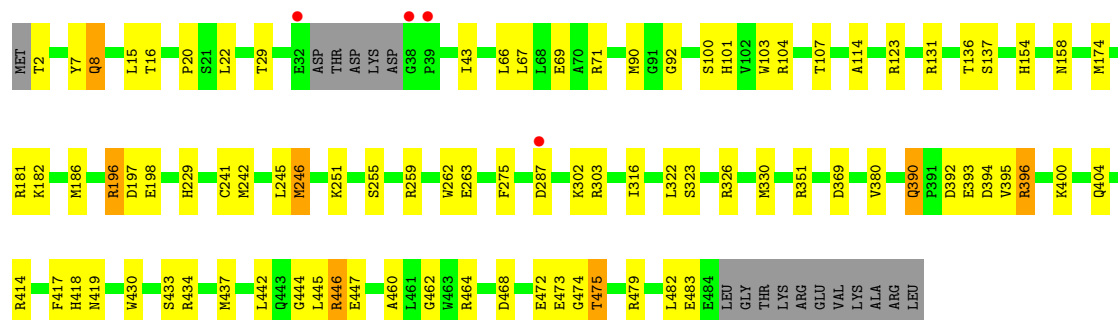
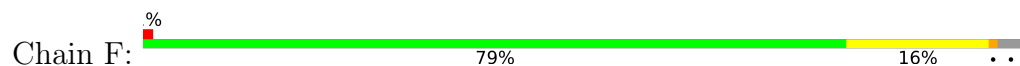
• Molecule 1: MONOAMINE OXIDASE N



• Molecule 1: MONOAMINE OXIDASE N

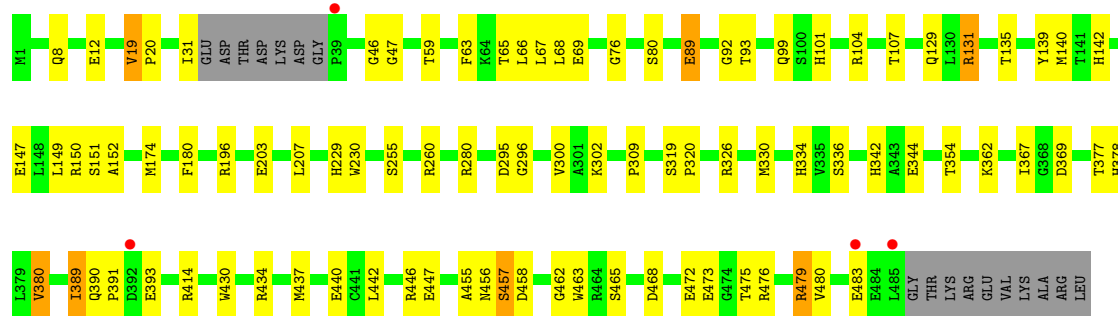


• Molecule 1: MONOAMINE OXIDASE N



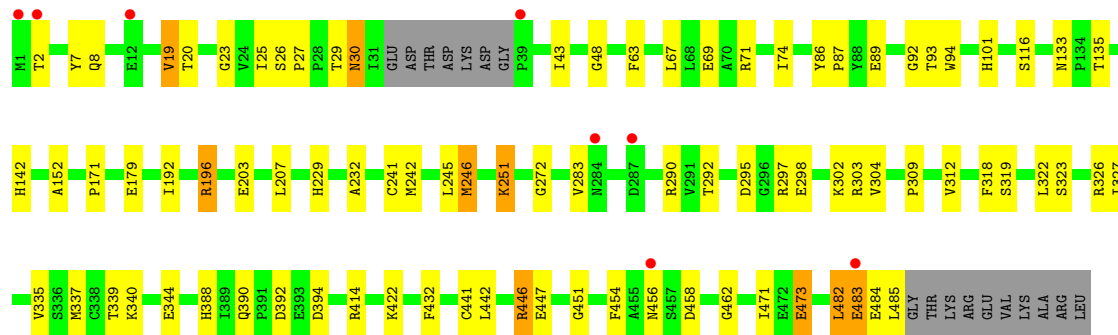
• Molecule 1: MONOAMINE OXIDASE N

Chain H:  78% 17% ..



• Molecule 2: MONOAMINE OXIDASE N

Chain G:  79% 16% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.29Å 187.25Å 132.43Å 90.00° 90.10° 90.00°	Depositor
Resolution (Å)	132.45 – 2.45 132.43 – 2.45	Depositor EDS
% Data completeness (in resolution range)	97.1 (132.45-2.45) 97.3 (132.43-2.45)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.85 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.4.0065	Depositor
R, R_{free}	0.182 , 0.236 (Not available) , 0.231	Depositor DCC
R_{free} test set	9016 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.636	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 30.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.148 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	31496	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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: EDO, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.21	33/3885 (0.8%)	1.11	27/5266 (0.5%)
1	B	1.19	30/3873 (0.8%)	1.18	26/5250 (0.5%)
1	C	1.13	21/3882 (0.5%)	1.21	39/5263 (0.7%)
1	D	1.18	30/3879 (0.8%)	1.13	22/5259 (0.4%)
1	E	1.06	18/3881 (0.5%)	1.10	25/5261 (0.5%)
1	F	1.11	27/3886 (0.7%)	1.13	34/5269 (0.6%)
1	H	1.19	27/3889 (0.7%)	1.10	25/5272 (0.5%)
2	G	1.17	24/3888 (0.6%)	1.07	16/5270 (0.3%)
All	All	1.16	210/31063 (0.7%)	1.13	214/42110 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	2
1	C	0	2
1	D	0	2
1	F	0	1
1	H	0	1
All	All	0	12

All (210) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	483	GLU	C-N	-23.80	1.03	1.33
1	C	4	ARG	C-N	-16.82	1.11	1.33
1	H	455	ALA	C-N	-16.36	1.13	1.33
1	A	196	ARG	C-N	-15.25	1.13	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	104	ARG	C-N	-15.16	1.14	1.33
1	H	67	LEU	C-N	-15.07	1.13	1.33
1	C	303	ARG	C-N	-14.91	1.14	1.33
1	B	393	GLU	C-N	-13.71	1.14	1.33
1	D	196	ARG	C-N	-13.45	1.15	1.33
1	A	143	GLU	C-N	-13.28	1.15	1.33
1	B	303	ARG	C-N	-12.61	1.17	1.33
1	F	393	GLU	C-N	-12.39	1.16	1.33
1	H	391	PRO	C-N	-12.24	1.15	1.33
1	H	66	LEU	C-N	-11.72	1.17	1.33
2	G	471	ILE	C-N	-11.45	1.19	1.33
1	E	394	ASP	C-N	-11.42	1.19	1.34
2	G	303	ARG	C-N	-11.32	1.19	1.33
1	C	99	GLN	C-N	-11.01	1.20	1.33
2	G	340	LYS	C-N	-10.28	1.20	1.33
1	E	393	GLU	C-N	-10.05	1.20	1.34
1	F	475	THR	C-N	-9.90	1.21	1.33
1	F	67	LEU	C-N	-9.74	1.20	1.33
1	A	340	LYS	C-N	-9.42	1.21	1.33
1	H	68	LEU	C-N	-9.31	1.20	1.33
1	D	472	GLU	C-N	-9.28	1.21	1.33
1	D	471	ILE	C-N	-9.15	1.20	1.33
1	D	246	MET	C-O	-8.99	1.17	1.23
1	B	7	TYR	C-N	-8.68	1.20	1.33
2	G	339	THR	C-N	-8.65	1.22	1.33
1	B	339	THR	C-N	-8.54	1.22	1.33
1	F	198	GLU	C-N	-8.52	1.21	1.33
1	E	246	MET	C-O	-8.50	1.17	1.23
1	B	246	MET	C-O	-8.30	1.15	1.24
1	F	103	TRP	C-N	8.19	1.43	1.33
1	H	89	GLU	C-N	-8.12	1.22	1.34
1	D	202	ASN	C-N	-8.08	1.22	1.33
1	H	280	ARG	C-N	-8.01	1.23	1.33
1	D	246	MET	CA-C	7.99	1.59	1.52
1	A	393	GLU	C-N	-7.96	1.21	1.33
1	F	396	ARG	C-N	-7.76	1.23	1.33
2	G	29	THR	N-CA	-7.75	1.35	1.45
1	C	202	ASN	C-N	-7.71	1.22	1.33
1	F	395	VAL	C-N	-7.68	1.24	1.33
1	B	31	ILE	CG1-CD1	-7.62	1.22	1.51
1	C	376	ASN	C-N	-7.46	1.23	1.33
1	B	340	LYS	C-N	-7.46	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	203	GLU	C-O	-7.45	1.15	1.24
1	D	31	ILE	CG1-CD1	-7.41	1.22	1.51
1	A	389	ILE	C-O	-7.36	1.16	1.24
1	D	6	GLY	C-O	-7.29	1.17	1.23
1	B	472	GLU	C-N	-7.24	1.24	1.33
2	G	473	GLU	C-O	-7.23	1.15	1.24
1	A	246	MET	C-O	-7.21	1.16	1.24
1	F	104	ARG	C-N	-7.19	1.24	1.33
1	F	197	ASP	C-N	-7.09	1.22	1.33
1	C	3	SER	C-N	-7.03	1.23	1.33
1	B	105	GLU	C-O	-6.99	1.15	1.24
1	D	26	SER	CA-C	-6.99	1.47	1.52
1	H	377	THR	C-N	6.96	1.43	1.33
1	D	298	GLU	N-CA	-6.90	1.37	1.46
1	D	390	GLN	C-O	-6.87	1.18	1.24
1	E	202	ASN	C-O	-6.83	1.16	1.24
1	A	403	GLY	C-O	-6.81	1.15	1.24
1	C	80	SER	C-O	-6.77	1.15	1.23
1	H	302	LYS	C-N	-6.77	1.24	1.33
1	F	8	GLN	C-N	-6.76	1.24	1.33
1	H	390	GLN	C-O	-6.73	1.16	1.24
1	A	15	LEU	C-O	-6.73	1.15	1.24
1	E	389	ILE	C-O	-6.73	1.17	1.24
1	E	442	LEU	C-O	-6.71	1.16	1.24
1	B	149	LEU	C-O	-6.70	1.16	1.24
2	G	458	ASP	C-O	-6.64	1.15	1.24
1	H	139	TYR	C-N	-6.53	1.25	1.33
1	D	389	ILE	C-O	-6.53	1.17	1.24
1	A	142	HIS	C-O	-6.50	1.15	1.24
1	H	203	GLU	C-O	-6.45	1.16	1.24
1	D	16	THR	CA-C	-6.42	1.44	1.52
1	D	99	GLN	C-O	-6.40	1.16	1.24
1	A	462	GLY	C-O	-6.37	1.17	1.24
1	A	98	HIS	C-O	-6.35	1.15	1.24
1	D	195	ILE	C-N	-6.32	1.26	1.33
1	C	202	ASN	C-O	-6.31	1.16	1.24
1	F	474	GLY	C-N	-6.28	1.26	1.33
1	A	178	PRO	C-N	-6.28	1.25	1.33
1	B	385	ASP	C-O	-6.28	1.15	1.24
1	A	56	ARG	C-O	-6.26	1.16	1.24
1	E	197	ASP	C-O	-6.25	1.15	1.24
1	F	246	MET	C-O	-6.19	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	195	ILE	C-N	-6.19	1.26	1.33
1	H	389	ILE	C-O	-6.18	1.17	1.24
1	E	390	GLN	C-O	-6.14	1.16	1.24
1	A	103	TRP	C-O	-6.13	1.16	1.24
2	G	142	HIS	C-O	-6.06	1.16	1.24
1	B	131	ARG	C-O	-6.06	1.17	1.24
1	D	16	THR	N-CA	-6.05	1.38	1.46
1	B	103	TRP	C-O	-6.04	1.16	1.24
1	F	316	ILE	C-O	-6.04	1.16	1.24
1	B	147	GLU	C-O	-6.03	1.16	1.24
2	G	394	ASP	C-O	-6.00	1.17	1.23
1	A	104	ARG	C-O	-6.00	1.17	1.24
1	D	202	ASN	C-O	-5.99	1.16	1.24
1	C	29	THR	C-O	-5.98	1.16	1.23
1	B	187	SER	C-O	-5.94	1.16	1.23
1	A	67	LEU	C-O	-5.93	1.16	1.24
1	B	105	GLU	N-CA	-5.93	1.39	1.46
1	D	246	MET	N-CA	5.92	1.52	1.47
1	F	479	ARG	C-O	-5.88	1.17	1.24
1	H	230	TRP	C-O	-5.87	1.17	1.24
1	F	174	MET	C-O	-5.86	1.16	1.24
2	G	394	ASP	CA-C	-5.84	1.47	1.53
1	E	316	ILE	N-CA	-5.84	1.39	1.46
1	D	245	LEU	CA-C	-5.83	1.45	1.52
1	D	195	ILE	C-O	-5.83	1.17	1.24
1	D	317	GLN	C-O	-5.81	1.17	1.23
1	D	11	PRO	C-O	-5.77	1.17	1.24
1	C	3	SER	N-CA	-5.76	1.38	1.45
1	A	202	ASN	C-O	-5.76	1.17	1.24
1	B	390	GLN	C-O	-5.75	1.17	1.24
1	B	311	ASN	C-O	-5.74	1.16	1.24
1	E	481	VAL	C-O	-5.72	1.17	1.24
1	C	317	GLN	C-O	-5.72	1.17	1.24
1	A	203	GLU	C-O	-5.70	1.17	1.24
1	B	68	LEU	C-O	-5.69	1.17	1.24
1	D	149	LEU	C-O	-5.68	1.17	1.24
1	A	445	LEU	C-O	-5.65	1.16	1.24
1	H	142	HIS	C-N	-5.63	1.26	1.33
1	A	250	PHE	C-O	-5.63	1.17	1.23
1	H	131	ARG	C-O	-5.62	1.17	1.24
1	B	146	ASP	C-O	-5.62	1.17	1.24
1	F	182	LYS	C-O	-5.58	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	196	ARG	C-O	-5.58	1.17	1.24
1	H	473	GLU	C-O	-5.57	1.17	1.24
1	D	16	THR	C-O	-5.55	1.17	1.23
1	F	131	ARG	C-O	-5.54	1.17	1.24
1	H	19	VAL	C-O	-5.54	1.18	1.24
1	H	475	THR	C-O	-5.53	1.17	1.24
1	E	196	ARG	C-O	-5.51	1.17	1.24
1	B	481	VAL	CB-CG1	-5.50	1.34	1.52
2	G	20	THR	CA-CB	-5.49	1.44	1.53
1	C	481	VAL	C-O	-5.48	1.17	1.24
1	F	390	GLN	C-O	-5.47	1.17	1.24
1	H	440	GLU	C-O	-5.44	1.17	1.24
1	D	251	LYS	C-O	-5.41	1.17	1.24
1	F	392	ASP	C-O	-5.41	1.17	1.24
1	E	303	ARG	C-N	5.39	1.40	1.33
2	G	482	LEU	C-O	-5.39	1.17	1.24
1	B	473	GLU	C-O	-5.38	1.17	1.24
1	A	390	GLN	C-O	-5.37	1.17	1.24
1	B	452	VAL	C-O	-5.37	1.18	1.24
2	G	19	VAL	C-O	-5.37	1.18	1.24
1	B	150[A]	ARG	C-O	-5.34	1.18	1.24
1	B	150[B]	ARG	C-O	-5.34	1.18	1.24
1	D	5	ASP	C-O	-5.34	1.17	1.24
1	C	136	THR	C-N	-5.33	1.25	1.33
1	E	472	GLU	C-O	-5.32	1.17	1.24
1	E	19	VAL	C-O	-5.32	1.17	1.24
1	F	196	ARG	C-O	-5.31	1.18	1.24
1	H	380	VAL	CA-CB	5.31	1.60	1.54
2	G	446	ARG	C-O	-5.31	1.17	1.24
1	D	396	ARG	C-O	-5.29	1.18	1.24
2	G	451	GLY	C-O	-5.29	1.19	1.24
1	D	334	HIS	C-O	-5.28	1.16	1.23
1	B	376	ASN	C-O	-5.27	1.17	1.23
1	E	104	ARG	C-O	-5.26	1.18	1.24
1	F	395	VAL	C-O	-5.26	1.17	1.24
1	D	104	ARG	C-O	-5.26	1.17	1.24
1	B	99	GLN	C-O	-5.25	1.17	1.23
1	A	25	ILE	CG1-CD1	-5.25	1.31	1.51
1	F	29	THR	C-O	-5.25	1.17	1.23
1	H	472	GLU	C-O	-5.25	1.17	1.24
1	H	149	LEU	C-O	-5.24	1.18	1.24
1	A	146	ASP	C-O	-5.24	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	178	PRO	C-O	-5.24	1.17	1.24
1	H	104	ARG	C-O	-5.23	1.18	1.24
2	G	246	MET	C-O	-5.23	1.17	1.23
2	G	203	GLU	C-O	-5.22	1.18	1.24
2	G	7	TYR	C-O	-5.22	1.17	1.23
2	G	251	LYS	C-O	-5.21	1.17	1.24
1	C	478	ALA	C-O	-5.20	1.18	1.24
1	B	42	VAL	CA-C	-5.19	1.46	1.52
1	F	393	GLU	C-O	-5.19	1.17	1.24
1	C	251	LYS	C-O	-5.17	1.18	1.24
1	C	98	HIS	C-O	-5.17	1.17	1.24
1	F	262	TRP	C-O	-5.17	1.18	1.24
1	A	260	ARG	C-O	-5.17	1.18	1.24
1	B	104	ARG	C-N	-5.17	1.27	1.34
1	A	182	LYS	C-O	-5.14	1.17	1.24
1	E	446	ARG	CZ-NH2	-5.14	1.26	1.33
1	B	188	TYR	C-O	-5.12	1.18	1.24
1	H	196	ARG	C-O	-5.12	1.18	1.24
1	A	178	PRO	C-O	-5.12	1.17	1.24
1	F	181	ARG	C-O	-5.11	1.18	1.24
1	A	251	LYS	C-O	-5.11	1.17	1.24
1	F	137	SER	C-O	-5.10	1.18	1.23
1	D	67	LEU	C-O	-5.09	1.17	1.24
2	G	67	LEU	C-O	-5.09	1.17	1.24
1	F	263	GLU	C-O	-5.08	1.18	1.24
2	G	390	GLN	C-O	-5.05	1.17	1.24
1	H	457	SER	C-O	-5.05	1.17	1.24
1	E	15	LEU	C-O	-5.05	1.17	1.24
1	A	439	SER	C-N	-5.04	1.27	1.33
1	H	142	HIS	C-O	-5.04	1.17	1.24
1	A	473	GLU	C-O	-5.03	1.18	1.24
1	C	377	THR	C-N	5.03	1.40	1.33
2	G	29	THR	CA-C	-5.03	1.46	1.52
1	A	392	ASP	C-N	-5.03	1.27	1.33
1	A	280	ARG	C-O	-5.03	1.16	1.23
1	A	441	CYS	C-O	-5.02	1.17	1.24
1	C	182	LYS	CG-CD	-5.01	1.37	1.52
1	A	445	LEU	C-N	-5.00	1.26	1.33

All (214) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	136	THR	O-C-N	-23.42	96.49	122.96
1	B	297	ARG	O-C-N	20.90	148.58	122.87
1	B	297	ARG	CA-C-N	-13.37	101.07	122.73
1	B	297	ARG	C-N-CA	-13.37	101.07	122.73
1	E	376	ASN	CA-C-N	11.80	137.48	120.95
1	E	376	ASN	C-N-CA	11.80	137.48	120.95
1	E	446	ARG	CA-C-N	11.72	140.84	121.39
1	E	446	ARG	C-N-CA	11.72	140.84	121.39
2	G	302	LYS	CA-C-N	10.94	139.68	122.62
2	G	302	LYS	C-N-CA	10.94	139.68	122.62
1	B	303	ARG	O-C-N	10.89	135.90	123.27
1	H	139	TYR	O-C-N	-10.80	109.49	123.21
1	D	196	ARG	O-C-N	-10.57	109.42	122.20
1	F	482	LEU	CA-C-N	10.43	134.62	120.54
1	F	482	LEU	C-N-CA	10.43	134.62	120.54
1	E	394	ASP	O-C-N	-10.37	113.04	123.62
1	D	5	ASP	CA-C-N	-10.34	112.03	122.27
1	D	5	ASP	C-N-CA	-10.34	112.03	122.27
1	D	246	MET	N-CA-C	10.14	127.41	113.21
1	D	296	GLY	CA-C-N	10.05	134.97	120.71
1	D	296	GLY	C-N-CA	10.05	134.97	120.71
2	G	302	LYS	O-C-N	-9.83	108.89	122.46
1	F	104	ARG	O-C-N	9.79	132.55	122.08
1	C	135	THR	CA-C-N	9.48	137.12	121.39
1	C	135	THR	C-N-CA	9.48	137.12	121.39
1	F	474	GLY	CA-C-N	9.43	133.09	120.65
1	F	474	GLY	C-N-CA	9.43	133.09	120.65
1	D	203	GLU	CA-C-N	9.32	133.52	120.29
1	D	203	GLU	C-N-CA	9.32	133.52	120.29
1	B	104	ARG	CA-C-N	-9.27	106.93	120.28
1	B	104	ARG	C-N-CA	-9.27	106.93	120.28
1	H	135	THR	N-CA-C	9.25	125.98	112.94
1	C	99	GLN	CA-C-N	9.09	132.82	120.54
1	C	99	GLN	C-N-CA	9.09	132.82	120.54
1	C	202	ASN	CA-C-O	9.07	130.35	120.10
1	H	139	TYR	CA-C-N	9.05	137.41	121.75
1	H	139	TYR	C-N-CA	9.05	137.41	121.75
1	C	195	ILE	CA-C-O	9.02	126.50	119.46
1	A	286	ARG	N-CA-C	-8.98	96.39	109.59
1	A	287	ASP	N-CA-C	8.90	123.72	112.86
1	B	303	ARG	CA-C-N	-8.63	111.83	123.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	303	ARG	C-N-CA	-8.63	111.83	123.14
1	F	15	LEU	CA-C-N	8.57	135.80	122.94
1	F	15	LEU	C-N-CA	8.57	135.80	122.94
1	F	15	LEU	O-C-N	-8.45	113.15	123.04
1	C	99	GLN	O-C-N	-8.44	112.33	122.63
1	C	203	GLU	CA-C-N	8.24	131.99	120.29
1	C	203	GLU	C-N-CA	8.24	131.99	120.29
2	G	446	ARG	CA-C-N	8.12	133.68	120.94
2	G	446	ARG	C-N-CA	8.12	133.68	120.94
1	D	202	ASN	CA-C-O	8.08	129.23	120.10
1	C	376	ASN	CA-C-N	8.01	133.11	122.30
1	C	376	ASN	C-N-CA	8.01	133.11	122.30
1	F	395	VAL	CA-C-N	7.97	130.80	120.44
1	F	395	VAL	C-N-CA	7.97	130.80	120.44
1	D	5	ASP	N-CA-C	7.88	120.96	111.82
1	F	474	GLY	CA-C-O	7.87	128.90	120.40
1	F	395	VAL	CA-C-O	7.75	128.86	120.57
1	B	7	TYR	CA-C-N	7.70	134.64	122.62
1	B	7	TYR	C-N-CA	7.70	134.64	122.62
1	H	302	LYS	CA-C-N	7.65	134.92	122.29
1	H	302	LYS	C-N-CA	7.65	134.92	122.29
1	F	396	ARG	O-C-N	-7.64	114.20	122.07
1	C	4	ARG	O-C-N	-7.62	112.11	122.33
1	C	136	THR	CA-C-N	7.57	135.38	122.37
1	C	136	THR	C-N-CA	7.57	135.38	122.37
1	D	31	ILE	CB-CG1-CD1	7.55	129.65	113.80
1	A	26	SER	CA-C-N	7.50	128.11	120.38
1	A	26	SER	C-N-CA	7.50	128.11	120.38
1	D	203	GLU	O-C-N	-7.48	112.20	122.30
1	H	393	GLU	N-CA-C	7.47	119.43	111.28
1	D	245	LEU	CA-C-O	7.45	127.33	119.14
1	A	178	PRO	CA-C-O	7.39	130.78	119.55
1	C	3	SER	N-CA-C	-7.37	100.60	110.55
1	F	287	ASP	CB-CA-C	-7.33	99.50	110.06
1	A	228	LEU	CD1-CG-CD2	7.32	126.90	110.80
1	F	396	ARG	CA-C-N	7.29	130.06	120.28
1	F	396	ARG	C-N-CA	7.29	130.06	120.28
1	A	473	GLU	CA-C-N	7.28	128.21	119.99
1	A	473	GLU	C-N-CA	7.28	128.21	119.99
1	F	446	ARG	CA-C-N	7.25	131.71	120.75
1	F	446	ARG	C-N-CA	7.25	131.71	120.75
1	B	296	GLY	CA-C-N	7.24	130.99	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	296	GLY	C-N-CA	7.24	130.99	120.71
1	A	26	SER	N-CA-C	-7.22	90.79	111.00
1	H	302	LYS	O-C-N	-7.22	113.39	122.27
2	G	246	MET	N-CA-C	7.21	121.01	109.83
1	C	393	GLU	N-CA-C	7.20	118.78	111.07
1	C	195	ILE	CB-CA-C	-7.20	103.57	110.70
1	H	377	THR	O-C-N	7.01	131.25	123.04
1	B	7	TYR	O-C-N	-6.98	115.44	123.33
1	B	143	GLU	CG-CD-OE2	-6.97	102.37	118.40
1	H	142	HIS	CA-C-N	6.92	130.11	120.29
1	H	142	HIS	C-N-CA	6.92	130.11	120.29
1	C	203	GLU	O-C-N	-6.89	112.15	122.28
1	E	446	ARG	N-CA-C	6.88	121.84	113.38
1	F	104	ARG	CA-C-N	-6.75	111.14	120.38
1	F	104	ARG	C-N-CA	-6.75	111.14	120.38
1	E	447	GLU	O-C-N	-6.74	115.34	122.96
1	B	143	GLU	CG-CD-OE1	6.73	133.87	118.40
1	E	376	ASN	O-C-N	-6.69	115.57	123.06
1	C	195	ILE	CA-C-N	6.66	130.80	120.82
1	C	195	ILE	C-N-CA	6.66	130.80	120.82
1	C	302	LYS	N-CA-C	6.60	118.48	111.28
1	H	19	VAL	N-CA-C	6.60	116.37	108.45
1	C	197	ASP	N-CA-C	-6.46	105.37	113.18
1	H	377	THR	CA-C-N	-6.40	113.89	122.72
1	H	377	THR	C-N-CA	-6.40	113.89	122.72
1	F	446	ARG	O-C-N	-6.37	114.53	122.24
1	H	479[A]	ARG	N-CA-C	6.36	118.22	111.28
1	H	479[B]	ARG	N-CA-C	6.36	118.22	111.28
1	C	303	ARG	CA-C-N	-6.36	114.81	123.14
1	C	303	ARG	C-N-CA	-6.36	114.81	123.14
1	E	394	ASP	CA-C-N	6.35	129.48	120.53
1	E	394	ASP	C-N-CA	6.35	129.48	120.53
2	G	29	THR	CA-C-O	6.33	128.60	121.51
1	B	447	GLU	N-CA-C	6.33	119.09	110.55
1	H	447	GLU	N-CA-C	6.31	118.86	110.53
1	A	142	HIS	CA-C-N	6.31	129.02	120.44
1	A	142	HIS	C-N-CA	6.31	129.02	120.44
1	A	4	ARG	CA-C-N	6.30	131.84	121.39
1	A	4	ARG	C-N-CA	6.30	131.84	121.39
1	F	100	SER	N-CA-C	6.22	118.57	111.11
1	E	316	ILE	CA-C-O	6.22	128.05	120.84
1	C	377	THR	CA-C-N	-6.21	114.52	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	377	THR	C-N-CA	-6.21	114.52	122.77
1	C	303	ARG	O-C-N	6.19	130.86	123.24
2	G	482	LEU	CA-C-N	6.17	131.01	120.71
2	G	482	LEU	C-N-CA	6.17	131.01	120.71
1	H	66	LEU	O-C-N	-6.17	116.19	123.22
1	A	317	GLN	CB-CG-CD	6.15	123.06	112.60
1	A	440	GLU	O-C-N	-6.13	115.66	122.03
1	B	104	ARG	O-C-N	-6.13	115.76	122.07
1	C	104	ARG	O-C-N	6.12	128.40	122.03
1	E	287	ASP	CB-CA-C	-6.10	98.29	110.42
1	B	13	THR	CA-C-N	-6.08	114.97	122.75
1	B	13	THR	C-N-CA	-6.08	114.97	122.75
1	H	260	ARG	CA-C-N	6.04	128.37	120.28
1	H	260	ARG	C-N-CA	6.04	128.37	120.28
1	D	6	GLY	N-CA-C	6.04	121.46	112.41
1	H	142	HIS	CA-C-O	6.00	126.76	119.38
1	B	19	VAL	CA-C-N	5.97	127.30	119.84
1	B	19	VAL	C-N-CA	5.97	127.30	119.84
1	D	11	PRO	CA-C-O	5.96	128.10	119.34
1	D	451	GLY	N-CA-C	-5.95	105.27	115.61
1	C	104	ARG	CA-C-N	-5.92	112.35	120.28
1	C	104	ARG	C-N-CA	-5.92	112.35	120.28
1	F	475	THR	CA-C-N	-5.92	112.27	120.38
1	F	475	THR	C-N-CA	-5.92	112.27	120.38
1	B	69	GLU	O-C-N	5.88	130.83	123.19
1	E	377	THR	CA-C-N	-5.87	114.96	122.77
1	E	377	THR	C-N-CA	-5.87	114.96	122.77
1	E	429	ALA	N-CA-C	-5.87	100.89	109.63
1	F	483	GLU	O-C-N	-5.85	116.00	122.09
1	A	179	GLU	O-C-N	-5.85	114.79	122.39
1	A	149	LEU	N-CA-C	5.77	117.65	111.36
1	D	296	GLY	N-CA-C	5.77	126.85	113.18
2	G	196	ARG	N-CA-C	5.70	118.27	111.71
1	H	458	ASP	N-CA-C	5.70	119.75	112.34
1	F	136	THR	N-CA-C	5.70	118.97	110.14
1	F	393	GLU	N-CA-C	5.66	118.65	111.69
1	C	3	SER	CA-C-O	5.65	128.47	121.81
1	A	202	ASN	N-CA-C	5.63	117.42	111.28
1	E	483	GLU	N-CA-C	5.62	126.74	111.00
1	F	474	GLY	N-CA-C	5.62	120.61	113.24
1	E	316	ILE	CA-C-N	5.61	130.23	122.77
1	E	316	ILE	C-N-CA	5.61	130.23	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	ILE	CA-C-O	5.61	124.26	119.38
1	H	300	VAL	CG1-CB-CG2	5.56	123.03	110.80
2	G	48	GLY	N-CA-C	-5.54	104.13	112.60
1	B	482	LEU	CA-C-N	5.52	131.63	121.70
1	B	482	LEU	C-N-CA	5.52	131.63	121.70
1	F	7	TYR	CA-C-N	5.52	131.39	122.29
1	F	7	TYR	C-N-CA	5.52	131.39	122.29
1	E	303	ARG	CA-C-N	5.51	130.81	122.98
1	E	303	ARG	C-N-CA	5.51	130.81	122.98
1	E	12	GLU	N-CA-C	5.46	118.16	111.82
1	C	442	LEU	CA-C-O	5.46	126.53	120.63
1	A	100	SER	N-CA-C	5.45	116.90	111.07
2	G	458	ASP	N-CA-C	5.45	118.72	111.75
1	B	413	LYS	CD-CE-NZ	5.44	129.31	111.90
1	D	196	ARG	CA-C-N	5.44	129.30	120.60
1	D	196	ARG	C-N-CA	5.44	129.30	120.60
1	B	312	VAL	N-CA-C	-5.42	108.22	113.53
2	G	30	ASN	N-CA-C	-5.42	105.97	113.18
1	E	183	TYR	N-CA-C	5.39	117.24	111.36
1	A	440	GLU	CA-C-N	-5.34	113.02	122.26
1	A	440	GLU	C-N-CA	-5.34	113.02	122.26
1	C	3	SER	CA-C-N	5.28	129.66	120.68
1	C	3	SER	C-N-CA	5.28	129.66	120.68
1	C	182	LYS	CB-CG-CD	5.26	123.39	111.30
2	G	447	GLU	N-CA-C	5.25	117.90	110.50
1	E	4	ARG	CB-CG-CD	-5.25	99.24	111.30
1	E	428	GLY	N-CA-C	-5.21	104.76	110.96
2	G	312	VAL	N-CA-C	-5.21	108.43	113.53
1	H	135	THR	CB-CA-C	-5.18	101.72	110.64
2	G	441	CYS	N-CA-C	5.18	120.25	113.30
1	A	146	ASP	CA-C-N	5.16	129.40	120.58
1	A	146	ASP	C-N-CA	5.16	129.40	120.58
1	H	12	GLU	N-CA-C	5.11	117.98	111.69
1	F	483	GLU	CA-C-N	-5.11	112.50	121.70
1	F	483	GLU	C-N-CA	-5.11	112.50	121.70
1	D	23	GLY	N-CA-C	5.07	120.30	114.16
1	D	245	LEU	CA-C-N	5.07	127.86	119.35
1	D	245	LEU	C-N-CA	5.07	127.86	119.35
1	F	16	THR	CA-C-N	-5.06	115.59	122.93
1	F	16	THR	C-N-CA	-5.06	115.59	122.93
1	A	312	VAL	N-CA-C	-5.04	108.59	113.53
1	C	478	ALA	N-CA-C	5.04	116.78	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	445	LEU	CA-C-O	5.02	125.56	119.49
1	A	24	VAL	N-CA-C	5.01	115.45	108.84
1	C	177	VAL	CA-C-N	5.01	125.03	119.32
1	C	177	VAL	C-N-CA	5.01	125.03	119.32
1	E	442	LEU	N-CA-C	5.00	117.11	111.11

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	196	ARG	Mainchain
1	A	25	ILE	Peptide
1	A	26	SER	Peptide
1	A	440	GLU	Mainchain
1	B	150[A]	ARG	Sidechain
1	B	150[B]	ARG	Sidechain
1	C	4	ARG	Mainchain
1	C	482	LEU	Peptide
1	D	196	ARG	Mainchain
1	D	482	LEU	Peptide
1	F	475	THR	Mainchain
1	H	140	MET	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3782	0	3631	47	0
1	B	3770	0	3617	61	0
1	C	3778	0	3618	69	0
1	D	3778	0	3618	55	0
1	E	3777	0	3626	58	0
1	F	3782	0	3622	50	0
1	H	3785	0	3634	52	0
2	G	3785	0	3636	49	0
3	A	53	0	30	5	0
3	B	53	0	30	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	53	0	30	5	0
3	D	53	0	30	4	0
3	E	53	0	31	4	0
3	F	53	0	30	4	0
3	G	53	0	31	5	0
3	H	53	0	30	4	0
4	A	4	0	6	0	0
4	C	8	0	12	1	0
4	D	4	0	6	0	0
4	F	4	0	6	0	0
4	G	8	0	12	3	0
5	A	118	0	0	1	0
5	B	134	0	0	1	0
5	C	95	0	0	0	0
5	D	102	0	0	2	0
5	E	122	0	0	1	0
5	F	103	0	0	1	0
5	G	53	0	0	0	0
5	H	80	0	0	1	0
All	All	31496	0	29286	439	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 (439) 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:C:481:VAL:C	1:C:482:LEU:HD12	1.44	1.41
1:B:483:GLU:O	1:B:484:GLU:HG2	1.40	1.20
1:E:481:VAL:C	1:E:482:LEU:HD12	1.78	1.07
1:B:482:LEU:HD12	1:B:482:LEU:N	1.69	1.06
1:D:483:GLU:O	1:D:484:GLU:HB3	1.49	1.05
1:C:481:VAL:O	1:C:482:LEU:HD12	1.55	1.04
1:E:482:LEU:N	1:E:482:LEU:CD1	2.18	1.01
1:C:481:VAL:C	1:C:482:LEU:CD1	2.35	0.99
1:C:482:LEU:CD1	1:C:482:LEU:N	2.25	0.96
1:B:481:VAL:C	1:B:482:LEU:HD12	1.92	0.95
1:F:242:MET:HE1	1:F:246:MET:CE	1.94	0.95
1:B:482:LEU:N	1:B:482:LEU:CD1	2.29	0.94
1:B:104:ARG:HD3	1:C:104:ARG:HD2	1.48	0.94
1:D:482:LEU:N	1:D:482:LEU:CD1	2.29	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:482:LEU:HD12	1:C:482:LEU:N	1.75	0.94
1:C:351:ARG:HE	4:C:601:EDO:H22	1.35	0.90
2:G:242:MET:HE1	2:G:246:MET:HE3	1.51	0.90
1:E:481:VAL:C	1:E:482:LEU:CD1	2.44	0.90
1:H:434:ARG:HG3	1:H:437:MET:HE3	1.54	0.89
3:G:600:FAD:H2'	3:G:600:FAD:H9	1.54	0.89
1:D:482:LEU:N	1:D:482:LEU:HD12	1.87	0.88
1:B:104:ARG:CD	1:C:104:ARG:CD	2.52	0.88
1:B:104:ARG:HD3	1:C:104:ARG:CD	2.03	0.87
1:F:196:ARG:HG2	5:F:2056:HOH:O	1.75	0.87
1:E:242:MET:HE1	1:E:246:MET:CE	2.04	0.87
1:D:481:VAL:C	1:D:482:LEU:HD12	2.00	0.86
1:E:482:LEU:N	1:E:482:LEU:HD13	1.87	0.86
1:B:483:GLU:C	1:B:484:GLU:HG2	1.95	0.86
1:H:342:HIS:HD2	1:H:378:HIS:NE2	1.75	0.85
1:B:284:ASN:HD21	1:B:451:GLY:H	1.23	0.84
1:H:309:PRO:HA	1:H:456:ASN:ND2	1.93	0.84
3:B:600:FAD:H2'	3:B:600:FAD:H9	1.59	0.84
1:E:482:LEU:HD12	1:E:482:LEU:N	1.88	0.83
1:H:89:GLU:HG3	1:H:93:THR:HG23	1.61	0.82
1:C:337:MET:HE2	1:C:421:VAL:HG13	1.62	0.81
1:F:242:MET:HE1	1:F:246:MET:HE3	1.61	0.81
3:C:600:FAD:H2'	3:C:600:FAD:H9	1.61	0.80
1:H:8:GLN:HE21	1:H:414:ARG:HE	1.29	0.80
1:C:337:MET:HE3	1:C:421:VAL:HG22	1.64	0.80
3:F:600:FAD:H2'	3:F:600:FAD:H9	1.64	0.80
2:G:309:PRO:HA	2:G:456:ASN:ND2	1.98	0.79
3:E:600:FAD:H2'	3:E:600:FAD:H9	1.64	0.78
1:B:104:ARG:CD	1:C:104:ARG:HD2	2.11	0.78
1:C:337:MET:CE	1:C:421:VAL:HG13	2.14	0.78
1:B:104:ARG:O	1:B:105:GLU:C	2.20	0.77
3:D:600:FAD:H2'	3:D:600:FAD:H9	1.66	0.77
1:H:434:ARG:HG3	1:H:437:MET:CE	2.16	0.75
1:C:433:SER:HA	1:C:437:MET:HE3	1.67	0.74
3:H:600:FAD:H2'	3:H:600:FAD:H9	1.69	0.74
1:C:442:LEU:O	1:C:446:ARG:HG3	1.87	0.74
1:F:8:GLN:HE21	1:F:414:ARG:HE	1.33	0.74
1:A:147:GLU:OE1	1:A:150[A]:ARG:NH1	2.21	0.74
1:D:483:GLU:O	1:D:484:GLU:CB	2.30	0.73
1:B:483:GLU:O	1:B:484:GLU:CG	2.30	0.73
1:B:483:GLU:C	1:B:484:GLU:CG	2.62	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:GLN:NE2	1:B:414:ARG:HH21	1.87	0.73
1:C:481:VAL:O	1:C:481:VAL:HG12	1.89	0.73
1:H:150:ARG:HG3	1:H:151:SER:N	2.03	0.72
2:G:485:LEU:N	2:G:485:LEU:HD12	2.04	0.72
1:B:104:ARG:CD	1:C:104:ARG:HD3	2.20	0.72
1:F:434:ARG:H	1:F:437:MET:HE2	1.55	0.71
1:D:186:MET:HE3	1:D:191:ARG:HB2	1.72	0.71
1:E:67:LEU:HD23	1:E:262:TRP:HZ3	1.53	0.71
1:F:322:LEU:HD13	1:F:330:MET:HE1	1.73	0.70
1:A:334:HIS:HD2	1:A:336:SER:H	1.40	0.70
1:C:323:SER:O	1:C:327:ILE:HG12	1.91	0.70
1:A:69:GLU:OE2	1:A:71:ARG:HG3	1.92	0.70
1:A:390:GLN:HG3	1:A:419:ASN:HD21	1.57	0.69
1:E:25:ILE:HD13	1:E:275:PHE:CZ	2.26	0.69
1:C:314:SER:HA	1:C:330:MET:HE3	1.73	0.69
2:G:344:GLU:OE1	2:G:414:ARG:NH1	2.24	0.69
1:F:8:GLN:NE2	1:F:414:ARG:HE	1.90	0.69
1:A:26:SER:HB3	1:A:27:PRO:HD2	1.75	0.69
1:E:71:ARG:NH2	1:E:423:ASP:OD2	2.26	0.69
1:E:140:MET:HG2	1:E:144:ALA:HB3	1.75	0.69
1:F:69:GLU:OE2	1:F:71:ARG:HG3	1.93	0.69
2:G:482:LEU:HD12	2:G:482:LEU:C	2.18	0.68
1:D:302:LYS:O	1:D:303:ARG:HD3	1.93	0.68
1:B:104:ARG:HD2	1:C:104:ARG:HD3	1.76	0.68
1:C:434:ARG:H	1:C:437:MET:CE	2.05	0.68
1:A:323:SER:O	1:A:327:ILE:HG12	1.94	0.68
1:H:59:THR:CG2	1:H:65:THR:HG23	2.24	0.68
1:F:444:GLY:O	1:F:447:GLU:HG2	1.92	0.68
1:H:229:HIS:HE1	1:H:462:GLY:O	1.77	0.68
1:E:229:HIS:HE1	1:E:462:GLY:O	1.77	0.67
1:E:242:MET:HE1	1:E:246:MET:HE3	1.77	0.67
1:B:334:HIS:HD2	1:B:336:SER:H	1.41	0.67
1:F:229:HIS:HE1	1:F:462:GLY:O	1.77	0.67
2:G:482:LEU:HD12	2:G:482:LEU:O	1.95	0.67
1:B:242:MET:HE1	1:B:246:MET:HE3	1.78	0.66
1:D:186:MET:HE2	1:D:224:PHE:CD2	2.30	0.66
1:C:331:GLN:HA	1:C:331:GLN:NE2	2.10	0.66
1:A:284:ASN:HD21	1:A:451:GLY:H	1.44	0.66
3:A:600:FAD:H2'	3:A:600:FAD:H9	1.78	0.65
2:G:30:ASN:HD22	2:G:272:GLY:HA2	1.60	0.65
1:C:434:ARG:H	1:C:437:MET:HE2	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:442:LEU:O	2:G:446:ARG:HG3	1.97	0.65
2:G:2:THR:HG23	2:G:19:VAL:C	2.21	0.65
1:D:482:LEU:N	1:D:482:LEU:HD13	2.10	0.65
1:A:179:GLU:HG3	1:A:182:LYS:NZ	2.11	0.64
1:D:242:MET:HE1	1:D:246:MET:HE3	1.80	0.64
1:A:327:ILE:O	1:A:331:GLN:HG2	1.98	0.64
1:E:69:GLU:OE1	3:E:600:FAD:H3B	1.98	0.63
1:E:334:HIS:HD2	1:E:336:SER:H	1.46	0.63
1:F:123:ARG:HH21	4:G:601:EDO:HO2	1.47	0.63
1:A:25:ILE:HA	1:A:26:SER:HB2	1.81	0.63
1:C:215:SER:O	1:C:336:SER:HB2	1.98	0.63
1:F:351:ARG:HE	4:G:601:EDO:H11	1.62	0.62
2:G:26:SER:HA	2:G:27:PRO:C	2.23	0.62
2:G:323:SER:O	2:G:327:ILE:HG12	1.99	0.62
1:B:229:HIS:HE1	1:B:462:GLY:O	1.82	0.62
1:F:322:LEU:CD1	1:F:330:MET:HE1	2.29	0.62
1:A:140:MET:HG2	1:A:144:ALA:HB3	1.82	0.62
2:G:485:LEU:N	2:G:485:LEU:CD1	2.62	0.62
1:H:147:GLU:HA	1:H:150:ARG:HG2	1.81	0.62
1:H:59:THR:HG23	1:H:65:THR:CG2	2.30	0.61
1:A:25:ILE:HA	1:A:26:SER:CB	2.29	0.61
1:B:104:ARG:HD2	1:C:104:ARG:CD	2.27	0.61
1:H:46:GLY:HA2	1:H:69:GLU:OE1	2.01	0.61
1:C:482:LEU:N	1:C:482:LEU:HD13	2.14	0.61
1:D:482:LEU:HD13	1:D:482:LEU:H	1.65	0.61
1:F:390:GLN:HE21	1:F:419:ASN:HD21	1.49	0.60
1:F:22:LEU:O	1:F:259:ARG:HD3	2.01	0.60
1:E:482:LEU:HA	1:E:484:GLU:H	1.67	0.60
1:A:25:ILE:HG23	1:A:26:SER:HB2	1.83	0.60
1:F:433:SER:HA	1:F:437:MET:HE3	1.82	0.60
1:E:442:LEU:O	1:E:446:ARG:HG3	2.02	0.60
1:H:59:THR:HG23	1:H:65:THR:HG23	1.83	0.59
1:B:8:GLN:HE22	1:B:414:ARG:HH21	1.50	0.59
1:E:481:VAL:O	1:E:482:LEU:HD12	2.00	0.59
1:H:319:SER:HA	1:H:320:PRO:C	2.27	0.59
1:B:314:SER:HB3	1:B:330:MET:HG2	1.83	0.59
2:G:30:ASN:ND2	2:G:272:GLY:HA2	2.16	0.59
1:E:326:ARG:O	1:E:330:MET:HG2	2.03	0.59
1:E:284:ASN:HD21	1:E:452:VAL:HG23	1.67	0.59
1:B:46:GLY:HA2	1:B:69:GLU:OE1	2.03	0.58
1:B:92:GLY:HA2	3:B:600:FAD:C4X	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:8:GLN:NE2	1:H:414:ARG:HE	1.98	0.58
1:B:388:HIS:NE2	1:B:390:GLN:NE2	2.52	0.58
2:G:25:ILE:HD13	2:G:74:ILE:HG23	1.84	0.58
1:B:41:ASP:HB2	1:B:64:LYS:O	2.02	0.58
2:G:229:HIS:HE1	2:G:462:GLY:O	1.86	0.58
1:C:481:VAL:O	1:C:481:VAL:CG1	2.52	0.58
1:E:67:LEU:CD2	1:E:262:TRP:HZ3	2.15	0.58
1:C:480:VAL:O	1:C:483:GLU:HB2	2.03	0.58
1:H:59:THR:CG2	1:H:65:THR:CG2	2.82	0.57
1:A:26:SER:HB3	1:A:27:PRO:CD	2.33	0.57
2:G:89:GLU:HG3	2:G:93:THR:HG23	1.87	0.57
1:H:334:HIS:HD2	1:H:336:SER:H	1.53	0.57
1:B:179:GLU:O	1:B:179:GLU:HG2	2.04	0.56
1:E:67:LEU:HD23	1:E:262:TRP:CZ3	2.37	0.56
1:E:430:TRP:HB3	3:E:600:FAD:H1'1	1.86	0.56
2:G:192:ILE:O	2:G:196:ARG:HB3	2.06	0.56
1:A:101:HIS:HE1	1:E:107:THR:OG1	1.88	0.56
1:A:229:HIS:HE1	1:A:462:GLY:O	1.89	0.56
1:E:92:GLY:HA2	3:E:600:FAD:C4X	2.35	0.56
1:D:442:LEU:O	1:D:446:ARG:HG3	2.05	0.56
1:E:29:THR:HG22	1:E:273:TYR:O	2.04	0.56
1:E:482:LEU:HA	1:E:484:GLU:N	2.19	0.56
1:H:309:PRO:HA	1:H:456:ASN:HD21	1.71	0.56
1:E:330:MET:HE1	5:E:2089:HOH:O	2.05	0.56
1:F:2:THR:HA	1:F:20:PRO:HA	1.88	0.56
1:E:8:GLN:HE21	1:E:414:ARG:HE	1.54	0.55
2:G:309:PRO:HA	2:G:456:ASN:HD21	1.70	0.55
2:G:456:ASN:O	2:G:473:GLU:HG3	2.06	0.55
1:H:309:PRO:HA	1:H:456:ASN:HD22	1.69	0.55
1:D:142:HIS:O	1:D:145:GLU:HB3	2.06	0.55
1:E:150[B]:ARG:HH21	1:E:237:THR:HB	1.72	0.55
1:C:397:GLU:OE1	1:C:400:LYS:HE2	2.07	0.55
1:A:179:GLU:HG3	1:A:182:LYS:CE	2.37	0.54
1:D:79:TRP:CZ2	1:D:90:MET:HG3	2.42	0.54
1:H:47:GLY:N	1:H:69:GLU:OE1	2.40	0.54
2:G:133:ASN:OD1	2:G:135:THR:HG22	2.08	0.54
1:H:354:THR:HG22	1:H:367:ILE:HG22	1.89	0.54
1:F:302:LYS:O	1:F:303:ARG:HD3	2.07	0.54
2:G:69:GLU:OE1	3:G:600:FAD:H3B	2.07	0.54
1:H:369:ASP:HB2	1:H:380:VAL:HG12	1.89	0.54
1:D:101:HIS:HE1	1:H:107:THR:OG1	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:390:GLN:NE2	1:F:419:ASN:HD21	2.05	0.54
1:E:242:MET:HE1	1:E:246:MET:HE1	1.89	0.54
1:B:44:VAL:O	1:B:67:LEU:HA	2.08	0.53
1:C:92:GLY:HA2	3:C:600:FAD:C4X	2.38	0.53
1:C:97:TRP:HB3	1:C:103:TRP:CE2	2.44	0.53
1:D:8:GLN:NE2	1:D:414:ARG:HH21	2.06	0.53
1:F:400:LYS:O	1:F:404:GLN:HG3	2.08	0.53
1:C:8:GLN:HE21	1:C:414:ARG:HE	1.57	0.53
2:G:241:CYS:O	2:G:245:LEU:HG	2.09	0.53
1:D:229:HIS:HE1	1:D:462:GLY:O	1.92	0.53
2:G:482:LEU:O	2:G:482:LEU:CD1	2.56	0.53
1:D:90:MET:HE1	1:D:416:VAL:HG12	1.91	0.53
1:F:123:ARG:NH2	4:G:601:EDO:O2	2.32	0.53
1:C:152:ALA:HB1	1:C:207:LEU:HB2	1.91	0.52
1:F:442:LEU:O	1:F:446:ARG:HG3	2.10	0.52
2:G:94:TRP:CG	2:G:246:MET:HA	2.45	0.52
1:A:390:GLN:HG3	1:A:419:ASN:ND2	2.24	0.52
1:B:283:VAL:HG22	1:B:319:SER:HB2	1.91	0.52
1:D:107:THR:OG1	1:H:101:HIS:HE1	1.92	0.52
1:F:90:MET:HE2	1:F:418:HIS:HB2	1.91	0.52
2:G:92:GLY:HA2	3:G:600:FAD:C4X	2.39	0.52
1:A:191:ARG:HG2	1:A:224:PHE:CE1	2.44	0.52
1:E:242:MET:CE	1:E:246:MET:HE3	2.37	0.52
1:F:90:MET:CE	1:F:418:HIS:HB2	2.38	0.52
1:A:2:THR:HA	1:A:20:PRO:HA	1.91	0.52
1:F:43:ILE:HA	1:F:66:LEU:O	2.10	0.52
1:H:89:GLU:O	1:H:342:HIS:HE1	1.92	0.52
1:A:92:GLY:HA2	3:A:600:FAD:C4X	2.39	0.52
1:B:107:THR:OG1	1:C:101:HIS:HE1	1.93	0.52
3:G:600:FAD:H9	3:G:600:FAD:C2'	2.35	0.52
1:E:89:GLU:HG3	1:E:93:THR:HG23	1.91	0.52
1:D:56:ARG:HD3	1:D:264:GLU:OE1	2.10	0.52
1:H:342:HIS:CD2	1:H:378:HIS:NE2	2.67	0.52
1:C:8:GLN:NE2	1:C:414:ARG:HE	2.08	0.51
1:E:362:LYS:HB3	1:E:389:ILE:HB	1.92	0.51
1:C:5:ASP:OD2	1:C:71:ARG:HD3	2.11	0.51
3:B:600:FAD:H9	3:B:600:FAD:C2'	2.36	0.51
1:C:334:HIS:HD2	1:C:336:SER:H	1.58	0.51
1:C:326:ARG:HG2	1:C:445:LEU:HD23	1.93	0.51
1:F:430:TRP:HB3	3:F:600:FAD:H1'1	1.93	0.51
1:E:482:LEU:HD13	1:E:482:LEU:H	1.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:ALA:HB3	1:A:464:ARG:HA	1.93	0.51
1:D:92:GLY:HA2	3:D:600:FAD:C4X	2.41	0.50
1:F:369:ASP:HB2	1:F:380:VAL:HG12	1.93	0.50
1:F:69:GLU:OE1	3:F:600:FAD:H3B	2.10	0.50
2:G:482:LEU:C	2:G:482:LEU:CD1	2.84	0.50
1:H:19:VAL:HB	1:H:20:PRO:HD2	1.92	0.50
1:A:89:GLU:O	1:A:342:HIS:NE2	2.38	0.50
1:B:71:ARG:NH2	1:B:423:ASP:OD2	2.34	0.50
1:H:326:ARG:O	1:H:330:MET:HG2	2.12	0.50
1:D:314:SER:HB3	1:D:330:MET:HG2	1.93	0.50
1:D:326:ARG:O	1:D:330:MET:HB2	2.12	0.50
1:H:442:LEU:O	1:H:446:ARG:HG3	2.12	0.50
1:A:69:GLU:OE1	3:A:600:FAD:H3B	2.11	0.50
1:A:179:GLU:O	1:A:180:PHE:C	2.50	0.50
1:D:92:GLY:HA2	3:D:600:FAD:C5X	2.42	0.50
1:A:133:ASN:HB2	1:A:134:PRO:HD2	1.92	0.49
2:G:309:PRO:HA	2:G:456:ASN:HD22	1.74	0.49
1:D:79:TRP:CE2	1:D:90:MET:HG3	2.48	0.49
1:F:434:ARG:H	1:F:437:MET:CE	2.23	0.49
1:B:101:HIS:HE1	1:C:107:THR:OG1	1.95	0.49
1:F:90:MET:HB3	1:F:90:MET:HE3	1.50	0.49
1:A:287:ASP:OD1	1:A:287:ASP:O	2.30	0.49
1:E:89:GLU:O	1:E:342:HIS:NE2	2.41	0.49
1:F:101:HIS:HD2	1:F:468:ASP:OD2	1.95	0.49
3:C:600:FAD:H2'	3:C:600:FAD:C9	2.37	0.49
1:H:92:GLY:HA2	3:H:600:FAD:C4X	2.43	0.49
1:B:307:THR:HA	1:B:455:ALA:O	2.13	0.49
1:H:19:VAL:HB	1:H:20:PRO:CD	2.43	0.49
1:H:80:SER:HB3	1:H:255:SER:H	1.78	0.48
1:H:430:TRP:HB3	3:H:600:FAD:H1'1	1.95	0.48
1:E:242:MET:CE	1:E:246:MET:CE	2.86	0.48
1:B:481:VAL:O	1:B:484:GLU:HG3	2.13	0.48
1:F:154:HIS:O	1:F:158:ASN:HB2	2.13	0.48
1:D:396:ARG:HA	1:D:396:ARG:HD3	1.70	0.48
1:E:25:ILE:HD11	1:E:74:ILE:HG23	1.96	0.48
1:F:242:MET:CE	1:F:246:MET:HE3	2.37	0.48
2:G:392:ASP:OD1	2:G:422:LYS:NZ	2.39	0.48
1:H:63:PHE:O	1:H:65:THR:HG22	2.14	0.48
1:H:129:GLN:HE21	1:H:131:ARG:HD3	1.79	0.48
1:H:362:LYS:HB3	1:H:389:ILE:HB	1.95	0.48
1:D:220:GLU:CD	1:D:220:GLU:H	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:GLU:O	1:C:342:HIS:NE2	2.43	0.48
2:G:152:ALA:HB1	2:G:207:LEU:HB2	1.95	0.48
2:G:326:ARG:CZ	2:G:454:PHE:CD2	2.96	0.48
1:B:94:TRP:CD2	1:B:246:MET:HA	2.49	0.48
1:C:133:ASN:HB2	1:C:134:PRO:CD	2.44	0.48
1:F:90:MET:HE1	1:F:417:PHE:C	2.39	0.48
2:G:116:SER:OG	2:G:251:LYS:HB2	2.14	0.48
1:H:295:ASP:OD1	1:H:296:GLY:N	2.46	0.48
2:G:337:MET:O	2:G:388:HIS:HE1	1.96	0.48
1:B:284:ASN:HB2	1:B:320:PRO:HD3	1.96	0.47
1:F:107:THR:OG1	2:G:101:HIS:HE1	1.97	0.47
1:A:430:TRP:HB3	3:A:600:FAD:H1'1	1.95	0.47
1:C:89:GLU:HG3	1:C:93:THR:HG23	1.95	0.47
1:A:241:CYS:O	1:A:245:LEU:HG	2.14	0.47
1:C:26:SER:HA	1:C:27:PRO:C	2.39	0.47
1:H:76:GLY:HA2	3:H:600:FAD:O3B	2.15	0.47
1:E:473:GLU:OE1	1:E:476:ARG:NH2	2.36	0.47
1:E:181:ARG:O	1:E:182:LYS:C	2.55	0.47
1:C:116:SER:OG	1:C:251:LYS:HG3	2.15	0.46
1:H:479[A]:ARG:HE	1:H:479[A]:ARG:HB2	1.51	0.46
1:B:430:TRP:HB3	3:B:600:FAD:H1'1	1.98	0.46
1:D:390:GLN:HG3	1:D:419:ASN:HD21	1.80	0.46
5:B:2122:HOH:O	1:F:396:ARG:HD2	2.16	0.46
1:E:480:VAL:HG12	1:E:481:VAL:N	2.27	0.46
1:D:242:MET:HE1	1:D:246:MET:CE	2.44	0.46
1:F:394:ASP:OD1	1:F:396:ARG:HB3	2.15	0.46
1:D:336:SER:HB3	1:D:430:TRP:O	2.16	0.46
1:A:152:ALA:HB1	1:A:207:LEU:HB2	1.97	0.46
1:B:334:HIS:HB2	1:B:432:PHE:O	2.15	0.46
1:D:326:ARG:HG2	1:D:445:LEU:HD23	1.98	0.46
1:E:344:GLU:HB3	1:E:414:ARG:HB3	1.97	0.46
1:F:460:ALA:HB3	1:F:464:ARG:HA	1.97	0.46
1:F:323:SER:HB3	1:F:447:GLU:OE2	2.16	0.46
1:A:147:GLU:O	1:A:148:LEU:C	2.58	0.45
1:C:327:ILE:O	1:C:331:GLN:HG2	2.15	0.45
1:A:390:GLN:HG2	1:A:422:LYS:HD2	1.98	0.45
1:C:434:ARG:H	1:C:437:MET:HE3	1.79	0.45
1:A:396:ARG:HA	1:A:396:ARG:HD3	1.54	0.45
1:B:94:TRP:CG	1:B:246:MET:HA	2.52	0.45
1:B:9:TRP:O	1:B:414:ARG:HA	2.17	0.45
1:C:482:LEU:HA	1:C:484:GLU:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:THR:HA	1:B:297:ARG:O	2.17	0.45
1:B:322:LEU:HD12	1:B:330:MET:HE1	1.98	0.45
1:F:69:GLU:HB3	1:F:275:PHE:CD1	2.51	0.45
1:H:456:ASN:OD1	1:H:457:SER:N	2.50	0.45
1:E:336:SER:HB3	1:E:430:TRP:O	2.17	0.45
1:A:92:GLY:HA2	3:A:600:FAD:C5X	2.47	0.45
1:F:186:MET:HE3	1:F:186:MET:HB2	1.85	0.45
1:C:8:GLN:O	1:C:15:LEU:HA	2.17	0.45
1:B:482:LEU:CD1	1:B:482:LEU:H	2.22	0.45
1:D:259:ARG:HA	1:D:259:ARG:HD3	1.66	0.45
1:D:259:ARG:O	1:D:263:GLU:HG2	2.16	0.45
1:D:480:VAL:O	1:D:483:GLU:HB3	2.17	0.45
1:D:483:GLU:O	1:D:483:GLU:CG	2.66	0.44
1:H:89:GLU:O	1:H:342:HIS:CE1	2.69	0.44
1:B:104:ARG:C	1:B:106:ILE:N	2.70	0.44
1:B:480:VAL:O	1:B:483:GLU:HB2	2.17	0.44
1:C:456:ASN:O	1:C:473:GLU:HG3	2.17	0.44
1:B:400:LYS:O	1:B:404:GLN:HG3	2.17	0.44
1:D:260:ARG:NH2	5:D:2070:HOH:O	2.50	0.44
2:G:179:GLU:O	2:G:179:GLU:CG	2.64	0.44
1:B:326:ARG:HG2	1:B:445:LEU:HD23	2.00	0.44
1:B:186:MET:HB2	1:B:186:MET:HE3	1.88	0.44
1:C:433:SER:CA	1:C:437:MET:HE3	2.42	0.44
1:C:283:VAL:HG13	1:C:319:SER:HB2	2.00	0.44
2:G:484:GLU:O	2:G:485:LEU:HB2	2.18	0.44
1:A:186:MET:HE3	1:A:186:MET:HB2	1.87	0.43
1:F:446:ARG:NH2	1:F:473:GLU:OE2	2.50	0.43
2:G:335:VAL:HG22	2:G:432:PHE:O	2.18	0.43
1:F:8:GLN:NE2	1:F:414:ARG:HH21	2.16	0.43
1:H:479[B]:ARG:CZ	1:H:479[B]:ARG:HB3	2.48	0.43
1:B:326:ARG:O	1:B:330:MET:HE3	2.18	0.43
1:C:99:GLN:HG2	1:C:463:TRP:CE2	2.53	0.43
1:H:465:SER:HA	5:H:2075:HOH:O	2.19	0.43
1:C:86:TYR:HA	1:C:87:PRO:HD3	1.87	0.43
1:D:29:THR:HG22	1:D:274:VAL:HG22	2.00	0.43
1:A:107:THR:OG1	1:E:101:HIS:HE1	2.00	0.43
1:C:67:LEU:C	1:C:67:LEU:HD23	2.43	0.43
2:G:295:ASP:HB3	2:G:297:ARG:H	1.83	0.43
1:H:99:GLN:HG2	1:H:463:TRP:CE2	2.54	0.43
1:H:174:MET:HE3	1:H:180:PHE:HE2	1.84	0.43
1:E:483:GLU:O	1:E:484:GLU:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:ILE:HG12	1:C:66:LEU:HD23	2.00	0.43
1:C:440:GLU:O	1:C:440:GLU:HG2	2.19	0.43
1:D:188:TYR:CD2	1:D:211:ILE:HD12	2.54	0.43
1:D:369:ASP:HB2	1:D:380:VAL:HG12	2.01	0.43
1:E:212:LEU:HD22	1:E:217:GLY:O	2.18	0.43
1:F:92:GLY:HA2	3:F:600:FAD:C4X	2.49	0.43
1:F:101:HIS:N	1:F:468:ASP:OD1	2.50	0.43
2:G:290:ARG:HD3	2:G:298:GLU:OE1	2.19	0.43
1:A:326:ARG:O	1:A:330:MET:HE3	2.18	0.43
1:D:99:GLN:HG2	1:D:463:TRP:CE2	2.54	0.43
3:G:600:FAD:H2'	3:G:600:FAD:C9	2.37	0.43
1:H:344:GLU:OE1	1:H:414:ARG:NH1	2.50	0.43
1:A:25:ILE:CD1	1:A:74:ILE:HG23	2.49	0.42
1:A:259:ARG:HD2	1:A:259:ARG:HA	1.83	0.42
1:C:482:LEU:HA	1:C:484:GLU:H	1.83	0.42
1:B:333:GLY:O	1:B:437:MET:HE1	2.20	0.42
2:G:8:GLN:NE2	2:G:414:ARG:HE	2.17	0.42
1:C:344:GLU:HB3	1:C:414:ARG:HB3	2.01	0.42
1:B:482:LEU:N	1:B:482:LEU:HD13	2.29	0.42
1:B:69:GLU:HG3	1:B:71:ARG:H	1.85	0.42
1:D:456:ASN:O	1:D:473:GLU:HG3	2.20	0.42
1:H:101:HIS:HD2	1:H:468:ASP:OD2	2.03	0.42
1:D:133:ASN:ND2	1:D:136:THR:HG22	2.35	0.42
1:E:77:ARG:HA	1:E:420:TRP:CH2	2.55	0.42
1:F:255:SER:O	1:F:259:ARG:HG2	2.19	0.42
1:B:281:SER:HA	1:B:317:GLN:O	2.19	0.42
1:D:245:LEU:HA	1:D:245:LEU:HD23	1.78	0.42
1:E:46:GLY:O	1:E:51:GLY:HA3	2.19	0.42
1:F:241:CYS:O	1:F:245:LEU:HG	2.19	0.42
1:A:430:TRP:CD1	1:A:430:TRP:C	2.97	0.42
1:C:133:ASN:HB2	1:C:134:PRO:HD2	2.01	0.42
1:D:26:SER:HA	1:D:27:PRO:C	2.45	0.42
1:D:430:TRP:HB3	3:D:600:FAD:H1'1	2.01	0.42
2:G:171:PRO:HG3	2:G:232:ALA:HB1	2.02	0.42
1:H:31:ILE:HG21	1:H:31:ILE:HD13	1.64	0.42
1:B:69:GLU:OE2	1:B:71:ARG:HG3	2.19	0.42
1:E:25:ILE:CD1	1:E:74:ILE:HG23	2.49	0.42
1:E:481:VAL:C	1:E:482:LEU:HD13	2.31	0.42
1:F:101:HIS:CD2	1:F:472:GLU:HB2	2.55	0.42
1:A:43:ILE:HG13	1:A:301:ALA:HB2	2.01	0.41
1:B:25:ILE:HG13	1:B:275:PHE:CZ	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:319:SER:HA	1:E:320:PRO:C	2.43	0.41
1:B:482:LEU:HA	1:B:484:GLU:N	2.35	0.41
1:E:94:TRP:CD2	1:E:246:MET:HA	2.55	0.41
1:E:157:THR:HG21	1:E:231:TRP:CE2	2.55	0.41
1:C:430:TRP:HB3	3:C:600:FAD:H1'1	2.02	0.41
1:D:192:ILE:O	1:D:196:ARG:HB2	2.20	0.41
1:A:330:MET:HB3	1:A:330:MET:HE2	1.76	0.41
1:C:141:THR:HB	1:C:143:GLU:OE1	2.19	0.41
1:D:29:THR:HB	1:D:31:ILE:H	1.86	0.41
1:F:114:ALA:O	1:F:251:LYS:HG2	2.20	0.41
2:G:283:VAL:HG13	2:G:319:SER:HB2	2.03	0.41
2:G:318:PHE:CD2	2:G:322:LEU:HD11	2.55	0.41
1:C:309:PRO:O	1:C:310:LEU:C	2.64	0.41
1:B:179:GLU:O	1:B:179:GLU:CG	2.67	0.41
1:D:292:THR:HA	1:D:297:ARG:O	2.20	0.41
1:E:8:GLN:NE2	1:E:414:ARG:HE	2.16	0.41
1:E:464:ARG:O	1:E:465:SER:CB	2.66	0.41
1:A:395:VAL:HG23	5:A:2102:HOH:O	2.21	0.41
1:C:215:SER:HB2	1:C:432:PHE:CD1	2.55	0.41
1:D:150:ARG:NH2	5:D:2039:HOH:O	2.45	0.41
1:A:25:ILE:CA	1:A:26:SER:HB2	2.49	0.41
1:B:152:ALA:HB1	1:B:207:LEU:HB2	2.03	0.41
1:D:154:HIS:O	1:D:158:ASN:HB2	2.20	0.41
2:G:43:ILE:HB	2:G:304:VAL:HG22	2.02	0.41
2:G:63:PHE:HE2	2:G:482:LEU:HD22	1.85	0.41
1:H:152:ALA:HB1	1:H:207:LEU:HB2	2.01	0.41
1:A:141:THR:HB	1:A:143:GLU:OE1	2.21	0.41
1:D:90:MET:HE1	1:D:416:VAL:CG1	2.50	0.41
1:E:342:HIS:O	1:E:415:LEU:HA	2.20	0.41
1:E:367:ILE:HG13	1:E:380:VAL:HG12	2.03	0.41
2:G:23:GLY:O	2:G:25:ILE:HD12	2.20	0.41
2:G:86:TYR:HA	2:G:87:PRO:HD3	1.99	0.41
2:G:292:THR:HG23	2:G:298:GLU:HG2	2.03	0.41
1:H:476:ARG:O	1:H:480:VAL:HG23	2.21	0.41
1:C:40:TRP:O	1:C:301:ALA:HA	2.21	0.41
1:C:76:GLY:HA2	3:C:600:FAD:O3B	2.21	0.41
1:C:331:GLN:NE2	1:C:331:GLN:CA	2.76	0.41
1:D:9:TRP:O	1:D:414:ARG:HA	2.20	0.41
1:D:89:GLU:O	1:D:342:HIS:NE2	2.50	0.41
1:A:90:MET:HE3	1:A:418:HIS:HB2	2.02	0.40
1:A:179:GLU:HG3	1:A:182:LYS:HZ1	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:482:LEU:H	1:B:482:LEU:HD13	1.86	0.40
1:E:152:ALA:HB1	1:E:207:LEU:HB2	2.03	0.40
1:F:326:ARG:HG2	1:F:445:LEU:HD23	2.02	0.40
2:G:69:GLU:OE2	2:G:71:ARG:HG3	2.21	0.40
1:H:59:THR:HG22	1:H:65:THR:CG2	2.51	0.40
1:B:89:GLU:HA	1:B:89:GLU:OE1	2.22	0.40
1:B:101:HIS:HD2	1:B:468:ASP:OD2	2.05	0.40
1:C:77:ARG:HA	1:C:420:TRP:CH2	2.56	0.40
1:D:25:ILE:HG13	1:D:275:PHE:CZ	2.57	0.40
1:D:446:ARG:CZ	1:D:461:LEU:HD13	2.51	0.40
1:C:22:LEU:O	1:C:259:ARG:HD3	2.22	0.40
1:C:334:HIS:HA	1:C:437:MET:HE1	2.04	0.40
1:E:481:VAL:HG12	1:E:482:LEU:CD1	2.52	0.40
2:G:483:GLU:C	2:G:484:GLU:O	2.60	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	475/495 (96%)	454 (96%)	20 (4%)	1 (0%)	43	54
1	B	473/495 (96%)	457 (97%)	16 (3%)	0	100	100
1	C	474/495 (96%)	453 (96%)	19 (4%)	2 (0%)	30	37
1	D	474/495 (96%)	458 (97%)	16 (3%)	0	100	100
1	E	474/495 (96%)	451 (95%)	22 (5%)	1 (0%)	43	54
1	F	475/495 (96%)	456 (96%)	19 (4%)	0	100	100
1	H	475/495 (96%)	460 (97%)	15 (3%)	0	100	100
2	G	475/495 (96%)	449 (94%)	26 (6%)	0	100	100
All	All	3795/3960 (96%)	3638 (96%)	153 (4%)	4 (0%)	48	61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	SER
1	E	481	VAL
1	C	481	VAL
1	C	179	GLU

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

15 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	FAD	E	600	-	58,58,58	1.59	12 (20%)	85,89,89	2.36	29 (34%)
3	FAD	D	600	-	58,58,58	1.45	9 (15%)	85,89,89	2.29	24 (28%)
4	EDO	A	601	-	3,3,3	0.41	0	2,2,2	0.73	0
3	FAD	B	600	-	58,58,58	1.53	8 (13%)	85,89,89	2.68	32 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FAD	G	600	-	58,58,58	1.62	11 (18%)	85,89,89	2.36	26 (30%)
3	FAD	C	600	-	58,58,58	1.51	8 (13%)	85,89,89	2.20	26 (30%)
3	FAD	H	600	-	58,58,58	1.62	11 (18%)	85,89,89	2.25	31 (36%)
4	EDO	F	601	-	3,3,3	0.38	0	2,2,2	0.68	0
3	FAD	A	600	-	58,58,58	1.52	11 (18%)	85,89,89	2.41	26 (30%)
3	FAD	F	600	-	58,58,58	1.69	10 (17%)	85,89,89	2.20	28 (32%)
4	EDO	D	601	-	3,3,3	0.40	0	2,2,2	0.27	0
4	EDO	G	601	-	3,3,3	0.41	0	2,2,2	0.80	0
4	EDO	G	602	-	3,3,3	0.46	0	2,2,2	0.42	0
4	EDO	C	601	-	3,3,3	0.38	0	2,2,2	0.67	0
4	EDO	C	602	-	3,3,3	0.44	0	2,2,2	0.43	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	E	600	-	3/3/9/9	13/34/50/50	0/6/6/6
3	FAD	D	600	-	3/3/9/9	10/34/50/50	0/6/6/6
4	EDO	A	601	-	-	1/1/1/1	-
3	FAD	B	600	-	3/3/9/9	9/34/50/50	0/6/6/6
3	FAD	G	600	-	3/3/9/9	17/34/50/50	0/6/6/6
3	FAD	C	600	-	3/3/9/9	9/34/50/50	0/6/6/6
3	FAD	H	600	-	3/3/9/9	9/34/50/50	0/6/6/6
4	EDO	F	601	-	-	1/1/1/1	-
3	FAD	A	600	-	3/3/9/9	10/34/50/50	0/6/6/6
3	FAD	F	600	-	3/3/9/9	9/34/50/50	0/6/6/6
4	EDO	D	601	-	-	1/1/1/1	-
4	EDO	G	601	-	-	1/1/1/1	-
4	EDO	G	602	-	-	1/1/1/1	-
4	EDO	C	601	-	-	1/1/1/1	-
4	EDO	C	602	-	-	1/1/1/1	-

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	600	FAD	C4X-N5	6.19	1.44	1.30
3	F	600	FAD	C4X-N5	6.07	1.43	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	600	FAD	C4X-N5	5.87	1.43	1.30
3	C	600	FAD	C4X-N5	5.78	1.43	1.30
3	G	600	FAD	P-O3P	5.75	1.65	1.59
3	D	600	FAD	C4X-N5	5.55	1.42	1.30
3	G	600	FAD	C4X-N5	5.34	1.42	1.30
3	F	600	FAD	P-O3P	5.10	1.65	1.59
3	H	600	FAD	C4X-N5	5.04	1.41	1.30
3	A	600	FAD	P-O3P	4.95	1.64	1.59
3	H	600	FAD	PA-O3P	4.74	1.64	1.59
3	C	600	FAD	P-O3P	4.71	1.64	1.59
3	A	600	FAD	C4X-N5	4.60	1.40	1.30
3	H	600	FAD	P-O3P	4.05	1.63	1.59
3	E	600	FAD	O4B-C1B	3.99	1.51	1.42
3	H	600	FAD	O4B-C1B	3.78	1.50	1.42
3	F	600	FAD	PA-O3P	3.63	1.63	1.59
3	B	600	FAD	O4B-C4B	3.40	1.52	1.45
3	D	600	FAD	C10-N1	3.28	1.39	1.33
3	H	600	FAD	C10-N1	3.24	1.39	1.33
3	F	600	FAD	O4B-C1B	3.22	1.49	1.42
3	A	600	FAD	C10-N1	3.21	1.39	1.33
3	E	600	FAD	PA-O3P	3.12	1.62	1.59
3	B	600	FAD	C10-N1	3.06	1.39	1.33
3	F	600	FAD	C4A-N9A	-3.05	1.31	1.37
3	B	600	FAD	C5A-N7A	-2.98	1.33	1.39
3	F	600	FAD	C10-N1	2.93	1.39	1.33
3	E	600	FAD	P-O1P	2.92	1.60	1.50
3	D	600	FAD	C5A-N7A	-2.91	1.33	1.39
3	G	600	FAD	O4B-C1B	2.90	1.48	1.42
3	B	600	FAD	O4B-C1B	2.90	1.48	1.42
3	E	600	FAD	P-O3P	2.83	1.62	1.59
3	G	600	FAD	C10-N1	2.80	1.38	1.33
3	G	600	FAD	C5A-N7A	-2.79	1.34	1.39
3	C	600	FAD	C4A-N9A	-2.78	1.31	1.37
3	E	600	FAD	C5A-N7A	-2.78	1.34	1.39
3	C	600	FAD	O4B-C1B	2.73	1.48	1.42
3	F	600	FAD	C5A-N7A	-2.71	1.34	1.39
3	D	600	FAD	P-O1P	2.71	1.60	1.50
3	G	600	FAD	C8A-N9A	-2.69	1.33	1.37
3	C	600	FAD	C5A-N7A	-2.67	1.34	1.39
3	C	600	FAD	C10-N1	2.66	1.38	1.33
3	B	600	FAD	P-O1P	2.64	1.60	1.50
3	D	600	FAD	O4B-C4B	2.64	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	600	FAD	P-O1P	2.60	1.59	1.50
3	H	600	FAD	C5A-N7A	-2.54	1.34	1.39
3	A	600	FAD	P-O1P	2.53	1.59	1.50
3	G	600	FAD	PA-O3P	2.52	1.62	1.59
3	F	600	FAD	C8M-C8	2.45	1.55	1.51
3	A	600	FAD	C8A-N9A	-2.45	1.33	1.37
3	H	600	FAD	P-O1P	2.42	1.59	1.50
3	D	600	FAD	C4A-N9A	-2.41	1.32	1.37
3	B	600	FAD	C8A-N9A	-2.39	1.33	1.37
3	H	600	FAD	C8A-N9A	-2.37	1.33	1.37
3	D	600	FAD	PA-O3P	2.35	1.62	1.59
3	A	600	FAD	C7M-C7	2.33	1.55	1.51
3	F	600	FAD	O4B-C4B	2.31	1.50	1.45
3	A	600	FAD	O4B-C1B	2.26	1.47	1.42
3	E	600	FAD	C10-N1	2.26	1.37	1.33
3	H	600	FAD	C4A-N9A	-2.25	1.33	1.37
3	E	600	FAD	C2'-C3'	2.24	1.57	1.53
3	E	600	FAD	O5B-C5B	-2.23	1.36	1.44
3	D	600	FAD	O4B-C1B	2.23	1.47	1.42
3	D	600	FAD	C8A-N9A	-2.22	1.33	1.37
3	A	600	FAD	PA-O3P	2.20	1.61	1.59
3	C	600	FAD	PA-O3P	2.19	1.61	1.59
3	A	600	FAD	C5A-N7A	-2.18	1.35	1.39
3	G	600	FAD	O5B-C5B	-2.17	1.36	1.44
3	E	600	FAD	C8A-N9A	-2.16	1.33	1.37
3	H	600	FAD	C8M-C8	2.13	1.55	1.51
3	C	600	FAD	C8A-N9A	-2.10	1.34	1.37
3	A	600	FAD	C4A-N9A	-2.10	1.33	1.37
3	A	600	FAD	O4B-C4B	2.08	1.49	1.45
3	E	600	FAD	C8M-C8	2.08	1.54	1.51
3	E	600	FAD	C4A-N9A	-2.06	1.33	1.37
3	G	600	FAD	C4A-N9A	-2.04	1.33	1.37
3	H	600	FAD	C2'-C3'	2.03	1.57	1.53
3	G	600	FAD	O4B-C4B	2.03	1.49	1.45
3	B	600	FAD	C4A-N9A	-2.02	1.33	1.37
3	G	600	FAD	C8M-C8	2.01	1.54	1.51

All (222) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	FAD	C2B-C3B-C4B	-8.69	85.82	102.61
3	B	600	FAD	C2B-C3B-C4B	-8.43	86.32	102.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	600	FAD	C3B-C2B-C1B	-8.06	86.22	101.46
3	D	600	FAD	C2B-C3B-C4B	-8.02	87.10	102.61
3	B	600	FAD	C3B-C2B-C1B	-7.74	86.82	101.46
3	C	600	FAD	C2B-C3B-C4B	-7.63	87.86	102.61
3	F	600	FAD	C2B-C3B-C4B	-7.48	88.15	102.61
3	A	600	FAD	C3B-C2B-C1B	-7.42	87.44	101.46
3	E	600	FAD	C3B-C2B-C1B	-7.40	87.47	101.46
3	H	600	FAD	C2B-C3B-C4B	-7.26	88.58	102.61
3	G	600	FAD	C2B-C3B-C4B	-7.13	88.83	102.61
3	E	600	FAD	C2B-C3B-C4B	-7.00	89.09	102.61
3	C	600	FAD	C3B-C2B-C1B	-6.85	88.51	101.46
3	H	600	FAD	C3B-C2B-C1B	-6.70	88.78	101.46
3	A	600	FAD	O4B-C4B-C3B	-6.41	92.44	105.15
3	D	600	FAD	C3B-C2B-C1B	-6.34	89.46	101.46
3	B	600	FAD	O4B-C4B-C3B	-6.31	92.62	105.15
3	F	600	FAD	C3B-C2B-C1B	-6.29	89.57	101.46
3	C	600	FAD	O4B-C4B-C3B	-6.10	93.04	105.15
3	G	600	FAD	O4B-C4B-C5B	5.59	127.24	109.33
3	D	600	FAD	O4B-C4B-C3B	-5.58	94.07	105.15
3	B	600	FAD	O2A-PA-O5B	-5.53	82.52	107.57
3	B	600	FAD	O2A-PA-O3P	5.48	122.08	107.27
3	A	600	FAD	C5A-C4A-N3A	-5.22	119.53	126.72
3	F	600	FAD	N3A-C2A-N1A	-5.16	120.77	128.58
3	G	600	FAD	N3A-C2A-N1A	-5.10	120.87	128.58
3	D	600	FAD	N3A-C2A-N1A	-5.07	120.90	128.58
3	F	600	FAD	O4B-C4B-C3B	-4.91	95.40	105.15
3	H	600	FAD	N3A-C2A-N1A	-4.88	121.20	128.58
3	B	600	FAD	C5A-C4A-N3A	-4.87	120.02	126.72
3	G	600	FAD	O4B-C4B-C3B	-4.83	95.56	105.15
3	B	600	FAD	C5B-C4B-C3B	4.83	132.59	115.21
3	G	600	FAD	C5A-C4A-N3A	-4.82	120.09	126.72
3	B	600	FAD	N3A-C2A-N1A	-4.77	121.36	128.58
3	H	600	FAD	O4B-C4B-C3B	-4.66	95.90	105.15
3	E	600	FAD	C5A-C4A-N3A	-4.63	120.34	126.72
3	E	600	FAD	C4-C4X-N5	4.59	124.55	118.21
3	C	600	FAD	N3A-C2A-N1A	-4.50	121.78	128.58
3	D	600	FAD	C5A-C4A-N3A	-4.48	120.55	126.72
3	E	600	FAD	N3A-C2A-N1A	-4.47	121.81	128.58
3	E	600	FAD	O4B-C1B-N9A	4.46	116.65	108.09
3	H	600	FAD	C5A-C4A-N3A	-4.43	120.62	126.72
3	A	600	FAD	N9A-C8A-N7A	-4.40	107.70	113.94
3	A	600	FAD	C5B-C4B-C3B	4.38	131.00	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	600	FAD	O4B-C4B-C3B	-4.30	96.62	105.15
3	C	600	FAD	C5A-C4A-N3A	-4.23	120.90	126.72
3	G	600	FAD	C4B-O4B-C1B	-4.22	100.15	109.47
3	B	600	FAD	C9A-C5X-N5	-4.19	118.01	122.45
3	F	600	FAD	C5A-C4A-N3A	-4.07	121.11	126.72
3	B	600	FAD	N3A-C4A-N9A	4.06	134.07	127.17
3	B	600	FAD	O3B-C3B-C4B	4.05	122.72	111.08
3	A	600	FAD	N3A-C2A-N1A	-4.03	122.47	128.58
3	E	600	FAD	N9A-C8A-N7A	-4.00	108.26	113.94
3	D	600	FAD	N9A-C8A-N7A	-3.99	108.28	113.94
3	B	600	FAD	N9A-C8A-N7A	-3.99	108.28	113.94
3	B	600	FAD	C4B-O4B-C1B	-3.98	100.67	109.47
3	B	600	FAD	C5'-C4'-C3'	-3.98	104.71	112.22
3	G	600	FAD	C4-C4X-N5	3.98	123.70	118.21
3	H	600	FAD	C5B-C4B-C3B	3.94	129.39	115.21
3	F	600	FAD	C4-C4X-N5	3.92	123.62	118.21
3	E	600	FAD	C4'-C3'-C2'	3.91	120.08	113.57
3	B	600	FAD	C4'-C3'-C2'	3.90	120.06	113.57
3	E	600	FAD	O4B-C4B-C5B	3.89	121.80	109.33
3	E	600	FAD	C4B-O4B-C1B	-3.88	100.90	109.47
3	G	600	FAD	O4B-C1B-N9A	3.87	115.52	108.09
3	A	600	FAD	C4A-N9A-C8A	3.83	109.76	105.74
3	B	600	FAD	O5B-PA-O1A	-3.83	93.76	108.94
3	H	600	FAD	C4-N3-C2	-3.82	118.85	125.64
3	H	600	FAD	C4'-C3'-C2'	3.80	119.89	113.57
3	A	600	FAD	N3A-C4A-N9A	3.78	133.60	127.17
3	G	600	FAD	N3A-C4A-N9A	3.77	133.59	127.17
3	D	600	FAD	C5B-C4B-C3B	3.74	128.68	115.21
3	F	600	FAD	C4B-O4B-C1B	-3.73	101.22	109.47
3	G	600	FAD	N9A-C8A-N7A	-3.73	108.64	113.94
3	B	600	FAD	C4-N3-C2	-3.69	119.08	125.64
3	F	600	FAD	N9A-C8A-N7A	-3.67	108.72	113.94
3	B	600	FAD	C4A-N9A-C8A	3.65	109.57	105.74
3	C	600	FAD	C9A-C5X-N5	-3.65	118.58	122.45
3	H	600	FAD	C4B-O4B-C1B	-3.63	101.45	109.47
3	D	600	FAD	C5'-C4'-C3'	-3.63	105.37	112.22
3	A	600	FAD	C5'-C4'-C3'	-3.61	105.40	112.22
3	F	600	FAD	C4A-N9A-C8A	3.61	109.53	105.74
3	E	600	FAD	C4X-C10-N10	3.58	121.60	116.48
3	D	600	FAD	C9A-C5X-N5	-3.54	118.70	122.45
3	D	600	FAD	C4B-O4B-C1B	-3.53	101.68	109.47
3	D	600	FAD	C2A-N3A-C4A	3.52	120.43	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	600	FAD	C4-C4X-N5	3.52	123.07	118.21
3	A	600	FAD	C5A-N7A-C8A	3.49	108.94	103.45
3	G	600	FAD	C4A-N9A-C8A	3.49	109.40	105.74
3	G	600	FAD	C2A-N3A-C4A	3.48	120.33	111.83
3	A	600	FAD	C2A-N3A-C4A	3.47	120.31	111.83
3	B	600	FAD	O3P-P-O1P	-3.47	100.26	110.70
3	B	600	FAD	C2A-N3A-C4A	3.47	120.30	111.83
3	D	600	FAD	C4A-N9A-C8A	3.47	109.38	105.74
3	A	600	FAD	C4B-O4B-C1B	-3.46	101.83	109.47
3	E	600	FAD	N3A-C4A-N9A	3.46	133.05	127.17
3	H	600	FAD	N9A-C8A-N7A	-3.46	109.03	113.94
3	E	600	FAD	O2'-C2'-C3'	3.46	117.34	109.25
3	H	600	FAD	C2B-C1B-N9A	3.44	121.86	113.30
3	D	600	FAD	N3A-C4A-N9A	3.44	133.01	127.17
3	D	600	FAD	C4-C4X-N5	3.43	122.95	118.21
3	F	600	FAD	C5B-C4B-C3B	3.42	127.54	115.21
3	A	600	FAD	C4-C4X-N5	3.41	122.92	118.21
3	E	600	FAD	C10-C4X-N5	-3.40	117.88	124.81
3	C	600	FAD	N9A-C8A-N7A	-3.39	109.13	113.94
3	E	600	FAD	C5A-N7A-C8A	3.39	108.78	103.45
3	H	600	FAD	N3A-C4A-N9A	3.38	132.92	127.17
3	C	600	FAD	C4B-O4B-C1B	-3.38	102.01	109.47
3	F	600	FAD	C2A-N3A-C4A	3.36	120.05	111.83
3	A	600	FAD	C4A-C5A-N7A	-3.36	106.74	110.58
3	H	600	FAD	C2A-N3A-C4A	3.36	120.04	111.83
3	E	600	FAD	C4A-N9A-C8A	3.33	109.23	105.74
3	C	600	FAD	C4A-N9A-C8A	3.30	109.20	105.74
3	B	600	FAD	C5A-N7A-C8A	3.28	108.60	103.45
3	E	600	FAD	C2A-N3A-C4A	3.26	119.78	111.83
3	H	600	FAD	C4A-N9A-C8A	3.25	109.16	105.74
3	D	600	FAD	C4-N3-C2	-3.25	119.86	125.64
3	G	600	FAD	C5A-N7A-C8A	3.25	108.55	103.45
3	F	600	FAD	C10-C4X-N5	-3.24	118.19	124.81
3	F	600	FAD	N3A-C4A-N9A	3.19	132.59	127.17
3	A	600	FAD	O3B-C3B-C4B	3.19	120.23	111.08
3	G	600	FAD	C10-C4X-N5	-3.18	118.31	124.81
3	C	600	FAD	C2A-N3A-C4A	3.18	119.59	111.83
3	H	600	FAD	C5'-C4'-C3'	-3.18	106.22	112.22
3	F	600	FAD	C5'-C4'-C3'	-3.17	106.23	112.22
3	C	600	FAD	C5'-C4'-C3'	-3.17	106.24	112.22
3	C	600	FAD	N3A-C4A-N9A	3.17	132.55	127.17
3	G	600	FAD	C4'-C3'-C2'	3.15	118.81	113.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	600	FAD	C9A-C5X-N5	-3.12	119.14	122.45
3	G	600	FAD	C5'-C4'-C3'	-3.12	106.33	112.22
3	A	600	FAD	C9A-C5X-N5	-3.09	119.17	122.45
3	C	600	FAD	C5B-C4B-C3B	3.08	126.29	115.21
3	G	600	FAD	C4A-C5A-N7A	-3.06	107.08	110.58
3	A	600	FAD	O4B-C1B-C2B	-3.06	100.07	106.62
3	B	600	FAD	C4X-C4-N3	3.05	121.02	113.25
3	C	600	FAD	C10-C4X-N5	-3.05	118.59	124.81
3	D	600	FAD	C4X-C4-N3	3.03	120.98	113.25
3	E	600	FAD	C4A-C5A-N7A	-3.03	107.12	110.58
3	D	600	FAD	C4'-C3'-C2'	3.02	118.60	113.57
3	D	600	FAD	C5A-N7A-C8A	3.01	108.18	103.45
3	E	600	FAD	C4-N3-C2	-3.00	120.31	125.64
3	H	600	FAD	C4X-C4-N3	3.00	120.88	113.25
3	H	600	FAD	C10-C4X-N5	-2.99	118.70	124.81
3	A	600	FAD	C10-C4X-N5	-2.98	118.72	124.81
3	B	600	FAD	C4-C4X-N5	2.97	122.32	118.21
3	C	600	FAD	C4-N3-C2	-2.97	120.37	125.64
3	A	600	FAD	C4X-C10-N10	2.95	120.70	116.48
3	D	600	FAD	C10-C4X-N5	-2.90	118.89	124.81
3	F	600	FAD	C4'-C3'-C2'	2.89	118.38	113.57
3	G	600	FAD	C4X-C10-N10	2.82	120.52	116.48
3	G	600	FAD	C5B-C4B-C3B	-2.82	105.06	115.21
3	E	600	FAD	C5'-C4'-C3'	-2.82	106.90	112.22
3	H	600	FAD	O3B-C3B-C4B	2.80	119.11	111.08
3	E	600	FAD	C1'-N10-C9A	2.76	126.00	120.63
3	C	600	FAD	C4X-C4-N3	2.76	120.28	113.25
3	G	600	FAD	C9A-C5X-N5	-2.76	119.53	122.45
3	C	600	FAD	O3B-C3B-C4B	2.74	118.95	111.08
3	F	600	FAD	C4X-C10-N10	2.72	120.38	116.48
3	H	600	FAD	O2'-C2'-C3'	2.71	115.60	109.25
3	B	600	FAD	O4B-C1B-N9A	2.71	113.29	108.09
3	F	600	FAD	C9A-C5X-N5	-2.70	119.59	122.45
3	A	600	FAD	C4'-C3'-C2'	2.69	118.05	113.57
3	H	600	FAD	C5A-N7A-C8A	2.68	107.66	103.45
3	D	600	FAD	O3B-C3B-C4B	2.66	118.72	111.08
3	H	600	FAD	C9A-C5X-N5	-2.64	119.66	122.45
3	G	600	FAD	C4-N3-C2	-2.62	121.00	125.64
3	H	600	FAD	C4-C4X-N5	2.60	121.80	118.21
3	B	600	FAD	C4A-C5A-N7A	-2.58	107.63	110.58
3	B	600	FAD	O4B-C1B-C2B	-2.58	101.11	106.62
3	E	600	FAD	O2-C2-N1	-2.57	117.52	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	600	FAD	C4-N3-C2	-2.57	121.08	125.64
3	D	600	FAD	O4B-C1B-C2B	-2.57	101.12	106.62
3	B	600	FAD	C10-C4X-N5	-2.56	119.59	124.81
3	E	600	FAD	O4B-C1B-C2B	-2.53	101.20	106.62
3	H	600	FAD	C4A-C5A-N7A	-2.53	107.69	110.58
3	E	600	FAD	C4X-C4-N3	2.52	119.67	113.25
3	C	600	FAD	C4X-C10-N10	2.50	120.06	116.48
3	D	600	FAD	C4A-C5A-N7A	-2.50	107.73	110.58
3	B	600	FAD	O4-C4-C4X	-2.50	119.94	126.53
3	A	600	FAD	C4X-C4-N3	2.50	119.61	113.25
3	G	600	FAD	C4X-C4-N3	2.49	119.59	113.25
3	F	600	FAD	O4B-C1B-N9A	2.45	112.80	108.09
3	H	600	FAD	O4-C4-C4X	-2.44	120.10	126.53
3	B	600	FAD	C5X-C9A-N10	2.43	120.17	117.97
3	C	600	FAD	O4B-C1B-C2B	-2.42	101.44	106.62
3	C	600	FAD	C5A-N7A-C8A	2.42	107.25	103.45
3	H	600	FAD	O2A-PA-O3P	-2.40	100.78	107.27
3	C	600	FAD	C4A-C5A-N7A	-2.36	107.88	110.58
3	D	600	FAD	C4X-C10-N10	2.35	119.84	116.48
3	A	600	FAD	C4-N3-C2	-2.34	121.49	125.64
3	A	600	FAD	O2P-P-O3P	2.32	113.55	107.27
3	E	600	FAD	O2-C2-N3	2.32	123.04	118.58
3	F	600	FAD	C4X-C4-N3	2.32	119.15	113.25
3	G	600	FAD	O4B-C1B-C2B	-2.32	101.66	106.62
3	F	600	FAD	C5A-N7A-C8A	2.28	107.04	103.45
3	H	600	FAD	C4X-C10-N10	2.28	119.75	116.48
3	E	600	FAD	O5B-PA-O1A	2.24	117.82	108.94
3	H	600	FAD	O5'-P-O1P	-2.24	100.05	108.94
3	G	600	FAD	O2'-C2'-C3'	2.22	114.45	109.25
3	C	600	FAD	C6-C5X-C9A	2.22	122.10	119.05
3	A	600	FAD	C1'-N10-C9A	2.22	124.95	120.63
3	B	600	FAD	O2'-C2'-C3'	2.20	114.40	109.25
3	H	600	FAD	O4B-C1B-C2B	-2.17	101.98	106.62
3	D	600	FAD	O4-C4-C4X	-2.14	120.89	126.53
3	A	600	FAD	O4B-C1B-N9A	2.13	112.17	108.09
3	F	600	FAD	O4B-C1B-C2B	-2.12	102.08	106.62
3	C	600	FAD	C4A-N9A-C1B	-2.12	121.68	126.63
3	F	600	FAD	C4A-N9A-C1B	-2.10	121.73	126.63
3	F	600	FAD	O3B-C3B-C4B	2.10	117.10	111.08
3	F	600	FAD	O2P-P-O3P	2.10	112.94	107.27
3	C	600	FAD	O4B-C4B-C5B	2.06	115.94	109.33
3	F	600	FAD	O2-C2-N1	-2.05	118.39	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	600	FAD	O4'-C4'-C3'	2.05	114.05	109.25
3	C	600	FAD	C4'-C3'-C2'	2.04	116.97	113.57
3	B	600	FAD	O2A-PA-O1A	2.04	121.95	112.44
3	F	600	FAD	O4B-C4B-C5B	2.04	115.87	109.33
3	E	600	FAD	C1'-C2'-C3'	2.03	115.17	109.66
3	G	600	FAD	C1'-N10-C9A	2.03	124.58	120.63
3	H	600	FAD	O2A-PA-O1A	2.03	121.88	112.44
3	F	600	FAD	C1'-N10-C9A	2.03	124.58	120.63
3	H	600	FAD	O2-C2-N1	-2.03	118.43	121.80
3	B	600	FAD	O2P-P-O3P	2.01	112.70	107.27

All (24) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	600	FAD	C4B
3	A	600	FAD	C2'
3	A	600	FAD	C3B
3	B	600	FAD	C4B
3	B	600	FAD	C2'
3	B	600	FAD	C3B
3	C	600	FAD	C4B
3	C	600	FAD	C2'
3	C	600	FAD	C3B
3	D	600	FAD	C4B
3	D	600	FAD	C2'
3	D	600	FAD	C3B
3	E	600	FAD	C4B
3	E	600	FAD	C2'
3	E	600	FAD	C3B
3	F	600	FAD	C4B
3	F	600	FAD	C2'
3	F	600	FAD	C3B
3	G	600	FAD	C4B
3	G	600	FAD	C2'
3	G	600	FAD	C3B
3	H	600	FAD	C4B
3	H	600	FAD	C2'
3	H	600	FAD	C3B

All (93) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	600	FAD	C1'-C2'-C3'-O3'
3	A	600	FAD	C1'-C2'-C3'-C4'
3	A	600	FAD	O2'-C2'-C3'-O3'
3	A	600	FAD	O2'-C2'-C3'-C4'
3	A	600	FAD	PA-O3P-P-O5'
3	B	600	FAD	C1'-C2'-C3'-O3'
3	B	600	FAD	C1'-C2'-C3'-C4'
3	B	600	FAD	O2'-C2'-C3'-O3'
3	B	600	FAD	O2'-C2'-C3'-C4'
3	C	600	FAD	C1'-C2'-C3'-O3'
3	C	600	FAD	C1'-C2'-C3'-C4'
3	C	600	FAD	O2'-C2'-C3'-O3'
3	C	600	FAD	O2'-C2'-C3'-C4'
3	C	600	FAD	PA-O3P-P-O5'
3	D	600	FAD	C1'-C2'-C3'-O3'
3	D	600	FAD	C1'-C2'-C3'-C4'
3	D	600	FAD	O2'-C2'-C3'-O3'
3	D	600	FAD	O2'-C2'-C3'-C4'
3	E	600	FAD	C5B-O5B-PA-O1A
3	E	600	FAD	C5B-O5B-PA-O2A
3	E	600	FAD	C5B-O5B-PA-O3P
3	E	600	FAD	C1'-C2'-C3'-O3'
3	E	600	FAD	C1'-C2'-C3'-C4'
3	E	600	FAD	O2'-C2'-C3'-O3'
3	E	600	FAD	O2'-C2'-C3'-C4'
3	F	600	FAD	C1'-C2'-C3'-O3'
3	F	600	FAD	C1'-C2'-C3'-C4'
3	F	600	FAD	O2'-C2'-C3'-O3'
3	F	600	FAD	O2'-C2'-C3'-C4'
3	G	600	FAD	C5B-O5B-PA-O2A
3	G	600	FAD	C5B-O5B-PA-O3P
3	G	600	FAD	C2'-C1'-N10-C10
3	G	600	FAD	C1'-C2'-C3'-O3'
3	G	600	FAD	C1'-C2'-C3'-C4'
3	G	600	FAD	O2'-C2'-C3'-O3'
3	G	600	FAD	O2'-C2'-C3'-C4'
3	G	600	FAD	C5'-O5'-P-O2P
3	G	600	FAD	C5'-O5'-P-O3P
3	H	600	FAD	C1'-C2'-C3'-O3'
3	H	600	FAD	C1'-C2'-C3'-C4'
3	H	600	FAD	O2'-C2'-C3'-O3'
3	H	600	FAD	O2'-C2'-C3'-C4'
3	H	600	FAD	PA-O3P-P-O5'

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Mol	Chain	Res	Type	Atoms
3	E	600	FAD	C3B-C4B-C5B-O5B
3	A	600	FAD	C2'-C3'-C4'-C5'
3	E	600	FAD	C2'-C3'-C4'-O4'
3	G	600	FAD	C3B-C4B-C5B-O5B
3	B	600	FAD	C2'-C3'-C4'-C5'
3	D	600	FAD	C2'-C3'-C4'-C5'
3	E	600	FAD	C2'-C3'-C4'-C5'
3	F	600	FAD	C2'-C3'-C4'-C5'
3	G	600	FAD	C2'-C3'-C4'-C5'
3	H	600	FAD	C2'-C3'-C4'-C5'
3	A	600	FAD	C2'-C3'-C4'-O4'
3	F	600	FAD	C2'-C3'-C4'-O4'
3	H	600	FAD	C2'-C3'-C4'-O4'
3	B	600	FAD	C2'-C3'-C4'-O4'
3	G	600	FAD	O4B-C4B-C5B-O5B
3	D	600	FAD	C2'-C3'-C4'-O4'
3	G	600	FAD	C2'-C3'-C4'-O4'
3	E	600	FAD	O4B-C4B-C5B-O5B
3	G	600	FAD	O3'-C3'-C4'-C5'
3	G	600	FAD	C2'-C1'-N10-C9A
3	A	600	FAD	O3'-C3'-C4'-C5'
3	C	600	FAD	C2'-C3'-C4'-C5'
3	D	600	FAD	PA-O3P-P-O5'
3	F	600	FAD	PA-O3P-P-O5'
4	C	601	EDO	O1-C1-C2-O2
3	C	600	FAD	O4B-C4B-C5B-O5B
3	C	600	FAD	C2'-C3'-C4'-O4'
3	D	600	FAD	C4B-C5B-O5B-PA
4	F	601	EDO	O1-C1-C2-O2
3	G	600	FAD	C4B-C5B-O5B-PA
3	H	600	FAD	C4B-C5B-O5B-PA
3	F	600	FAD	O3'-C3'-C4'-C5'
3	G	600	FAD	O3'-C3'-C4'-O4'
3	E	600	FAD	O3'-C3'-C4'-C5'
4	G	602	EDO	O1-C1-C2-O2
3	A	600	FAD	C4B-C5B-O5B-PA
3	E	600	FAD	C4B-C5B-O5B-PA
3	B	600	FAD	PA-O3P-P-O5'
3	C	600	FAD	C4B-C5B-O5B-PA
3	F	600	FAD	C4B-C5B-O5B-PA
3	D	600	FAD	O3'-C3'-C4'-C5'
3	H	600	FAD	O3'-C3'-C4'-C5'

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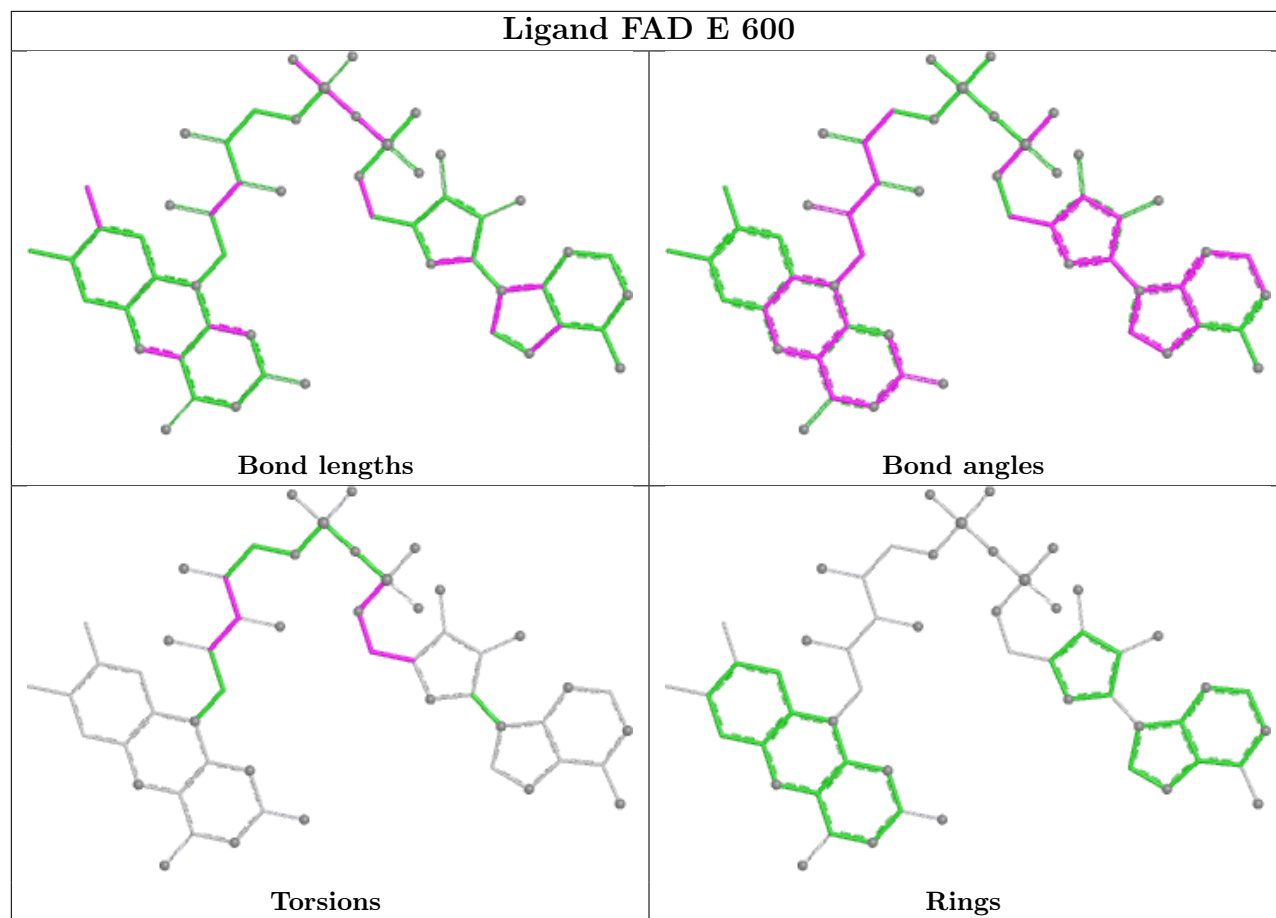
Mol	Chain	Res	Type	Atoms
4	G	601	EDO	O1-C1-C2-O2
3	A	600	FAD	O3'-C3'-C4'-O4'
3	B	600	FAD	C4B-C5B-O5B-PA
4	C	602	EDO	O1-C1-C2-O2
4	D	601	EDO	O1-C1-C2-O2
3	D	600	FAD	O4B-C4B-C5B-O5B
3	B	600	FAD	O3'-C3'-C4'-C5'
4	A	601	EDO	O1-C1-C2-O2

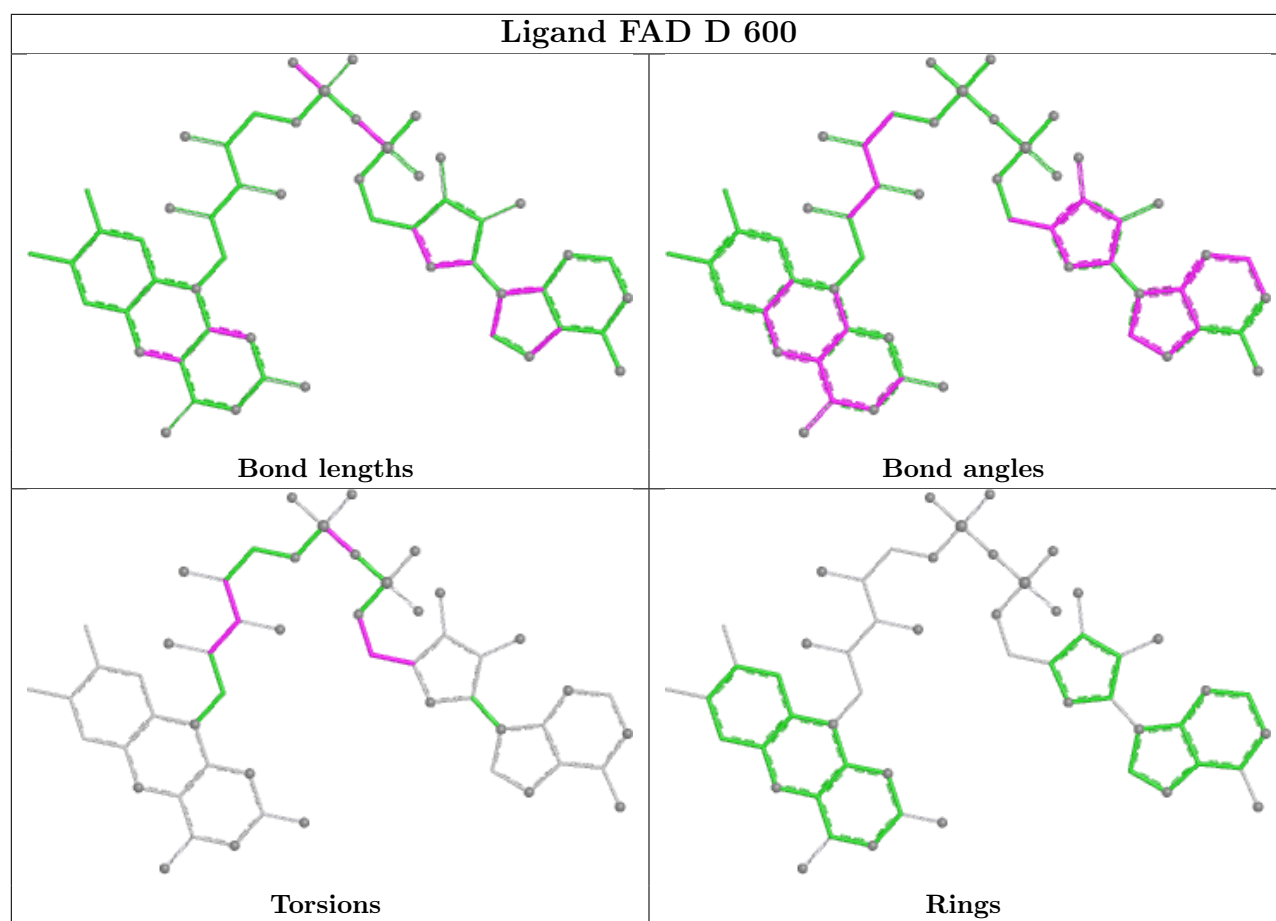
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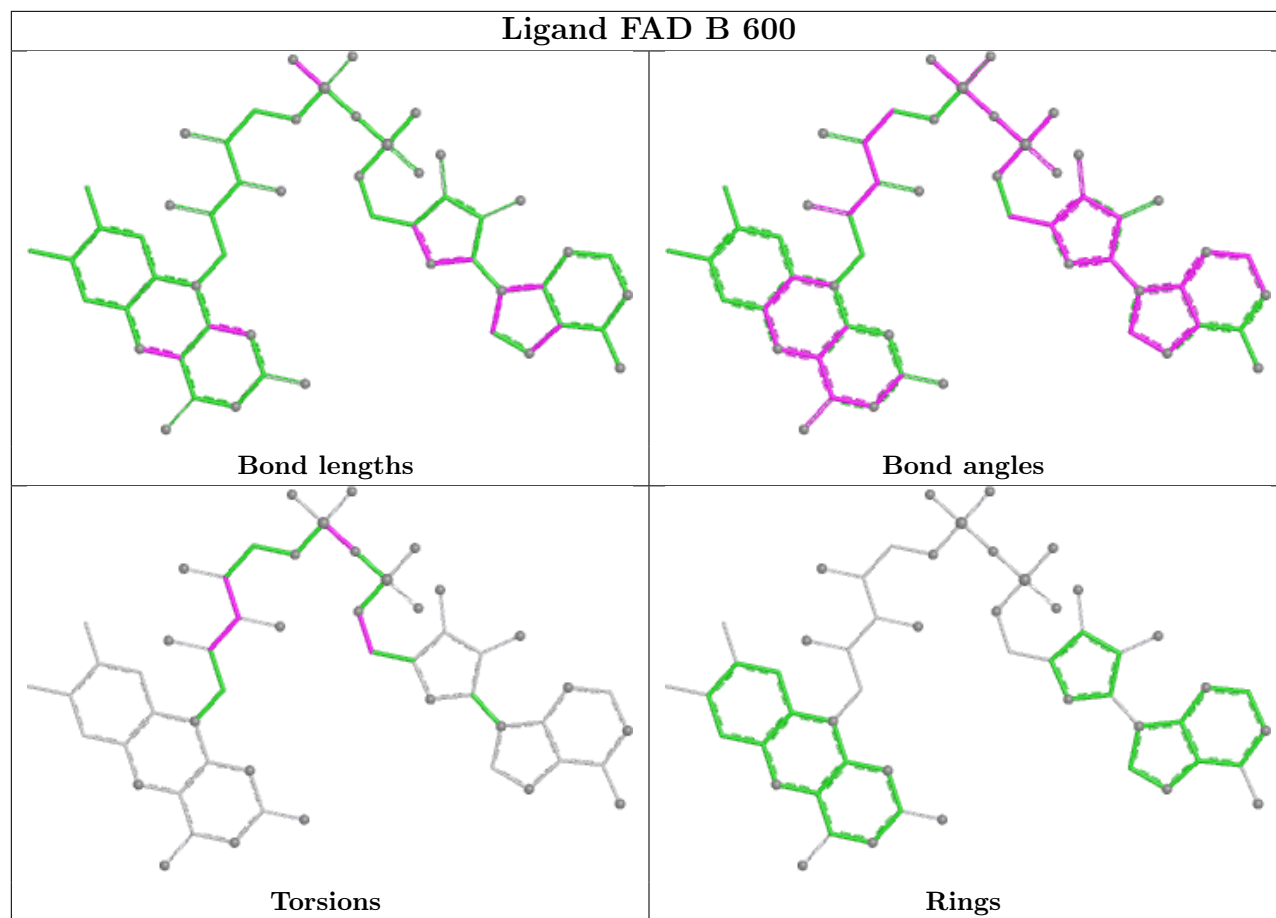
10 monomers are involved in 39 short contacts:

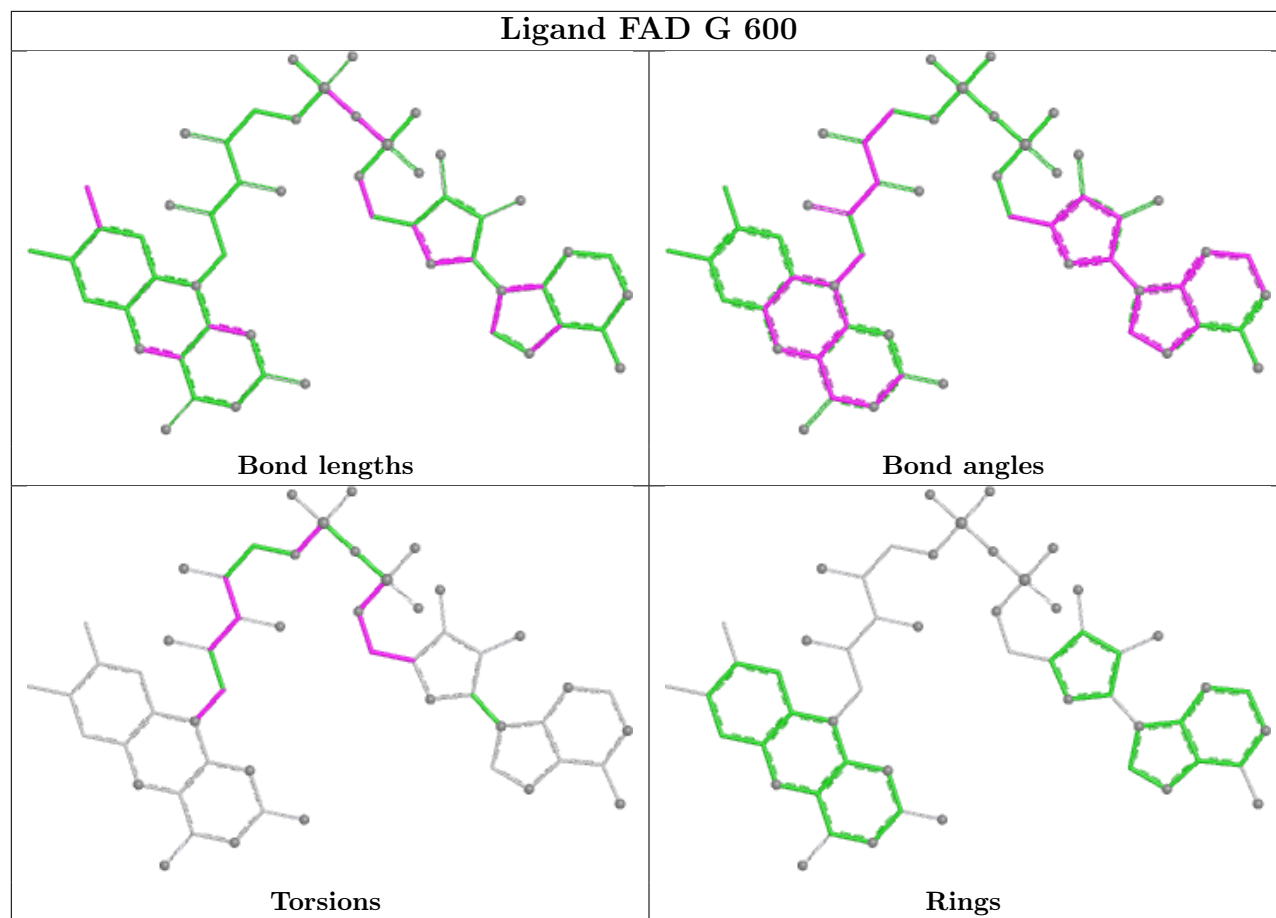
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	600	FAD	4	0
3	D	600	FAD	4	0
3	B	600	FAD	4	0
3	G	600	FAD	5	0
3	C	600	FAD	5	0
3	H	600	FAD	4	0
3	A	600	FAD	5	0
3	F	600	FAD	4	0
4	G	601	EDO	3	0
4	C	601	EDO	1	0

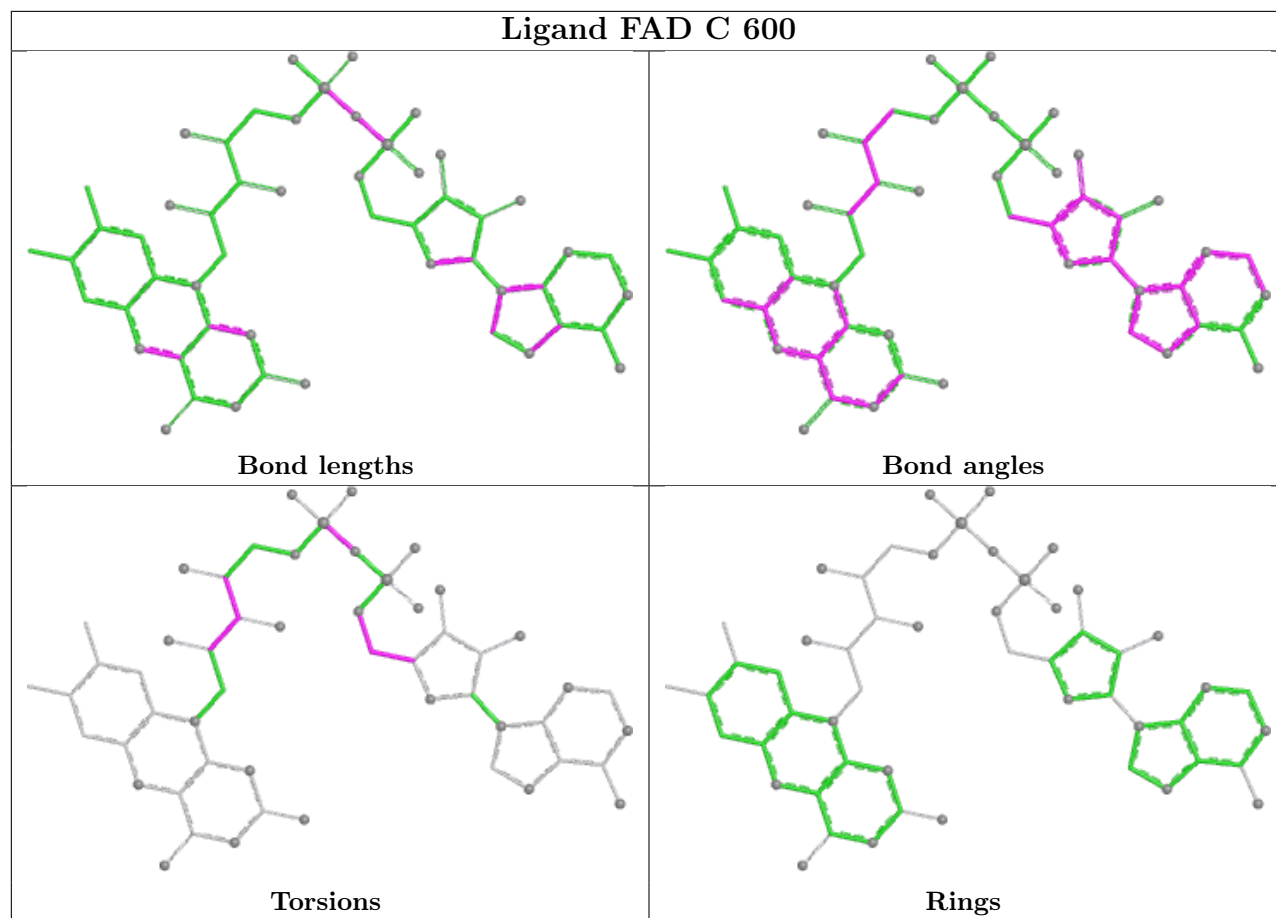
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

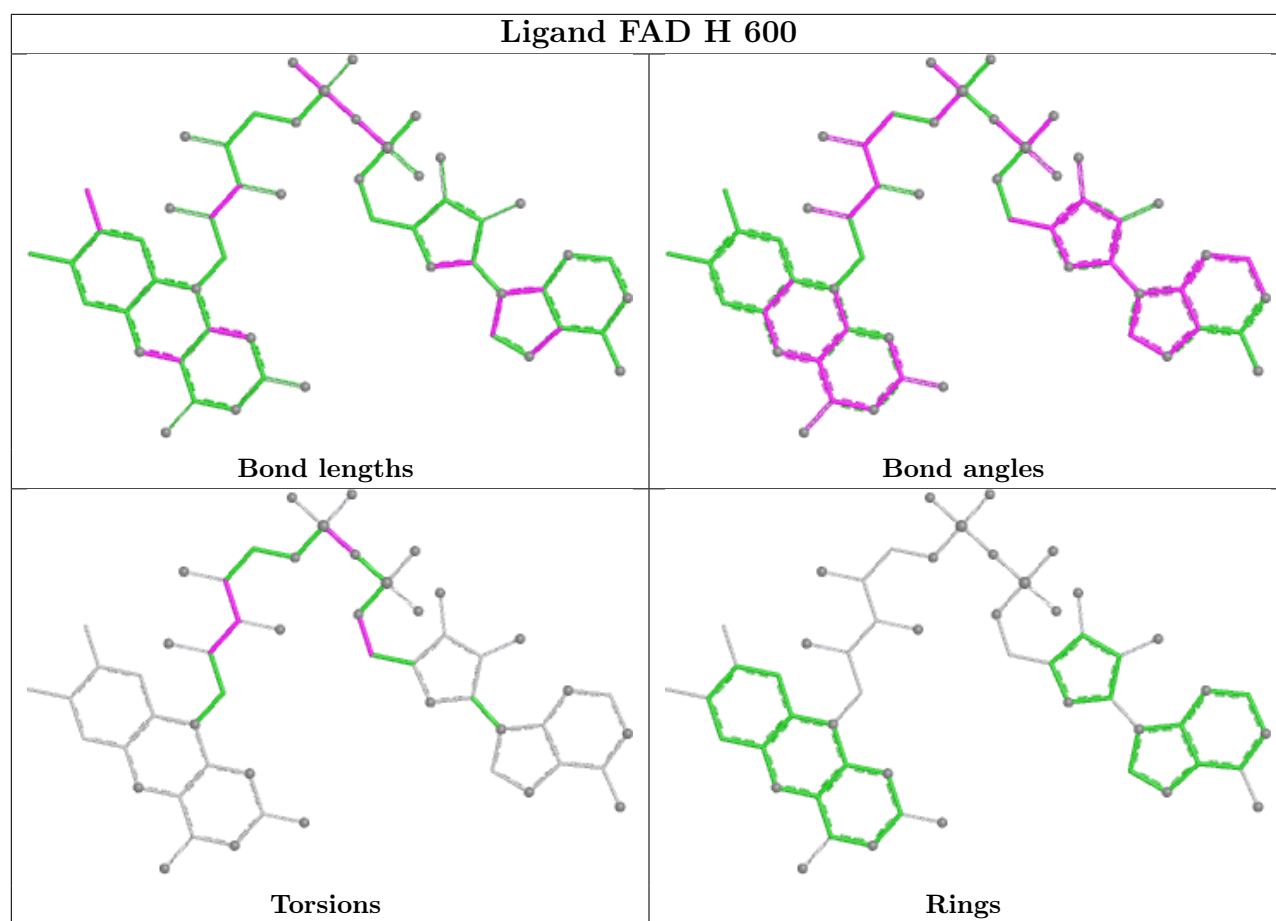


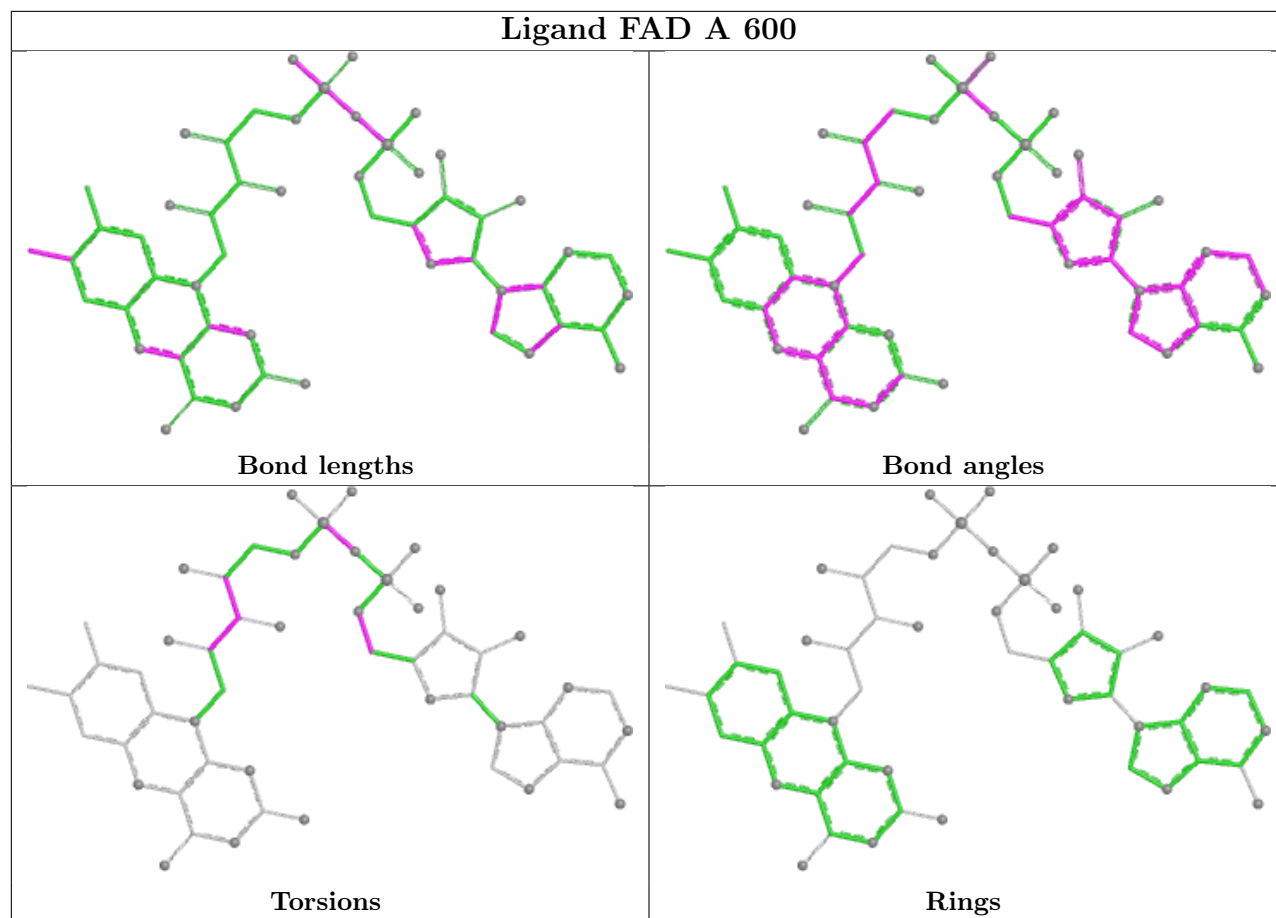


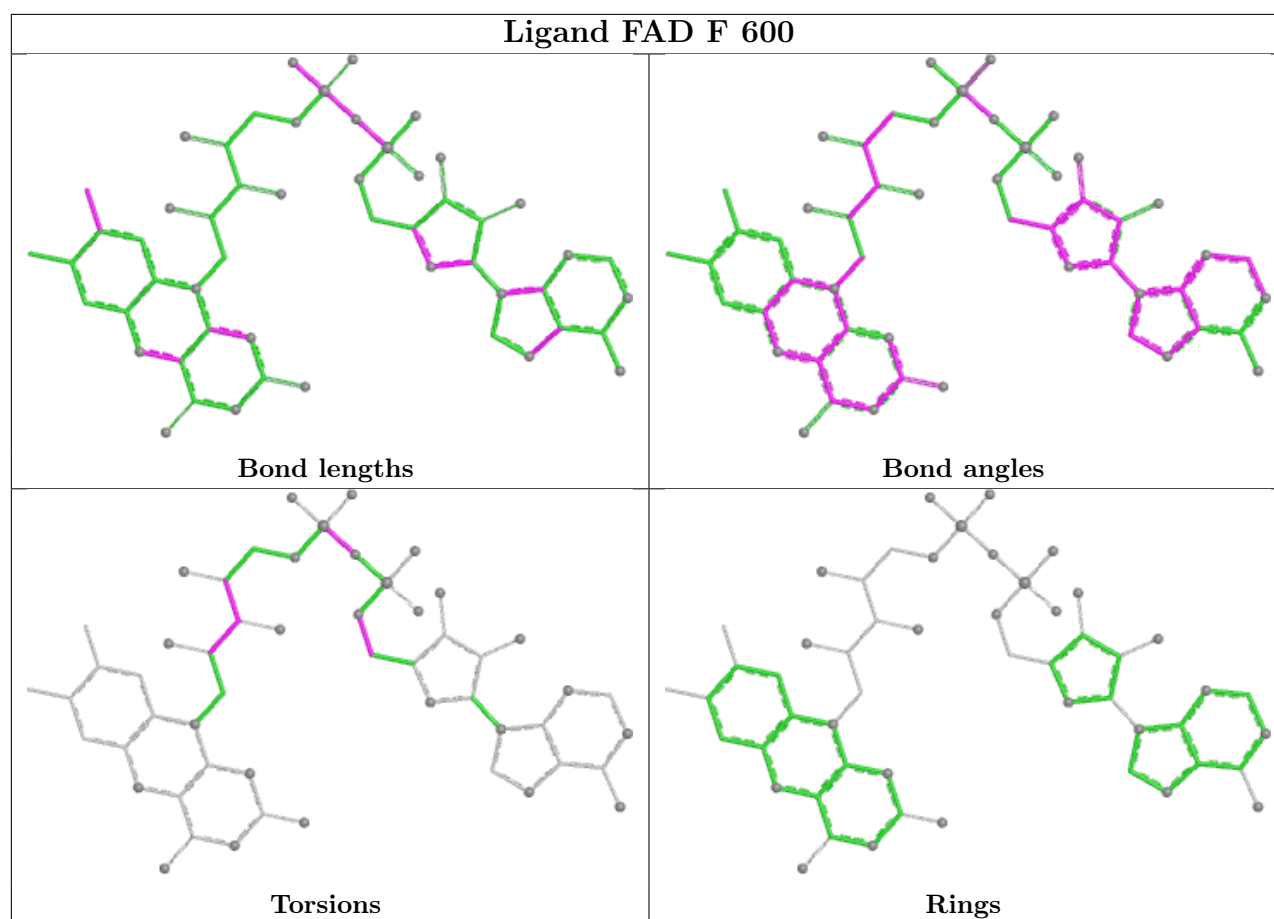












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	4
1	H	4
1	B	3
2	G	3
1	E	2
1	A	2
1	F	1
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	7:TYR	C	8:GLN	N	1.20
1	C	99:GLN	C	100:SER	N	1.20
1	E	393:GLU	C	394:ASP	N	1.20
1	E	394:ASP	C	395:VAL	N	1.19
1	G	303:ARG	C	304:VAL	N	1.19
1	G	471:ILE	C	472:GLU	N	1.19
1	B	303:ARG	C	304:VAL	N	1.17
1	H	66:LEU	C	67:LEU	N	1.17
1	F	393:GLU	C	394:ASP	N	1.16
1	A	143:GLU	C	144:ALA	N	1.15
1	D	196:ARG	C	197:ASP	N	1.15
1	H	391:PRO	C	392:ASP	N	1.15
1	B	393:GLU	C	394:ASP	N	1.14
1	C	104:ARG	C	105:GLU	N	1.14
1	C	303:ARG	C	304:VAL	N	1.14
1	A	196:ARG	C	197:ASP	N	1.13
1	H	67:LEU	C	68:LEU	N	1.13
1	H	455:ALA	C	456:ASN	N	1.13
1	C	4:ARG	C	5:ASP	N	1.11
1	G	483:GLU	C	484:GLU	N	1.03

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	478/495 (96%)	-0.43	2 (0%) 88 89	8, 19, 30, 47	10 (2%)
1	B	476/495 (96%)	-0.36	3 (0%) 85 87	7, 19, 35, 48	14 (2%)
1	C	477/495 (96%)	-0.21	5 (1%) 79 80	7, 22, 38, 49	17 (3%)
1	D	478/495 (96%)	-0.20	11 (2%) 61 63	10, 22, 39, 56	18 (3%)
1	E	477/495 (96%)	-0.22	6 (1%) 75 77	8, 23, 40, 49	16 (3%)
1	F	478/495 (96%)	-0.25	4 (0%) 82 83	8, 22, 37, 46	17 (3%)
1	H	478/495 (96%)	-0.08	4 (0%) 82 83	12, 26, 43, 52	19 (3%)
2	G	478/495 (96%)	-0.20	8 (1%) 69 71	10, 22, 38, 51	15 (3%)
All	All	3820/3960 (96%)	-0.25	43 (1%) 78 79	7, 22, 39, 56	126 (3%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	486	GLY	4.8
1	E	482	LEU	3.7
2	G	1	MET	3.6
1	H	485	LEU	3.6
2	G	39	PRO	3.6
1	C	482	LEU	3.5
2	G	2	THR	3.4
1	D	1	MET	3.1
1	B	1	MET	3.1
1	C	32	GLU	3.1
1	F	32	GLU	2.9
1	B	482	LEU	2.9
1	D	482	LEU	2.8
1	H	483	GLU	2.8
2	G	284	ASN	2.8
1	E	287	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	287	ASP	2.5
1	E	198	GLU	2.5
1	D	324	THR	2.5
1	D	286	ARG	2.5
1	C	2	THR	2.4
1	E	39	PRO	2.4
1	B	287	ASP	2.4
2	G	287	ASP	2.4
1	D	39	PRO	2.3
1	D	450	GLY	2.3
1	E	1	MET	2.3
1	C	286	ARG	2.3
1	D	481	VAL	2.2
1	D	296	GLY	2.2
1	F	38	GLY	2.2
1	H	392	ASP	2.2
1	D	325	GLU	2.1
1	F	39	PRO	2.1
1	D	484	GLU	2.1
1	D	32	GLU	2.1
1	C	39	PRO	2.1
1	E	447	GLU	2.1
2	G	12	GLU	2.1
2	G	483	GLU	2.1
1	A	286	ARG	2.0
2	G	456	ASN	2.0
1	H	39	PRO	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,

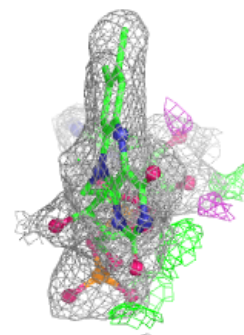
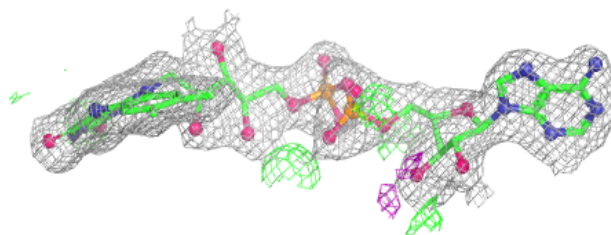
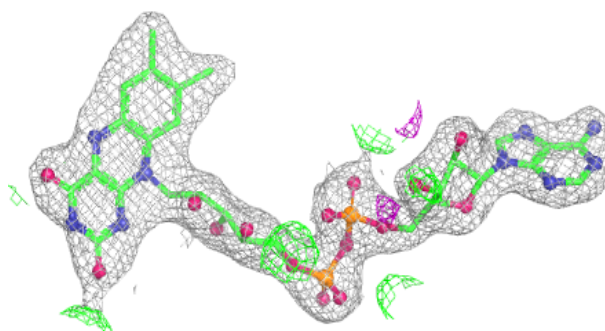
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	G	601	4/4	0.84	0.23	26,28,31,34	0
4	EDO	C	601	4/4	0.89	0.18	24,27,31,32	0
4	EDO	D	601	4/4	0.95	0.09	20,23,25,27	0
4	EDO	C	602	4/4	0.95	0.09	29,32,33,33	0
3	FAD	C	600	53/53	0.96	0.07	13,19,27,28	0
3	FAD	G	600	53/53	0.96	0.08	17,22,32,32	0
3	FAD	H	600	53/53	0.96	0.07	19,24,29,30	0
4	EDO	F	601	4/4	0.96	0.09	21,24,27,31	0
4	EDO	A	601	4/4	0.96	0.07	23,25,26,26	0
4	EDO	G	602	4/4	0.96	0.08	29,31,31,31	0
3	FAD	D	600	53/53	0.97	0.06	10,19,26,27	0
3	FAD	E	600	53/53	0.97	0.07	14,19,29,30	0
3	FAD	F	600	53/53	0.97	0.07	15,20,25,25	0
3	FAD	B	600	53/53	0.97	0.06	10,18,22,23	0
3	FAD	A	600	53/53	0.98	0.06	13,18,20,22	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.

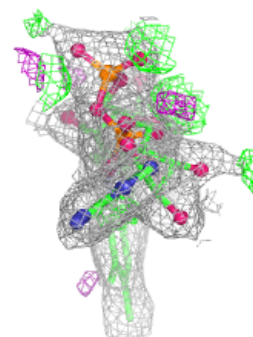
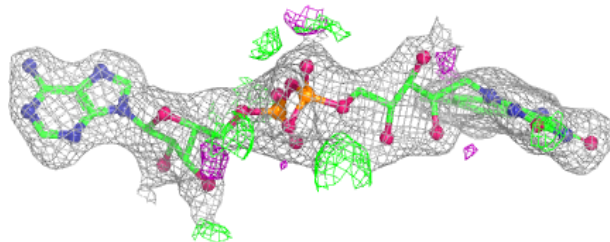
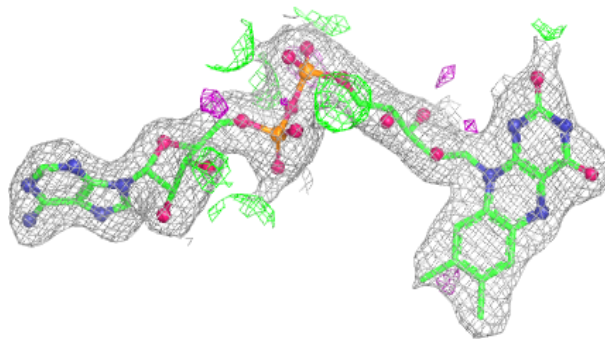
Electron density around FAD C 600:

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

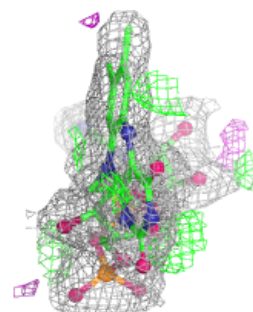
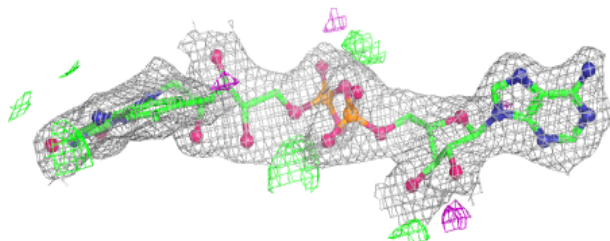
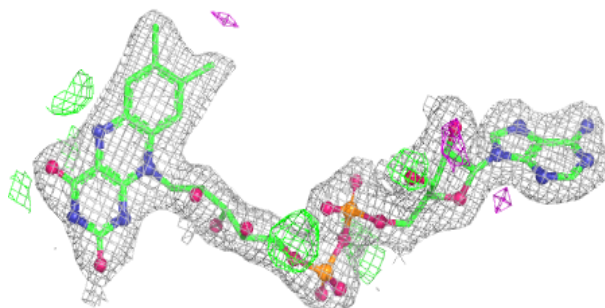


Electron density around FAD G 600:

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

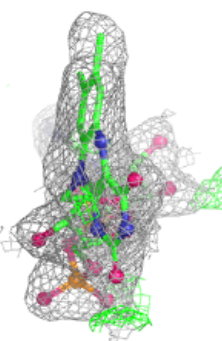
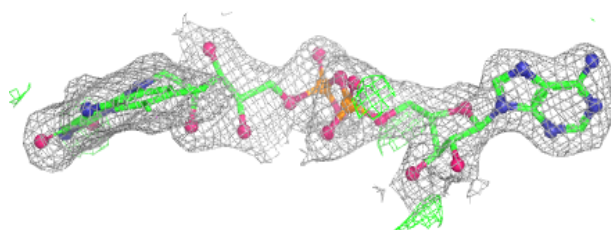
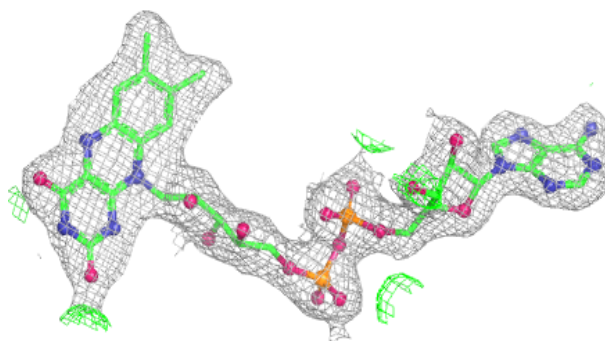
**Electron density around FAD H 600:**

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

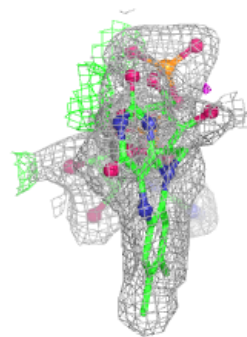
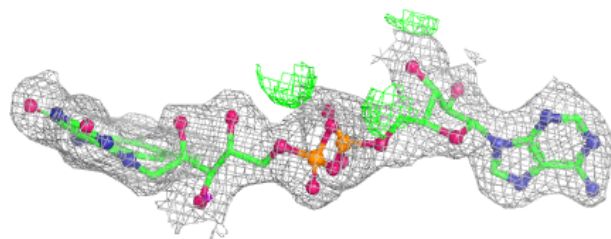
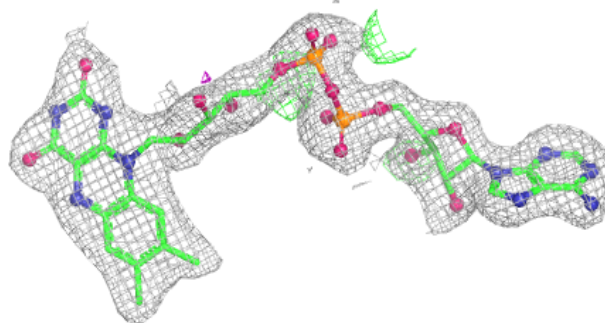


Electron density around FAD D 600:

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

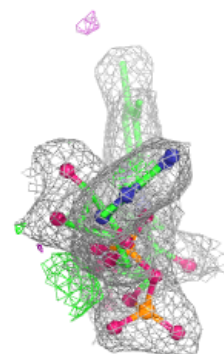
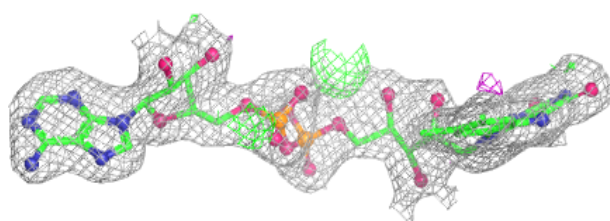
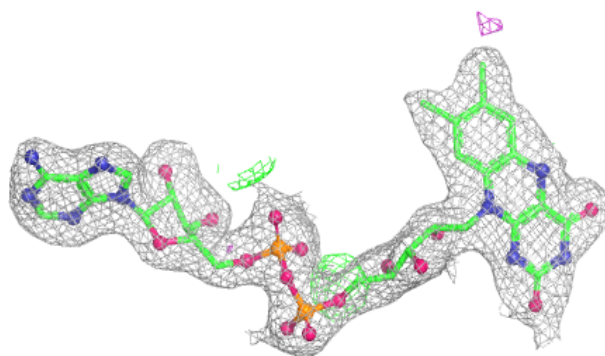
**Electron density around FAD E 600:**

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

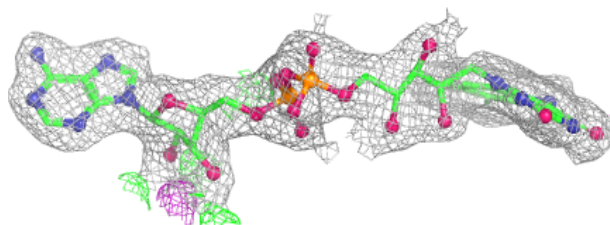
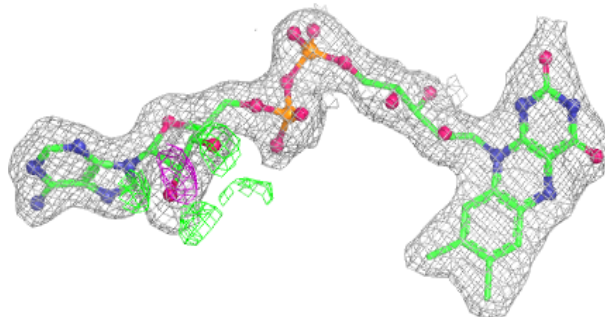


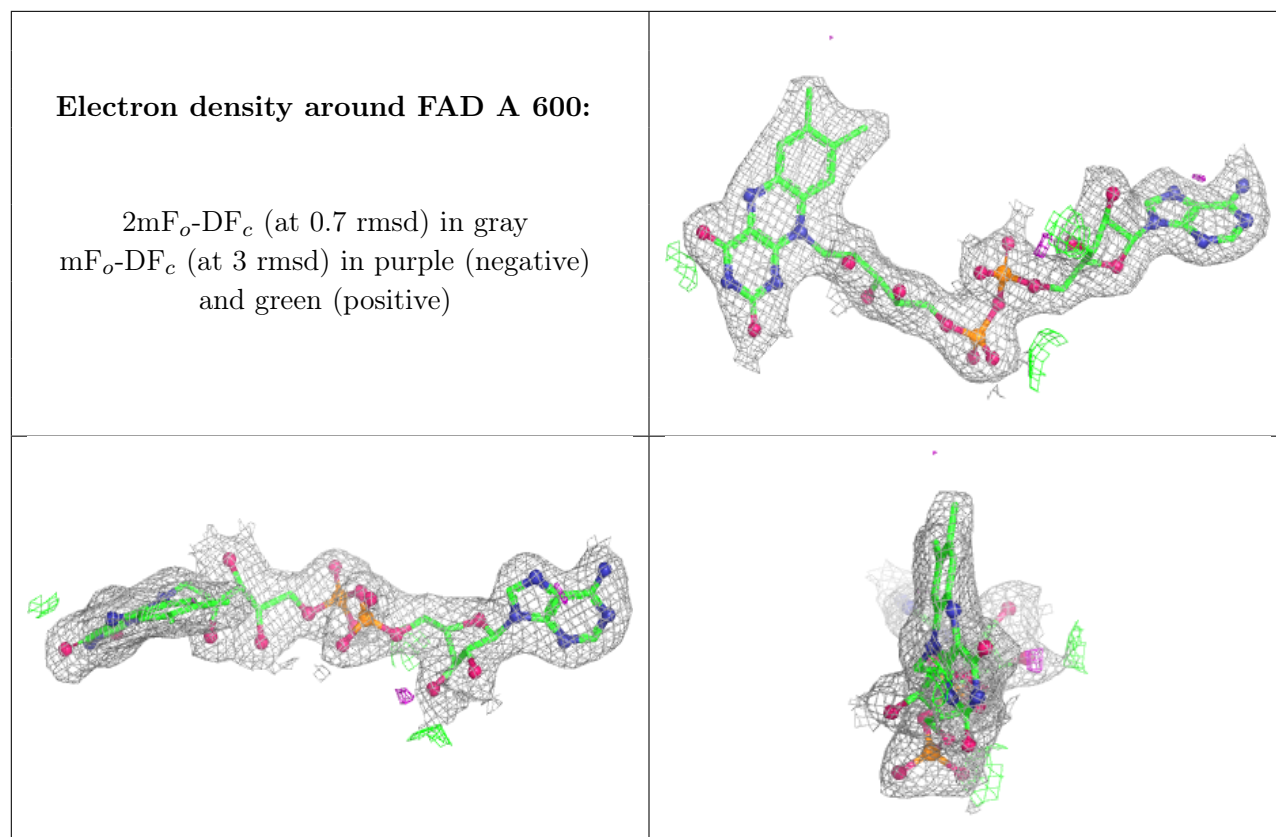
Electron density around FAD F 600:

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

**Electron density around FAD B 600:**

$2mF_o-DF_c$ (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.