



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 07:51 AM EDT

PDB ID : 2IGM / pdb_00002igm
Title : Crystal structure of recombinant pyranose 2-oxidase H548N mutant
Authors : Divne, C.
Deposited on : 2006-09-22
Resolution : 1.90 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)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

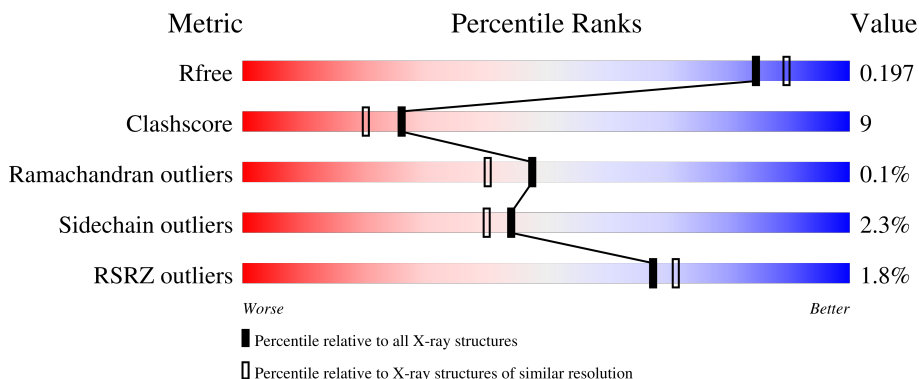
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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.



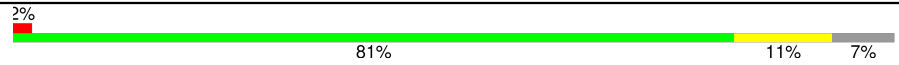

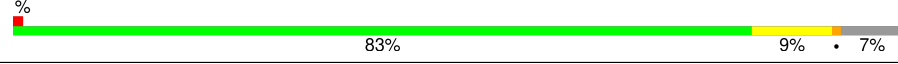
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	623	 2% 81% 10% • 7%
1	B	623	 0% 81% 10% • 7%
1	C	623	 2% 81% 10% • 7%
1	D	623	 0% 82% 10% • 7%
1	E	623	 0% 82% 10% • 7%

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Mol	Chain	Length	Quality of chain
1	F	623	 2% 81% 11% 7%
1	G	623	 3% 81% 10% 7%
1	H	623	 % 83% 9% 7%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 41255 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.

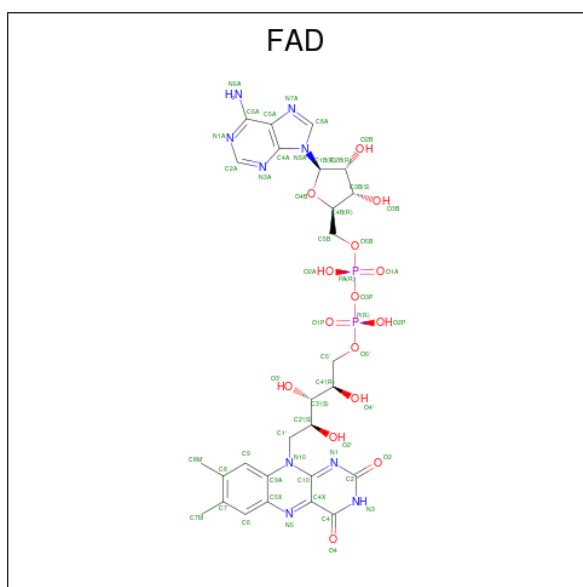
- Molecule 1 is a protein called Pyranose oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	577	4561	2879	779	878	25	0	2	0
1	B	577	4562	2881	779	877	25	0	2	0
1	D	577	4569	2883	780	881	25	0	3	0
1	C	577	4555	2876	778	876	25	0	1	0
1	E	577	4561	2879	779	878	25	0	2	0
1	F	577	4555	2876	778	876	25	0	1	0
1	G	577	4562	2881	779	877	25	0	2	0
1	H	577	4555	2876	778	876	25	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

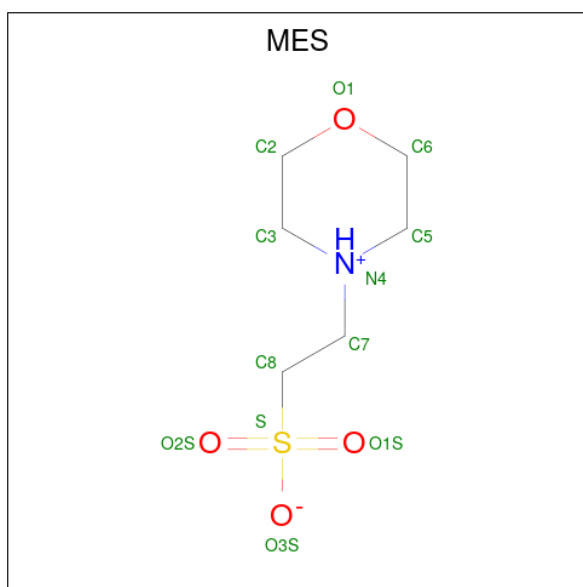
Chain	Residue	Modelled	Actual	Comment	Reference
A	548	ASN	HIS	engineered mutation	UNP Q7ZA32
B	548	ASN	HIS	engineered mutation	UNP Q7ZA32
C	548	ASN	HIS	engineered mutation	UNP Q7ZA32
D	548	ASN	HIS	engineered mutation	UNP Q7ZA32
E	548	ASN	HIS	engineered mutation	UNP Q7ZA32
F	548	ASN	HIS	engineered mutation	UNP Q7ZA32
G	548	ASN	HIS	engineered mutation	UNP Q7ZA32
H	548	ASN	HIS	engineered mutation	UNP Q7ZA32

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



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

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	572	Total	O	0	0
			572	572		
4	B	570	Total	O	0	0
			570	570		
4	D	546	Total	O	0	0
			546	546		
4	C	514	Total	O	0	0
			514	514		

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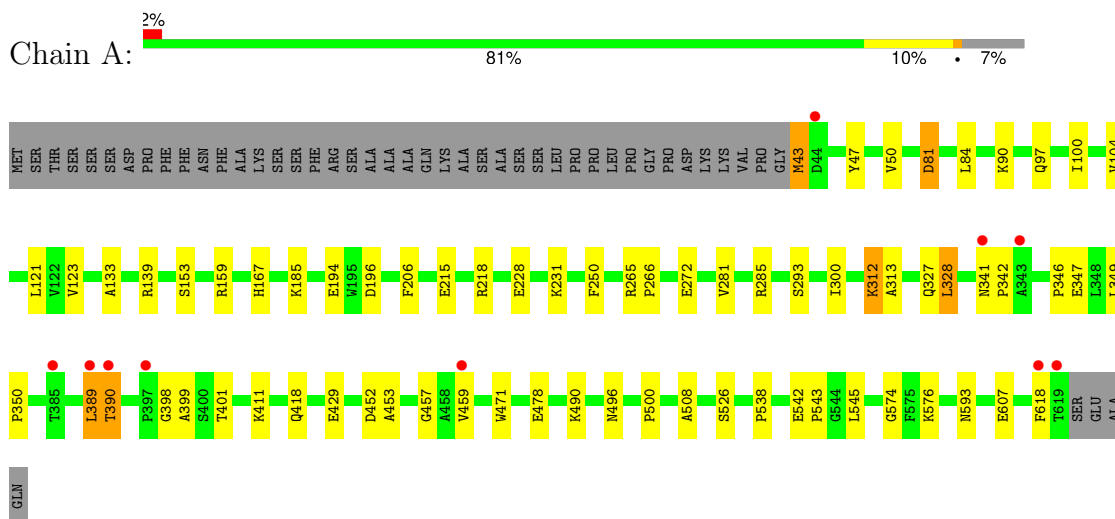
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	524	Total 524	O 524	0	0
4	F	472	Total 472	O 472	0	0
4	G	519	Total 519	O 519	0	0
4	H	538	Total 538	O 538	0	0

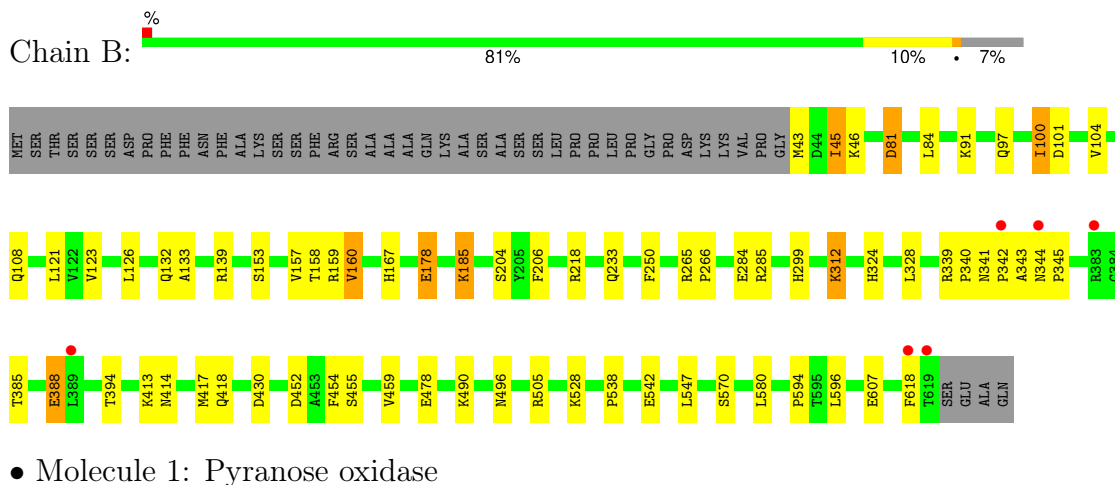
3 Residue-property plots [i](#)

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

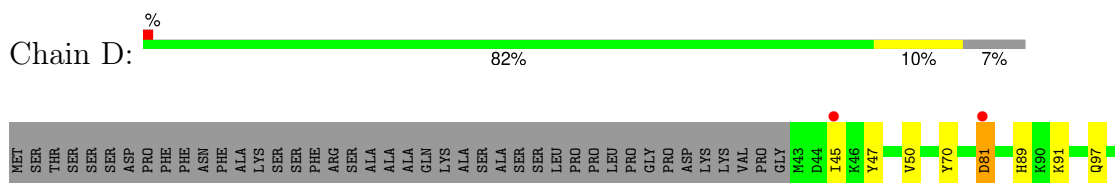
- Molecule 1: Pyranose oxidase

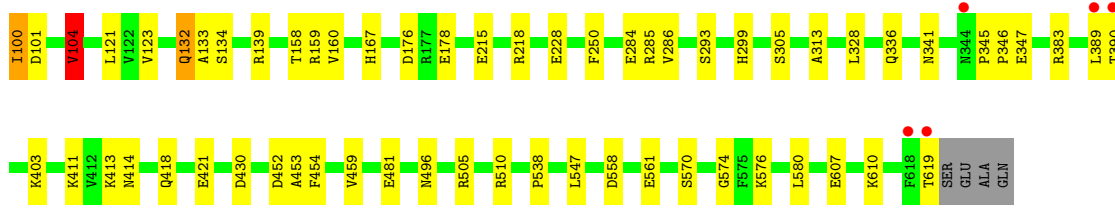


- Molecule 1: Pyranose oxidase

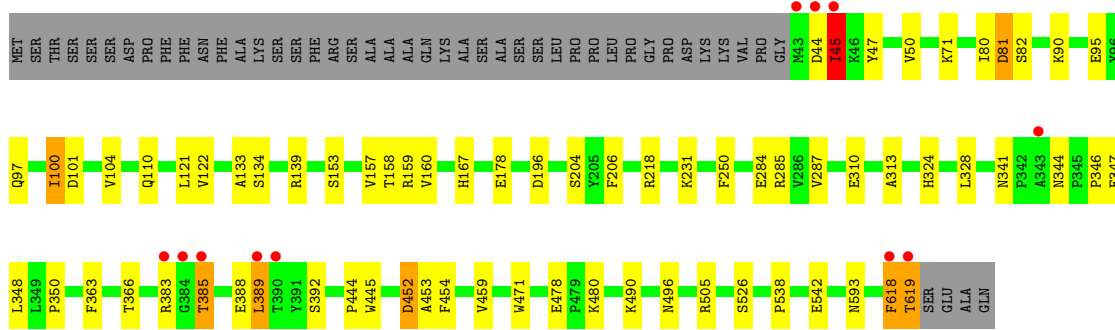
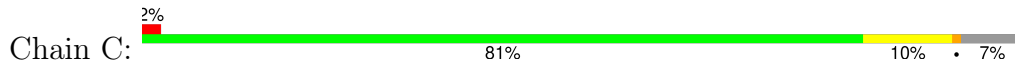


- Molecule 1: Pyranose oxidase

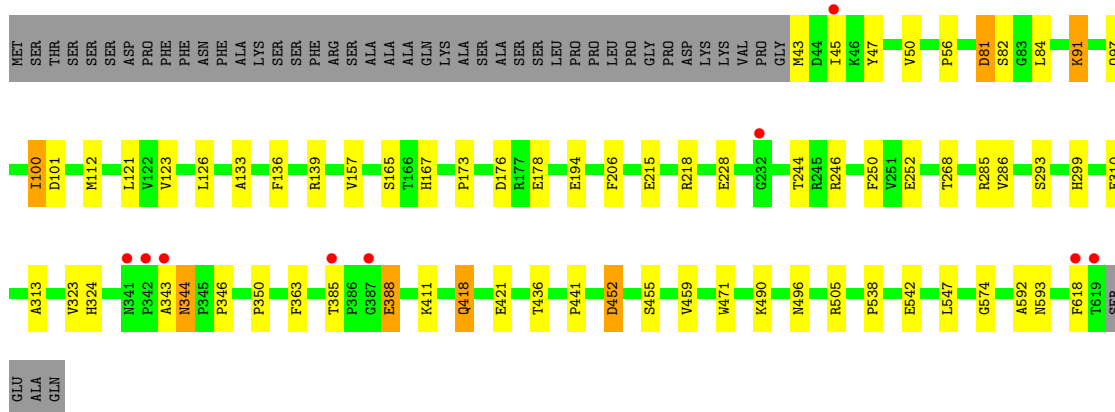
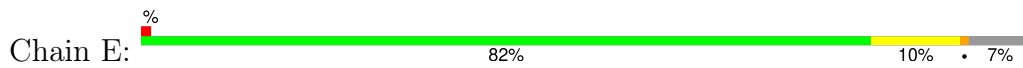




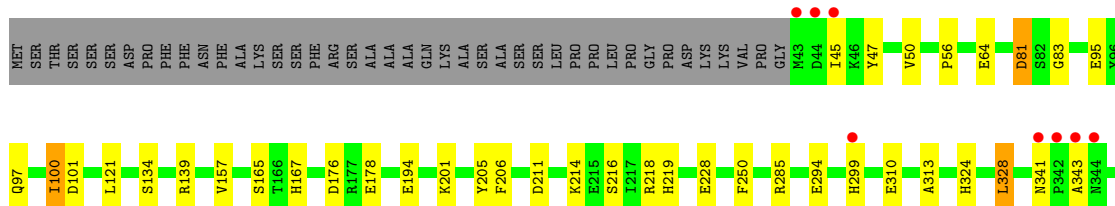
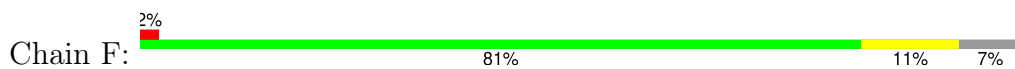
● Molecule 1: Pyranose oxidase

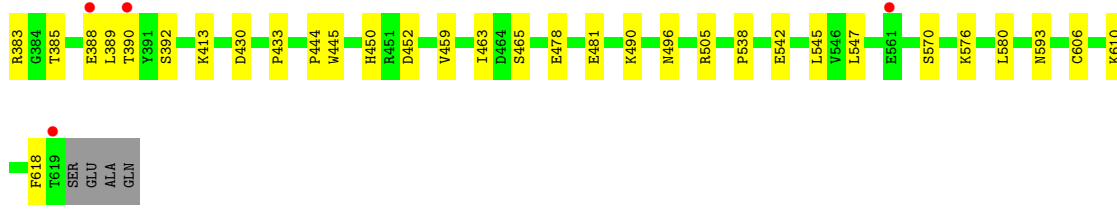


● Molecule 1: Pyranose oxidase

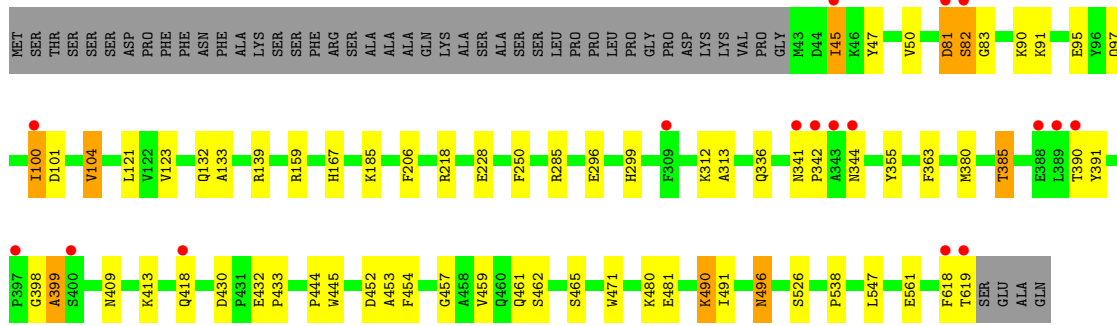
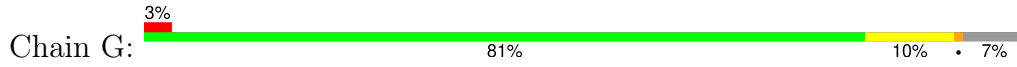


● Molecule 1: Pyranose oxidase

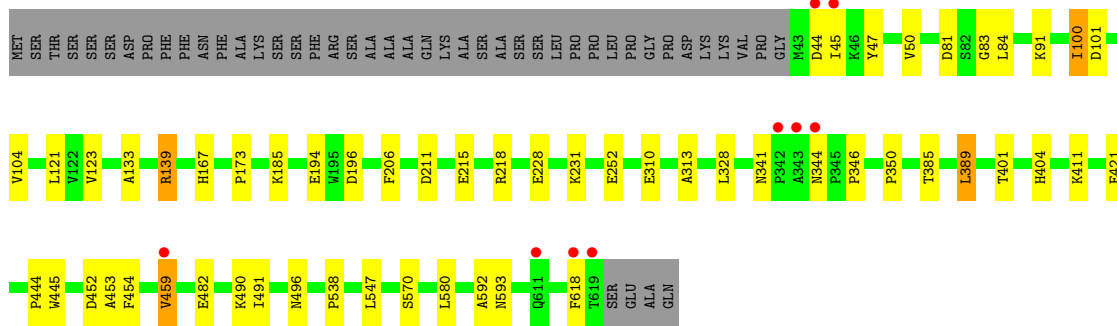
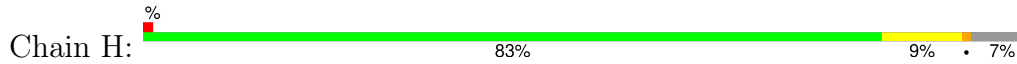




• Molecule 1: Pyranose oxidase



• Molecule 1: Pyranose oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	168.43Å 103.14Å 168.91Å 90.00° 106.08° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.7 (20.00-1.90) 96.7 (20.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 1.90Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.152 , 0.189 0.160 , 0.197	Depositor DCC
R_{free} test set	4236 reflections (0.97%)	wwPDB-VP
Wilson B-factor (Å ²)	16.9	Xtrriage
Anisotropy	0.160	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.015 for l,-k,h	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	41255	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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

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	1.07	4/4676 (0.1%)	0.97	2/6358 (0.0%)
1	B	1.07	3/4677 (0.1%)	0.97	4/6360 (0.1%)
1	C	1.02	5/4670 (0.1%)	0.97	5/6350 (0.1%)
1	D	1.03	3/4684 (0.1%)	0.97	5/6369 (0.1%)
1	E	1.00	1/4676 (0.0%)	0.93	3/6358 (0.0%)
1	F	0.99	2/4670 (0.0%)	0.95	4/6350 (0.1%)
1	G	1.03	5/4677 (0.1%)	0.95	4/6360 (0.1%)
1	H	1.02	1/4670 (0.0%)	0.95	3/6350 (0.0%)
All	All	1.03	24/37400 (0.1%)	0.96	30/50855 (0.1%)

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	E	0	1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	81	ASP	CA-C	9.33	1.65	1.52
1	D	345	PRO	CA-C	7.02	1.56	1.52
1	D	139	ARG	CD-NE	-6.73	1.36	1.46
1	B	139	ARG	CD-NE	-6.67	1.36	1.46
1	G	45	ILE	CA-CB	6.48	1.62	1.54
1	H	139	ARG	CD-NE	-6.36	1.37	1.46
1	C	139	ARG	CD-NE	-6.20	1.37	1.46
1	F	81	ASP	CA-C	6.19	1.61	1.52
1	G	82	SER	N-CA	6.13	1.53	1.46
1	C	81	ASP	CA-C	6.01	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	81	ASP	CA-C	5.96	1.60	1.52
1	B	81	ASP	CA-C	5.92	1.60	1.52
1	G	139	ARG	CD-NE	-5.90	1.38	1.46
1	G	82	SER	C-O	5.89	1.31	1.24
1	F	139	ARG	CD-NE	-5.84	1.38	1.46
1	A	139	ARG	CD-NE	-5.77	1.38	1.46
1	E	81	ASP	CA-C	5.72	1.60	1.52
1	A	508	ALA	CA-CB	5.65	1.62	1.53
1	C	80	ILE	CA-CB	5.57	1.60	1.53
1	A	349	LEU	C-O	5.29	1.26	1.23
1	A	81	ASP	CA-C	5.28	1.59	1.52
1	C	45	ILE	CA-CB	5.24	1.61	1.54
1	B	160	VAL	CA-CB	5.17	1.61	1.55
1	C	366	THR	CA-CB	5.12	1.63	1.53

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	139	ARG	NE-CZ-NH2	-11.93	108.46	119.20
1	C	139	ARG	NE-CZ-NH2	-11.89	108.49	119.20
1	F	139	ARG	NE-CZ-NH2	-11.43	108.92	119.20
1	G	139	ARG	NE-CZ-NH2	-10.98	109.32	119.20
1	H	139	ARG	NE-CZ-NH2	-9.68	110.49	119.20
1	B	139	ARG	NE-CZ-NH2	-9.51	110.64	119.20
1	A	139	ARG	NE-CZ-NH2	-9.05	111.06	119.20
1	C	139	ARG	NE-CZ-NH1	8.59	130.09	121.50
1	E	139	ARG	NE-CZ-NH2	-8.57	111.48	119.20
1	G	139	ARG	NE-CZ-NH1	8.12	129.62	121.50
1	H	139	ARG	NE-CZ-NH1	7.59	129.09	121.50
1	D	139	ARG	NE-CZ-NH1	7.43	128.93	121.50
1	D	104	VAL	CB-CA-C	-7.09	101.17	112.16
1	C	139	ARG	CD-NE-CZ	6.52	133.53	124.40
1	G	139	ARG	CD-NE-CZ	6.49	133.48	124.40
1	D	139	ARG	CD-NE-CZ	6.28	133.19	124.40
1	B	139	ARG	NE-CZ-NH1	6.06	127.56	121.50
1	D	139	ARG	CG-CD-NE	-6.03	98.73	112.00
1	C	139	ARG	CA-CB-CG	5.84	125.78	114.10
1	F	139	ARG	CG-CD-NE	-5.75	99.36	112.00
1	F	139	ARG	NE-CZ-NH1	5.68	127.18	121.50
1	H	139	ARG	CD-NE-CZ	5.68	132.36	124.40
1	C	452	ASP	CB-CA-C	5.58	122.83	111.11
1	E	139	ARG	CG-CD-NE	-5.45	100.00	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	139	ARG	CG-CD-NE	-5.44	100.04	112.00
1	A	139	ARG	NE-CZ-NH1	5.41	126.91	121.50
1	G	139	ARG	CG-CD-NE	-5.31	100.31	112.00
1	B	594	PRO	N-CA-C	5.16	121.24	114.27
1	F	139	ARG	CA-CB-CG	5.15	124.40	114.10
1	E	139	ARG	NE-CZ-NH1	5.08	126.58	121.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	436	THR	Peptide

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	4561	0	4408	93	0
1	B	4562	0	4412	114	0
1	C	4555	0	4404	89	0
1	D	4569	0	4411	89	0
1	E	4561	0	4408	104	0
1	F	4555	0	4404	97	0
1	G	4562	0	4412	107	0
1	H	4555	0	4404	79	0
2	A	53	0	30	6	0
2	B	53	0	29	13	0
2	C	53	0	28	8	0
2	D	53	0	29	8	0
2	E	53	0	30	11	0
2	F	53	0	29	9	0
2	G	53	0	29	10	0
2	H	53	0	28	6	0
3	A	12	0	12	1	0
3	B	12	0	12	1	0
3	C	12	0	12	0	0
3	D	12	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	12	0	12	4	0
3	F	12	0	12	0	0
3	G	12	0	12	2	0
3	H	12	0	12	1	0
4	A	572	0	0	40	0
4	B	570	0	0	37	0
4	C	514	0	0	22	0
4	D	546	0	0	46	0
4	E	524	0	0	43	0
4	F	472	0	0	31	0
4	G	519	0	0	38	0
4	H	538	0	0	31	0
All	All	41255	0	35591	673	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 9.

All (673) 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:G:167:HIS:HE2	2:G:801:FAD:C8M	0.98	1.61
1:E:167:HIS:HE2	2:E:801:FAD:C8M	1.01	1.60
1:D:167:HIS:HE2	2:D:801:FAD:C8M	0.97	1.59
1:B:167:HIS:HE2	2:B:801:FAD:C8M	0.97	1.57
1:F:167:HIS:HE2	2:F:801:FAD:C8M	0.96	1.54
1:C:167:HIS:HE2	2:C:801:FAD:C8M	0.92	1.53
1:A:167:HIS:HE2	2:A:801:FAD:C8M	0.90	1.52
1:H:167:HIS:HE2	2:H:801:FAD:C8M	0.98	1.52
1:E:121[B]:LEU:CD2	1:F:459:VAL:HG22	1.43	1.49
1:A:459:VAL:HG22	1:B:121[B]:LEU:CD2	1.52	1.40
1:E:167:HIS:NE2	2:E:801:FAD:HM82	1.09	1.38
1:H:167:HIS:NE2	2:H:801:FAD:HM82	1.06	1.36
1:A:459:VAL:CG2	1:B:121[B]:LEU:HD21	1.53	1.35
1:B:167:HIS:NE2	2:B:801:FAD:HM82	1.03	1.34
1:F:545:LEU:HD22	4:F:7392:HOH:O	1.26	1.33
1:G:167:HIS:NE2	2:G:801:FAD:HM82	1.00	1.32
1:A:104:VAL:HB	4:A:7508:HOH:O	1.26	1.31
1:B:452:ASP:HB2	4:B:7324:HOH:O	1.28	1.29
1:E:459:VAL:HG22	1:F:121[B]:LEU:CD2	1.62	1.29
1:E:121[B]:LEU:HD21	1:F:459:VAL:CG2	1.64	1.27
1:F:167:HIS:NE2	2:F:801:FAD:HM82	0.95	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:SER:CB	4:B:7545:HOH:O	1.72	1.26
1:G:121[B]:LEU:CD2	1:H:459:VAL:HG23	1.62	1.26
1:D:167:HIS:NE2	2:D:801:FAD:HM82	0.95	1.25
1:C:104:VAL:HB	4:C:7428:HOH:O	1.35	1.25
1:H:452:ASP:HB2	4:H:7281:HOH:O	1.33	1.24
1:H:389:LEU:HD12	4:H:7254:HOH:O	1.38	1.23
1:C:167:HIS:NE2	2:C:801:FAD:HM82	0.90	1.23
1:A:121[B]:LEU:CD2	1:B:459:VAL:HG22	1.70	1.21
1:A:327:GLN:NE2	4:A:7531:HOH:O	1.67	1.21
1:A:167:HIS:NE2	2:A:801:FAD:HM82	0.88	1.21
1:D:459:VAL:CG2	1:C:121[B]:LEU:HD21	1.70	1.20
1:D:121[B]:LEU:CD2	1:C:459:VAL:HG22	1.71	1.20
1:D:459:VAL:HG22	1:C:121[B]:LEU:CD2	1.71	1.20
1:G:465:SER:HB2	4:G:7441:HOH:O	1.06	1.19
1:C:100:ILE:HB	4:C:7356:HOH:O	1.41	1.19
1:G:453:ALA:HB1	4:G:7438:HOH:O	1.42	1.19
1:H:104:VAL:HB	4:H:7426:HOH:O	1.05	1.19
1:D:453:ALA:HB1	4:D:7506:HOH:O	1.43	1.18
1:B:417:MET:SD	4:B:7483:HOH:O	1.95	1.18
1:F:452:ASP:HB2	4:F:7275:HOH:O	1.41	1.17
1:G:452:ASP:HB2	4:G:7274:HOH:O	1.45	1.16
1:B:204:SER:HB2	4:B:7545:HOH:O	1.29	1.15
1:A:167:HIS:CD2	2:A:801:FAD:HM82	1.82	1.15
1:E:459:VAL:CG2	1:F:121[B]:LEU:HD21	1.79	1.12
1:D:121[B]:LEU:HD21	1:C:459:VAL:CG2	1.78	1.12
1:C:134:SER:HB2	4:C:7475:HOH:O	1.47	1.12
1:A:121[B]:LEU:HD21	1:B:459:VAL:HG22	1.23	1.10
1:A:97:GLN:HB2	4:A:7511:HOH:O	1.47	1.10
1:H:167:HIS:CD2	2:H:801:FAD:HM82	1.86	1.10
1:G:459:VAL:HG22	1:H:121[B]:LEU:HD21	1.19	1.10
1:C:178:GLU:OE1	4:C:7451:HOH:O	1.67	1.10
1:H:167:HIS:HE2	2:H:801:FAD:HM81	1.14	1.10
1:G:121[B]:LEU:HD23	1:H:459:VAL:HA	1.19	1.09
1:G:465:SER:CB	4:G:7441:HOH:O	1.66	1.09
1:C:452:ASP:HB2	4:C:7262:HOH:O	1.47	1.09
1:E:121[B]:LEU:HD23	1:F:459:VAL:HA	1.36	1.08
1:G:459:VAL:HG22	1:H:121[B]:LEU:CD2	1.84	1.07
1:G:121[B]:LEU:HD21	1:H:459:VAL:HG23	1.11	1.07
1:A:459:VAL:HA	1:B:121[B]:LEU:HD23	1.06	1.05
1:D:459:VAL:HG22	1:C:121[B]:LEU:HD21	1.07	1.03
1:F:121[A]:LEU:CD2	1:G:121[A]:LEU:CD2	2.37	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:7007:MES:H71	4:D:7447:HOH:O	1.56	1.03
1:C:167:HIS:CD2	2:C:801:FAD:HM82	1.94	1.02
1:A:459:VAL:HA	1:B:121[B]:LEU:CD2	1.89	1.02
1:G:121[B]:LEU:HD21	1:H:459:VAL:CG2	1.88	1.02
1:F:134:SER:HB2	4:F:7364:HOH:O	1.57	1.01
1:E:121[B]:LEU:CD2	1:F:459:VAL:CG2	2.32	1.00
1:B:285:ARG:HD3	4:B:7315:HOH:O	1.58	1.00
1:D:100:ILE:HD13	1:D:100:ILE:O	1.62	0.99
1:A:459:VAL:CA	1:B:121[B]:LEU:HD23	1.92	0.98
1:D:176:ASP:OD1	4:D:7499:HOH:O	1.81	0.98
1:F:167:HIS:CD2	2:F:801:FAD:HM82	1.98	0.98
1:E:452:ASP:CB	4:E:7267:HOH:O	2.09	0.97
1:E:452:ASP:HB3	4:E:7267:HOH:O	1.65	0.96
1:D:167:HIS:CD2	2:D:801:FAD:HM82	2.00	0.96
1:E:459:VAL:HG22	1:F:121[B]:LEU:HD21	0.97	0.96
1:B:121[A]:LEU:CD2	1:C:121[A]:LEU:CD2	2.43	0.96
1:A:167:HIS:HE2	2:A:801:FAD:HM81	1.31	0.96
1:A:418:GLN:HG3	4:A:7330:HOH:O	1.64	0.96
1:G:167:HIS:CD2	2:G:801:FAD:HM82	2.01	0.96
1:C:167:HIS:CE1	2:C:801:FAD:HM82	2.02	0.95
1:G:121[B]:LEU:CD2	1:H:459:VAL:HA	1.95	0.95
1:B:414:ASN:O	1:B:418:GLN:HG2	1.67	0.94
1:G:121[B]:LEU:CD2	1:H:459:VAL:CG2	2.45	0.94
1:G:418:GLN:HG3	4:G:7510:HOH:O	1.66	0.94
1:B:167:HIS:CD2	2:B:801:FAD:HM82	2.03	0.94
1:G:459:VAL:CG2	1:H:121[B]:LEU:HD21	1.97	0.94
1:E:126:LEU:HD11	4:E:7492:HOH:O	1.68	0.93
1:E:167:HIS:HE2	2:E:801:FAD:HM81	1.34	0.93
1:F:178:GLU:OE1	4:F:7427:HOH:O	1.87	0.92
1:A:121[B]:LEU:HD21	1:B:459:VAL:CG2	2.01	0.91
1:B:43:MET:N	4:B:7228:HOH:O	2.04	0.91
1:H:454:PHE:O	4:H:7503:HOH:O	1.89	0.91
1:D:167:HIS:CE1	2:D:801:FAD:HM82	2.07	0.90
1:E:167:HIS:CD2	2:E:801:FAD:HM82	2.07	0.89
1:G:100:ILE:HG12	4:G:7256:HOH:O	1.72	0.88
1:A:459:VAL:CB	1:B:121[B]:LEU:HD21	2.04	0.88
1:B:167:HIS:HE2	2:B:801:FAD:HM81	1.35	0.87
1:A:285:ARG:NH1	4:A:7463:HOH:O	2.06	0.87
1:A:194:GLU:HG2	4:A:7452:HOH:O	1.75	0.87
1:G:81:ASP:HA	4:G:7236:HOH:O	1.73	0.87
1:A:453:ALA:HB3	4:A:7490:HOH:O	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:7336:HOH:O	1:B:84:LEU:HD23	1.75	0.85
1:C:167:HIS:HE2	2:C:801:FAD:HM83	1.33	0.85
1:A:459:VAL:HG22	1:B:121[B]:LEU:HD21	0.85	0.85
1:D:121[B]:LEU:HD21	1:C:459:VAL:HG22	0.89	0.85
4:D:7493:HOH:O	1:C:160:VAL:HG13	1.76	0.85
1:F:167:HIS:CE1	2:F:801:FAD:HM82	2.08	0.85
1:D:178:GLU:HB3	4:D:7499:HOH:O	1.76	0.84
1:A:459:VAL:CG2	1:B:121[B]:LEU:CD2	2.30	0.83
1:B:121[A]:LEU:CD2	1:C:121[A]:LEU:HD23	2.08	0.83
1:G:121[B]:LEU:HD23	1:H:459:VAL:CA	2.04	0.83
1:E:459:VAL:CG2	1:F:121[B]:LEU:CD2	2.49	0.82
1:G:285:ARG:HD3	4:G:7371:HOH:O	1.80	0.81
4:E:7492:HOH:O	1:F:463:ILE:HD11	1.81	0.81
1:C:310:GLU:OE2	4:C:7438:HOH:O	1.99	0.81
1:G:167:HIS:HE2	2:G:801:FAD:HM81	1.39	0.80
1:F:176:ASP:OD2	4:F:7427:HOH:O	2.00	0.80
1:G:81:ASP:CA	4:G:7236:HOH:O	2.29	0.79
1:H:341:ASN:HD22	1:H:344:ASN:HB3	1.45	0.79
1:B:121[A]:LEU:HD21	1:C:121[A]:LEU:CD2	2.12	0.79
1:A:196:ASP:HB2	4:A:7411:HOH:O	1.83	0.79
1:D:286:VAL:HG22	4:D:7496:HOH:O	1.82	0.78
1:E:452:ASP:HB2	4:E:7267:HOH:O	1.77	0.78
1:A:121[B]:LEU:CD2	1:B:459:VAL:CG2	2.56	0.78
1:G:81:ASP:CA	4:G:7282:HOH:O	2.32	0.78
1:D:418:GLN:HG3	4:D:7275:HOH:O	1.83	0.77
1:B:133:ALA:O	4:B:7457:HOH:O	2.01	0.77
1:H:133:ALA:O	4:H:7369:HOH:O	2.02	0.77
1:D:101:ASP:OD1	4:D:7484:HOH:O	2.02	0.77
1:A:459:VAL:CB	1:B:121[B]:LEU:CD2	2.62	0.77
1:G:82:SER:N	4:G:7236:HOH:O	2.17	0.77
1:G:462:SER:OG	4:G:7489:HOH:O	2.03	0.76
1:A:500:PRO:HD3	4:A:7531:HOH:O	1.85	0.76
3:E:7004:MES:C7	4:E:7440:HOH:O	2.32	0.76
1:D:176:ASP:CG	4:D:7499:HOH:O	2.24	0.75
1:D:459:VAL:HG22	1:C:121[B]:LEU:CG	2.15	0.75
1:D:459:VAL:CG2	1:C:121[B]:LEU:CD2	2.47	0.75
1:F:81:ASP:HB2	4:F:7258:HOH:O	1.86	0.75
1:G:81:ASP:C	4:G:7236:HOH:O	2.29	0.74
1:A:429:GLU:HG2	4:A:7455:HOH:O	1.86	0.74
1:C:619:THR:O	1:C:619:THR:HG23	1.86	0.74
1:F:121[A]:LEU:HD21	1:G:121[A]:LEU:CD2	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:299:HIS:HE2	1:F:310:GLU:CD	1.96	0.74
1:D:100:ILE:HD13	1:D:100:ILE:C	2.11	0.74
1:D:178:GLU:CB	4:D:7499:HOH:O	2.32	0.74
1:E:121[B]:LEU:HD23	1:F:459:VAL:CA	2.16	0.74
1:A:459:VAL:HG22	1:B:121[B]:LEU:HD22	1.64	0.73
1:E:133:ALA:O	4:E:7440:HOH:O	2.05	0.73
1:E:121[B]:LEU:HD21	1:F:459:VAL:HG22	0.76	0.73
4:B:7457:HOH:O	1:C:505:ARG:NH2	2.22	0.73
1:G:167:HIS:CE1	2:G:801:FAD:HM82	2.12	0.72
1:B:167:HIS:CE1	2:B:801:FAD:HM82	2.14	0.72
1:B:542:GLU:HB2	4:B:7476:HOH:O	1.90	0.72
1:D:341:ASN:ND2	4:D:7479:HOH:O	2.19	0.72
1:E:176:ASP:OD2	4:E:7312:HOH:O	2.07	0.72
1:A:496:ASN:CG	4:A:7509:HOH:O	2.32	0.71
1:D:452[B]:ASP:OD1	4:D:7467:HOH:O	2.08	0.71
1:A:228:GLU:HG3	4:A:7294:HOH:O	1.90	0.71
1:E:133:ALA:C	4:E:7440:HOH:O	2.33	0.71
1:B:285:ARG:CD	4:B:7315:HOH:O	2.24	0.71
3:E:7004:MES:H72	4:E:7440:HOH:O	1.88	0.71
1:F:121[A]:LEU:CD2	1:G:121[A]:LEU:HD21	2.19	0.71
1:B:121[A]:LEU:HD21	1:C:121[A]:LEU:HD23	1.70	0.71
1:B:478:GLU:HB2	4:B:7501:HOH:O	1.90	0.71
1:G:121[B]:LEU:HD23	1:H:459:VAL:HG23	1.68	0.70
1:D:178:GLU:OE1	4:D:7294:HOH:O	2.08	0.70
1:G:123:VAL:HG22	1:H:459:VAL:HG22	1.72	0.70
1:E:121[B]:LEU:CD2	1:F:459:VAL:HA	2.19	0.70
1:E:323:VAL:HG21	4:E:7494:HOH:O	1.91	0.70
1:H:100:ILE:HG12	4:H:7283:HOH:O	1.92	0.70
1:B:385:THR:HG22	4:B:7411:HOH:O	1.91	0.70
1:F:167:HIS:HE2	2:F:801:FAD:HM81	1.39	0.70
1:A:459:VAL:CA	1:B:121[B]:LEU:CD2	2.58	0.69
1:B:505:ARG:NH2	4:C:7327:HOH:O	2.25	0.69
1:F:81:ASP:CA	4:F:7258:HOH:O	2.39	0.69
1:D:459:VAL:HG23	1:C:121[B]:LEU:HD21	1.72	0.69
1:G:81:ASP:C	4:G:7282:HOH:O	2.35	0.69
3:D:7007:MES:C7	4:D:7447:HOH:O	2.24	0.69
1:E:121[A]:LEU:CD2	1:H:121[A]:LEU:CD2	2.71	0.69
1:E:421:GLU:OE2	4:E:7504:HOH:O	2.11	0.68
1:E:121[B]:LEU:HD22	1:F:459:VAL:HG22	1.68	0.68
1:E:244:THR:O	4:E:7477:HOH:O	2.11	0.68
1:H:211:ASP:HB3	4:H:7331:HOH:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:GLU:HG3	4:B:7219:HOH:O	1.93	0.68
1:C:45:ILE:HG23	4:C:7267:HOH:O	1.92	0.68
1:G:101:ASP:O	1:G:104[A]:VAL:HG23	1.94	0.68
1:E:178:GLU:OE1	4:E:7312:HOH:O	2.11	0.68
1:F:299:HIS:NE2	1:F:310:GLU:CD	2.51	0.68
1:F:121[A]:LEU:HD21	1:G:121[A]:LEU:HD22	1.74	0.68
1:A:104:VAL:CB	4:A:7508:HOH:O	2.04	0.67
1:D:101:ASP:HA	4:D:7506:HOH:O	1.92	0.67
1:E:167:HIS:CE1	2:E:801:FAD:HM82	2.19	0.67
4:G:7299:HOH:O	1:H:84:LEU:HD23	1.95	0.67
1:A:250:PHE:CD2	4:A:7511:HOH:O	2.46	0.66
1:G:104[B]:VAL:HG13	4:G:7438:HOH:O	1.94	0.66
1:E:84:LEU:HD23	4:F:7219:HOH:O	1.94	0.66
1:B:339:ARG:HG3	4:B:7417:HOH:O	1.95	0.66
1:E:100:ILE:HB	4:E:7441:HOH:O	1.95	0.66
1:A:121[B]:LEU:HD23	1:B:459:VAL:HG22	1.72	0.66
1:D:418:GLN:CG	4:D:7275:HOH:O	2.41	0.66
1:E:82:SER:O	4:E:7256:HOH:O	2.14	0.66
1:E:133:ALA:CA	4:E:7440:HOH:O	2.43	0.66
1:C:82:SER:O	4:C:7311:HOH:O	2.12	0.66
1:F:97:GLN:HG3	1:F:250:PHE:CE2	2.30	0.66
1:B:528:LYS:HE3	4:B:7428:HOH:O	1.95	0.66
1:F:178:GLU:OE2	4:F:7347:HOH:O	2.14	0.66
1:A:496:ASN:CG	4:A:7324:HOH:O	2.37	0.66
1:E:121[B]:LEU:HD12	4:E:7181:HOH:O	1.95	0.66
1:E:133:ALA:HB3	4:E:7440:HOH:O	1.94	0.66
1:A:84:LEU:HD23	4:B:7307:HOH:O	1.95	0.66
1:C:133:ALA:O	4:C:7327:HOH:O	2.12	0.66
1:F:121[A]:LEU:CD2	1:G:121[A]:LEU:HD22	2.22	0.65
1:G:490:LYS:HD3	1:G:491:ILE:HD13	1.78	0.65
1:B:542:GLU:CB	4:B:7476:HOH:O	2.41	0.65
1:A:228:GLU:OE1	4:A:7390:HOH:O	2.15	0.65
1:E:97:GLN:HG3	1:E:250:PHE:CE2	2.32	0.65
1:H:310:GLU:OE1	4:H:7456:HOH:O	2.14	0.65
1:B:596:LEU:HD13	4:B:7543:HOH:O	1.97	0.65
1:G:81:ASP:C	1:G:81:ASP:OD1	2.37	0.65
1:G:121[B]:LEU:CD2	1:H:459:VAL:CA	2.70	0.65
1:D:100:ILE:C	1:D:100:ILE:CD1	2.70	0.64
3:E:7004:MES:H71	4:E:7440:HOH:O	1.94	0.64
1:E:167:HIS:HE2	2:E:801:FAD:HM82	0.50	0.64
1:D:91:LYS:CE	4:D:7373:HOH:O	2.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:81:ASP:CB	4:F:7258:HOH:O	2.45	0.64
1:F:121[A]:LEU:HD23	1:G:121[A]:LEU:CD2	2.27	0.64
1:H:459:VAL:HG13	4:H:7517:HOH:O	1.97	0.64
1:E:286:VAL:HG22	4:E:7444:HOH:O	1.97	0.64
1:E:91:LYS:CE	4:E:7268:HOH:O	2.47	0.63
1:F:121[A]:LEU:HD22	1:G:121[A]:LEU:CD2	2.27	0.63
1:E:97:GLN:HG3	1:E:250:PHE:CD2	2.34	0.63
1:A:121[B]:LEU:HD12	4:A:7267:HOH:O	1.96	0.63
1:D:133:ALA:HB3	4:D:7447:HOH:O	1.97	0.63
1:C:97:GLN:HG3	1:C:250:PHE:CE2	2.34	0.63
1:D:421:GLU:HG3	4:D:7367:HOH:O	1.99	0.63
1:B:91:LYS:CE	4:B:7302:HOH:O	2.47	0.62
1:C:100:ILE:HG12	4:C:7341:HOH:O	2.00	0.62
1:E:459:VAL:HA	1:F:121[B]:LEU:HD23	1.81	0.62
1:F:121[A]:LEU:HD22	1:G:121[A]:LEU:HD21	1.82	0.62
1:C:341:ASN:ND2	4:C:7416:HOH:O	2.32	0.62
1:G:459:VAL:CG2	1:H:121[B]:LEU:CD2	2.66	0.62
1:A:104:VAL:CG2	4:A:7508:HOH:O	2.42	0.62
1:B:121[A]:LEU:CD2	1:C:121[A]:LEU:HD21	2.29	0.62
1:G:101:ASP:HA	4:G:7438:HOH:O	1.99	0.62
1:A:194:GLU:CG	4:A:7452:HOH:O	2.39	0.62
1:F:81:ASP:C	4:F:7258:HOH:O	2.41	0.62
1:B:91:LYS:NZ	4:B:7302:HOH:O	2.28	0.61
1:B:97:GLN:HG3	1:B:250:PHE:CE2	2.34	0.61
1:G:561:GLU:HG3	4:G:7264:HOH:O	2.00	0.61
1:H:101:ASP:CG	4:H:7503:HOH:O	2.44	0.61
1:G:97:GLN:HG3	1:G:250:PHE:CE2	2.36	0.61
1:G:496:ASN:HB2	4:G:7476:HOH:O	2.00	0.61
1:B:618:PHE:HB3	4:B:7490:HOH:O	2.01	0.61
1:E:167:HIS:HE2	2:E:801:FAD:C8	2.02	0.61
1:D:561:GLU:HG2	4:D:7296:HOH:O	2.00	0.60
1:C:285:ARG:HD3	4:C:7309:HOH:O	2.01	0.60
1:G:121[B]:LEU:HD21	1:H:459:VAL:CB	2.31	0.60
1:B:547:LEU:CD1	2:B:801:FAD:HM83	2.32	0.60
1:D:123:VAL:HG22	1:C:459:VAL:CG1	2.31	0.60
1:A:341:ASN:HD22	1:A:342:PRO:HD2	1.66	0.60
1:E:505:ARG:NH2	4:E:7318:HOH:O	2.34	0.60
4:G:7261:HOH:O	1:H:81:ASP:HA	2.00	0.60
1:C:389:LEU:H	1:C:389:LEU:HD12	1.67	0.60
1:C:505:ARG:NH2	4:C:7312:HOH:O	2.35	0.59
1:A:133:ALA:O	4:A:7279:HOH:O	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:341:ASN:HB3	4:G:7527:HOH:O	2.03	0.59
1:B:284:GLU:C	1:B:285:ARG:HG2	2.27	0.59
1:B:413:LYS:HE3	4:B:7494:HOH:O	2.01	0.59
1:B:121[A]:LEU:HD22	1:C:121[A]:LEU:CD2	2.31	0.58
1:B:167:HIS:HE2	2:B:801:FAD:C8	2.01	0.58
1:G:104[A]:VAL:HG23	4:G:7438:HOH:O	2.03	0.58
1:G:121[B]:LEU:CD2	1:H:459:VAL:CB	2.80	0.58
1:E:246:ARG:NE	4:E:7477:HOH:O	2.36	0.58
4:A:7279:HOH:O	1:D:505:ARG:NH2	2.35	0.58
1:H:346:PRO:HG2	1:H:350:PRO:HA	1.85	0.58
1:C:50:VAL:HG13	1:C:313:ALA:HB2	1.86	0.58
1:H:91:LYS:NZ	4:H:7301:HOH:O	2.17	0.58
4:D:7493:HOH:O	1:C:160:VAL:CG1	2.44	0.58
1:G:104[A]:VAL:HG21	1:G:454:PHE:C	2.29	0.58
1:E:91:LYS:NZ	4:E:7268:HOH:O	2.34	0.58
1:B:341:ASN:HD22	1:B:342:PRO:N	2.03	0.57
1:C:167:HIS:CD2	2:C:801:FAD:C8M	2.71	0.57
1:E:299:HIS:CE1	1:E:310:GLU:HG2	2.39	0.57
1:F:83:GLY:N	4:F:7220:HOH:O	2.31	0.57
1:F:121[A]:LEU:CD2	1:G:121[A]:LEU:HD23	2.30	0.57
1:G:121[B]:LEU:HD23	1:H:459:VAL:CG2	2.27	0.57
1:A:50:VAL:HG13	1:A:313:ALA:HB2	1.86	0.57
1:B:81:ASP:OD1	1:B:81:ASP:C	2.44	0.57
1:D:121[B]:LEU:HD23	1:C:459:VAL:HA	1.86	0.57
1:G:398:GLY:O	1:G:399:ALA:C	2.47	0.57
1:E:505:ARG:NH2	4:H:7369:HOH:O	2.38	0.56
1:G:459:VAL:HA	1:H:121[B]:LEU:HD23	1.85	0.56
1:E:100:ILE:HD13	1:E:100:ILE:O	2.05	0.56
1:G:83:GLY:N	4:G:7261:HOH:O	2.21	0.56
4:F:7418:HOH:O	1:G:121[A]:LEU:HD11	2.03	0.56
1:B:167:HIS:HE2	2:B:801:FAD:HM82	0.40	0.56
1:B:121[A]:LEU:HD22	1:C:121[A]:LEU:HD21	1.87	0.56
1:F:505:ARG:NH2	4:G:7361:HOH:O	2.39	0.56
1:H:45:ILE:C	1:H:45:ILE:HD12	2.31	0.56
1:A:272:GLU:HG2	4:A:7368:HOH:O	2.04	0.56
1:F:481:GLU:HG2	4:F:7362:HOH:O	2.06	0.56
1:G:97:GLN:HG3	1:G:250:PHE:CD2	2.41	0.56
1:G:104[A]:VAL:CG2	4:G:7438:HOH:O	2.53	0.56
1:B:167:HIS:NE2	2:B:801:FAD:HM81	2.06	0.56
1:G:444:PRO:HD2	1:G:445:TRP:CZ3	2.41	0.55
1:F:50:VAL:HG13	1:F:313:ALA:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:231:LYS:HE3	4:H:7487:HOH:O	2.05	0.55
1:A:81:ASP:C	1:A:81:ASP:OD1	2.45	0.55
1:B:97:GLN:HG3	1:B:250:PHE:CD2	2.41	0.55
1:H:310:GLU:CD	4:H:7456:HOH:O	2.49	0.55
1:A:576:LYS:HE2	4:A:7432:HOH:O	2.07	0.55
1:B:341:ASN:ND2	1:B:343:ALA:H	2.04	0.55
1:H:45:ILE:HG22	4:H:7444:HOH:O	2.07	0.55
1:B:167:HIS:NE2	2:B:801:FAD:C8	2.66	0.54
1:E:441:PRO:HD3	4:E:7312:HOH:O	2.07	0.54
1:D:228:GLU:HG3	4:D:7312:HOH:O	2.07	0.54
1:G:418:GLN:CG	4:G:7510:HOH:O	2.36	0.54
1:D:97:GLN:HG3	1:D:250:PHE:CE2	2.43	0.54
1:E:323:VAL:CG2	4:E:7494:HOH:O	2.51	0.54
1:E:421:GLU:HG3	4:F:7340:HOH:O	2.07	0.54
1:A:390:THR:HG23	4:A:7528:HOH:O	2.08	0.54
1:B:101:ASP:O	1:B:104[B]:VAL:HG22	2.08	0.54
1:E:133:ALA:CB	4:E:7440:HOH:O	2.55	0.54
1:E:121[B]:LEU:CD2	1:F:459:VAL:CB	2.86	0.54
1:D:454:PHE:HB3	4:D:7484:HOH:O	2.08	0.54
1:A:121[A]:LEU:CD2	1:D:121[A]:LEU:CD2	2.86	0.53
1:E:246:ARG:HG2	4:E:7477:HOH:O	2.07	0.53
1:E:547:LEU:CD1	2:E:801:FAD:HM83	2.38	0.53
1:B:341:ASN:HD22	1:B:342:PRO:CD	2.21	0.53
1:D:305:SER:HB3	4:D:7472:HOH:O	2.06	0.53
1:A:121[B]:LEU:HD23	1:B:459:VAL:HA	1.90	0.53
1:B:43:MET:N	4:B:7389:HOH:O	2.40	0.53
1:D:133:ALA:CA	4:D:7447:HOH:O	2.56	0.53
1:D:576:LYS:CD	4:D:7295:HOH:O	2.55	0.53
1:B:45:ILE:HG23	4:B:7361:HOH:O	2.08	0.53
1:C:619:THR:O	1:C:619:THR:CG2	2.56	0.53
1:H:211:ASP:CB	4:H:7331:HOH:O	2.56	0.53
1:D:123:VAL:HG22	1:C:459:VAL:HG12	1.90	0.53
1:C:97:GLN:HG3	1:C:250:PHE:CD2	2.43	0.53
1:E:418:GLN:HE21	1:E:418:GLN:HA	1.73	0.53
1:B:341:ASN:HD22	1:B:342:PRO:HD2	1.73	0.53
1:G:167:HIS:CE1	2:G:801:FAD:C8M	2.84	0.53
1:E:133:ALA:N	4:E:7440:HOH:O	2.42	0.53
1:G:81:ASP:HA	4:G:7282:HOH:O	2.02	0.53
1:A:496:ASN:CB	4:A:7324:HOH:O	2.57	0.52
1:D:133:ALA:C	4:D:7447:HOH:O	2.52	0.52
1:G:341:ASN:HD22	1:G:342:PRO:HD2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:GLN:CD	4:B:7569:HOH:O	2.52	0.52
1:E:56:PRO:HD3	1:E:165:SER:HB3	1.91	0.52
1:E:244:THR:HB	4:E:7477:HOH:O	2.08	0.52
1:H:618:PHE:HB3	4:H:7438:HOH:O	2.10	0.52
1:A:121[B]:LEU:HD23	1:B:459:VAL:CG2	2.36	0.52
1:A:459:VAL:CG1	1:B:121[B]:LEU:HD21	2.39	0.52
1:C:618:PHE:CD1	1:C:618:PHE:C	2.88	0.52
1:E:268:THR:HG22	4:E:7484:HOH:O	2.10	0.52
1:F:383:ARG:HB2	1:F:392:SER:HB3	1.92	0.52
1:A:194:GLU:CD	4:A:7452:HOH:O	2.51	0.51
1:F:157:VAL:HG21	1:F:324:HIS:HE1	1.74	0.51
1:G:481:GLU:HG2	4:G:7262:HOH:O	2.10	0.51
1:G:547:LEU:CD1	2:G:801:FAD:HM83	2.39	0.51
4:D:7493:HOH:O	1:C:110:GLN:HB2	2.09	0.51
1:C:618:PHE:C	1:C:618:PHE:HD1	2.17	0.51
1:E:91:LYS:HE3	4:E:7268:HOH:O	2.10	0.51
1:E:167:HIS:NE2	2:E:801:FAD:C8	2.68	0.51
1:D:414:ASN:O	1:D:418:GLN:HG2	2.10	0.51
1:C:218:ARG:HD2	4:C:7083:HOH:O	2.09	0.51
1:F:201:LYS:NZ	4:F:7388:HOH:O	2.44	0.51
1:A:607:GLU:HG3	4:A:7438:HOH:O	2.09	0.51
1:B:104[B]:VAL:HG21	1:B:455:SER:HB3	1.93	0.51
1:E:459:VAL:HG22	1:F:121[B]:LEU:HD23	1.81	0.51
1:E:285:ARG:NH1	1:E:299:HIS:CD2	2.79	0.51
4:E:7492:HOH:O	1:F:463:ILE:CD1	2.47	0.51
1:B:121[A]:LEU:HD23	1:C:121[A]:LEU:HD23	1.92	0.51
1:C:153:SER:OG	1:C:542:GLU:HG3	2.11	0.51
1:A:285:ARG:HA	1:A:328:LEU:HD13	1.93	0.50
1:F:388:GLU:HB3	4:F:7431:HOH:O	2.10	0.50
1:D:121[B]:LEU:CD2	1:C:459:VAL:CG2	2.59	0.50
1:G:81:ASP:CB	4:G:7282:HOH:O	2.59	0.50
1:G:341:ASN:HD22	1:G:342:PRO:CD	2.25	0.50
1:F:390:THR:HG23	4:F:7431:HOH:O	2.10	0.50
1:A:97:GLN:CB	4:A:7511:HOH:O	2.28	0.50
1:G:121[B]:LEU:CG	1:H:459:VAL:HG23	2.32	0.50
1:D:158:THR:HG22	1:D:160:VAL:HG22	1.93	0.50
1:D:215:GLU:CD	4:D:7508:HOH:O	2.55	0.50
1:F:121[A]:LEU:HD23	1:G:121[A]:LEU:HD23	1.92	0.50
1:B:45:ILE:HD12	1:B:45:ILE:C	2.37	0.50
1:D:134:SER:HB2	4:D:7389:HOH:O	2.12	0.50
1:D:167:HIS:CE1	2:D:801:FAD:C8M	2.81	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:538:PRO:HG2	1:D:538:PRO:HG2	1.93	0.49
1:D:215:GLU:O	1:D:411:LYS:NZ	2.45	0.49
1:D:607:GLU:HG3	4:D:7304:HOH:O	2.12	0.49
1:F:45:ILE:HG22	1:F:45:ILE:O	2.11	0.49
1:A:43:MET:HE3	4:A:7361:HOH:O	2.12	0.49
1:F:285:ARG:HA	1:F:328:LEU:HD13	1.94	0.49
1:G:218:ARG:HD2	4:G:7043:HOH:O	2.12	0.49
1:B:45:ILE:HD12	1:B:45:ILE:O	2.12	0.49
1:F:97:GLN:HG3	1:F:250:PHE:CD2	2.47	0.49
1:H:44:ASP:HB3	4:H:7417:HOH:O	2.12	0.49
1:A:250:PHE:CE2	4:A:7511:HOH:O	2.65	0.49
1:A:542:GLU:OE1	1:A:545:LEU:HD13	2.12	0.49
1:E:346:PRO:HG2	1:E:350:PRO:HA	1.95	0.49
1:G:167:HIS:NE2	2:G:801:FAD:HM81	2.10	0.49
1:B:284:GLU:O	1:B:285:ARG:HG2	2.13	0.49
1:B:341:ASN:ND2	1:B:342:PRO:HD2	2.28	0.49
1:D:481:GLU:HG2	4:D:7272:HOH:O	2.13	0.49
1:C:157:VAL:HG21	1:C:324:HIS:HE1	1.78	0.49
1:D:284:GLU:C	1:D:328:LEU:CD1	2.86	0.49
1:E:167:HIS:NE2	2:E:801:FAD:HM81	2.07	0.49
1:H:459:VAL:CG1	4:H:7380:HOH:O	2.61	0.49
1:A:218:ARG:HD2	4:A:7091:HOH:O	2.13	0.49
1:D:453:ALA:HB3	4:D:7513:HOH:O	2.12	0.49
1:C:81:ASP:OD1	1:C:81:ASP:C	2.51	0.49
1:H:482:GLU:HG3	4:H:7357:HOH:O	2.12	0.49
1:H:547:LEU:CD1	2:H:801:FAD:HM83	2.43	0.48
1:C:385:THR:OG1	1:C:388:GLU:OE1	2.15	0.48
1:G:81:ASP:HB2	4:G:7282:HOH:O	2.12	0.48
1:G:91:LYS:HG2	4:G:7395:HOH:O	2.13	0.48
1:B:153:SER:OG	1:B:542:GLU:HG3	2.12	0.48
1:F:45:ILE:O	1:F:45:ILE:CG2	2.62	0.48
1:F:83:GLY:CA	4:F:7220:HOH:O	2.61	0.48
1:G:47:TYR:O	1:G:313:ALA:HA	2.13	0.48
1:G:457:GLY:O	1:G:461:GLN:HG3	2.13	0.48
1:A:312:LYS:HD2	4:A:7560:HOH:O	2.13	0.48
1:B:167:HIS:CE1	2:B:801:FAD:C8M	2.83	0.48
1:D:133:ALA:N	4:D:7447:HOH:O	2.46	0.48
1:E:100:ILE:CG2	1:E:101:ASP:N	2.77	0.48
1:H:91:LYS:CE	4:H:7301:HOH:O	2.60	0.48
1:E:215:GLU:O	1:E:411:LYS:NZ	2.47	0.48
1:D:101:ASP:O	1:D:104:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:459:VAL:HG22	1:F:121[B]:LEU:CG	2.39	0.48
1:H:411:LYS:HE3	4:H:7382:HOH:O	2.14	0.48
1:A:285:ARG:HA	1:A:328:LEU:CD1	2.44	0.48
1:A:389:LEU:HD12	1:A:389:LEU:H	1.79	0.48
1:D:561:GLU:CG	4:D:7296:HOH:O	2.61	0.48
1:C:287:VAL:HG22	4:C:7452:HOH:O	2.14	0.48
1:F:538:PRO:HG2	1:H:538:PRO:HG2	1.95	0.48
1:H:50:VAL:HG13	1:H:313:ALA:HB2	1.94	0.48
1:B:218:ARG:HD2	4:B:7023:HOH:O	2.14	0.47
1:C:619:THR:HG22	4:C:7283:HOH:O	2.13	0.47
1:F:47:TYR:O	1:F:313:ALA:HA	2.14	0.47
1:G:390:THR:HG23	4:G:7485:HOH:O	2.13	0.47
4:G:7236:HOH:O	1:H:83:GLY:N	2.47	0.47
1:H:228:GLU:HG3	4:H:7256:HOH:O	2.14	0.47
1:C:44:ASP:OD2	1:C:71:LYS:NZ	2.36	0.47
1:B:153:SER:OG	1:B:542:GLU:CG	2.61	0.47
1:E:100:ILE:HD13	1:E:100:ILE:C	2.39	0.47
1:E:100:ILE:HG23	1:E:101:ASP:N	2.28	0.47
1:E:547:LEU:HD12	2:E:801:FAD:HM83	1.96	0.47
1:G:459:VAL:HG22	1:H:121[B]:LEU:CG	2.43	0.47
1:C:104:VAL:CG2	1:C:453:ALA:C	2.87	0.47
1:F:83:GLY:HA2	4:F:7220:HOH:O	2.13	0.47
1:A:81:ASP:O	1:A:90:LYS:HE2	2.14	0.47
1:A:123:VAL:HG22	1:B:459:VAL:CG1	2.44	0.47
1:H:401:THR:HG23	4:H:7440:HOH:O	2.13	0.47
1:A:121[B]:LEU:CG	1:B:459:VAL:HG22	2.41	0.47
1:A:452:ASP:N	1:A:452:ASP:OD1	2.47	0.47
1:B:46:LYS:HE2	4:B:7320:HOH:O	2.15	0.47
1:D:91:LYS:NZ	4:D:7373:HOH:O	2.34	0.47
1:D:547:LEU:CD1	2:D:801:FAD:HM83	2.44	0.47
1:G:133:ALA:O	4:G:7361:HOH:O	2.20	0.47
1:E:43:MET:HE2	4:E:7461:HOH:O	2.14	0.47
1:H:215:GLU:O	1:H:411:LYS:NZ	2.47	0.47
1:C:478:GLU:HG2	1:C:480:LYS:HE2	1.96	0.47
1:F:385:THR:OG1	1:F:388:GLU:OE1	2.28	0.46
1:G:50:VAL:HG13	1:G:313:ALA:HB2	1.98	0.46
1:A:123:VAL:HG22	1:B:459:VAL:HG12	1.97	0.46
1:F:167:HIS:CE1	2:F:801:FAD:C8M	2.83	0.46
1:G:490:LYS:CD	1:G:491:ILE:HD13	2.45	0.46
1:A:341:ASN:HD22	1:A:342:PRO:CD	2.28	0.46
1:F:100:ILE:HG23	1:F:101:ASP:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:328:LEU:C	1:F:328:LEU:HD12	2.41	0.46
1:F:490:LYS:HE2	4:F:7441:HOH:O	2.15	0.46
1:H:570:SER:HB3	1:H:580:LEU:O	2.16	0.46
1:D:159:ARG:HA	2:D:801:FAD:O2B	2.16	0.46
1:C:100:ILE:HG23	1:C:101:ASP:N	2.30	0.46
1:C:196:ASP:HB2	4:C:7288:HOH:O	2.15	0.46
1:E:388:GLU:HG2	4:E:7463:HOH:O	2.15	0.46
1:D:50:VAL:HG13	1:D:313:ALA:HB2	1.96	0.46
1:H:167:HIS:CD2	2:H:801:FAD:C8M	2.70	0.46
1:B:339:ARG:CG	4:B:7417:HOH:O	2.59	0.46
1:D:167:HIS:NE2	2:D:801:FAD:C8	2.71	0.46
1:C:47:TYR:O	1:C:313:ALA:HA	2.15	0.46
1:C:285:ARG:NH1	4:C:7362:HOH:O	2.48	0.46
1:B:340:PRO:HD2	4:B:7417:HOH:O	2.16	0.45
1:G:218:ARG:HG3	1:G:430:ASP:OD2	2.16	0.45
1:A:542:GLU:HB2	4:D:7486:HOH:O	2.16	0.45
1:C:285:ARG:HA	1:C:328:LEU:CD1	2.46	0.45
1:E:121[A]:LEU:CD2	1:H:121[A]:LEU:HD21	2.46	0.45
1:B:312:LYS:HE2	4:B:7320:HOH:O	2.17	0.45
1:F:218:ARG:HG3	1:F:430:ASP:OD2	2.16	0.45
1:E:538:PRO:HG2	1:G:538:PRO:HG2	1.97	0.45
1:G:618:PHE:C	1:G:618:PHE:CD1	2.94	0.45
1:D:218:ARG:HD2	4:D:7043:HOH:O	2.16	0.45
1:D:293:SER:HA	1:D:574:GLY:O	2.17	0.45
1:E:47:TYR:O	1:E:313:ALA:HA	2.17	0.45
1:E:121[B]:LEU:HD23	1:F:459:VAL:CB	2.46	0.45
1:A:459:VAL:HG13	1:B:121[B]:LEU:CD2	2.46	0.45
1:E:112:MET:HE2	1:F:95:GLU:HG3	1.99	0.45
1:H:139:ARG:HD3	3:H:7002:MES:O3S	2.16	0.45
1:D:570:SER:HB3	1:D:580:LEU:O	2.16	0.45
1:F:64:GLU:OE1	4:F:7408:HOH:O	2.21	0.45
1:A:153:SER:OG	1:A:542:GLU:HG3	2.17	0.45
1:A:618:PHE:CD1	1:A:618:PHE:C	2.94	0.45
1:C:363:PHE:HA	1:C:471:TRP:O	2.17	0.45
1:F:211:ASP:HB2	1:F:214:LYS:HD3	1.98	0.45
1:A:459:VAL:CG1	1:B:123:VAL:HG22	2.46	0.45
1:D:505:ARG:NH2	4:D:7289:HOH:O	2.50	0.45
1:E:218:ARG:HD2	4:E:7084:HOH:O	2.17	0.45
1:F:121[A]:LEU:HD23	4:G:7292:HOH:O	2.16	0.45
1:F:167:HIS:NE2	2:F:801:FAD:HM81	2.12	0.45
1:B:185:LYS:HG2	4:B:7319:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:GLN:HB2	4:D:7436:HOH:O	2.16	0.45
1:C:285:ARG:HA	1:C:328:LEU:HD11	1.99	0.45
1:A:346:PRO:HG2	1:A:350:PRO:HA	1.99	0.44
1:C:383:ARG:HB3	1:C:392:SER:HB3	1.98	0.44
1:E:343:ALA:O	1:E:344:ASN:HB2	2.16	0.44
1:H:252:GLU:CD	4:H:7482:HOH:O	2.60	0.44
1:D:285:ARG:HG3	1:D:299:HIS:HB2	1.99	0.44
1:B:547:LEU:HD12	2:B:801:FAD:HM83	2.00	0.44
1:C:100:ILE:HG22	4:C:7271:HOH:O	2.17	0.44
1:C:285:ARG:CD	4:C:7309:HOH:O	2.64	0.44
1:F:167:HIS:NE2	2:F:801:FAD:C8	2.72	0.44
1:G:83:GLY:CA	4:G:7261:HOH:O	2.62	0.44
1:G:285:ARG:NH2	1:G:299:HIS:HD2	2.15	0.44
1:G:336:GLN:NE2	1:G:344:ASN:O	2.50	0.44
1:H:196:ASP:HB2	4:H:7258:HOH:O	2.17	0.44
1:B:104[A]:VAL:HG21	1:B:454:PHE:C	2.42	0.44
1:B:265:ARG:HA	1:B:266:PRO:C	2.43	0.44
1:B:341:ASN:HD22	1:B:341:ASN:C	2.26	0.44
3:A:7003:MES:H51	3:A:7003:MES:O1S	2.18	0.44
1:B:342:PRO:O	1:B:345:PRO:HD3	2.18	0.44
1:D:413:LYS:HE2	1:D:414:ASN:OD1	2.17	0.44
1:C:346:PRO:HG2	1:C:350:PRO:HA	1.99	0.44
1:G:81:ASP:CG	1:G:81:ASP:O	2.60	0.44
1:E:136:PHE:HA	4:E:7426:HOH:O	2.17	0.44
1:E:167:HIS:CD2	1:E:167:HIS:C	2.96	0.44
1:G:81:ASP:OD1	1:G:81:ASP:O	2.35	0.44
1:G:121[A]:LEU:HD23	4:G:7292:HOH:O	2.18	0.44
1:B:394:THR:OG1	4:B:7370:HOH:O	2.21	0.44
1:C:104:VAL:HG21	1:C:454:PHE:CA	2.48	0.44
1:B:159:ARG:HA	2:B:801:FAD:O2B	2.18	0.44
1:E:81:ASP:HA	4:F:7220:HOH:O	2.16	0.44
1:H:104:VAL:CG2	4:H:7426:HOH:O	2.49	0.44
1:C:385:THR:N	4:C:7487:HOH:O	2.48	0.44
1:E:459:VAL:CA	1:F:121[B]:LEU:HD23	2.48	0.44
1:H:444:PRO:HD2	1:H:445:TRP:CZ3	2.53	0.44
1:G:81:ASP:O	1:G:90:LYS:HE2	2.17	0.43
1:H:173:PRO:HG2	1:H:592:ALA:HB1	1.99	0.43
1:A:496:ASN:HB3	4:A:7324:HOH:O	2.17	0.43
1:E:246:ARG:CD	4:E:7477:HOH:O	2.66	0.43
1:H:100:ILE:C	1:H:100:ILE:HD13	2.43	0.43
1:A:167:HIS:CE1	2:A:801:FAD:C8M	2.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:285:ARG:HH12	1:E:299:HIS:CD2	2.36	0.43
1:A:478:GLU:HB2	4:A:7366:HOH:O	2.18	0.43
1:E:293:SER:HA	1:E:574:GLY:O	2.17	0.43
1:E:452:ASP:OD1	1:E:452:ASP:N	2.49	0.43
1:B:126:LEU:HD12	1:B:132:GLN:HG3	2.01	0.43
1:C:104:VAL:HG22	1:C:453:ALA:C	2.42	0.43
1:E:45:ILE:HG22	1:E:45:ILE:O	2.18	0.43
1:G:380:MET:HE1	1:G:409:ASN:O	2.18	0.43
1:D:89:HIS:CE1	1:D:91:LYS:HG2	2.54	0.43
1:C:167:HIS:NE2	2:C:801:FAD:HM83	2.04	0.43
3:E:7004:MES:H72	4:E:7426:HOH:O	2.19	0.43
1:F:64:GLU:OE2	1:F:205:TYR:OH	2.36	0.43
1:B:218:ARG:HG3	1:B:430:ASP:OD2	2.18	0.43
1:C:81:ASP:O	1:C:90:LYS:HE2	2.18	0.43
1:E:123:VAL:HB	4:E:7492:HOH:O	2.18	0.43
1:E:363:PHE:HA	1:E:471:TRP:O	2.19	0.43
1:A:538:PRO:HG2	1:C:538:PRO:HG2	2.00	0.43
1:B:158:THR:HG22	1:B:160:VAL:HG22	2.00	0.43
1:E:50:VAL:HG13	1:E:313:ALA:HB2	1.99	0.43
1:E:459:VAL:CG2	1:F:121[B]:LEU:HD23	2.45	0.43
1:B:100:ILE:CG1	4:B:7296:HOH:O	2.67	0.43
1:D:100:ILE:HG23	1:D:101:ASP:N	2.34	0.43
1:H:104:VAL:HG22	1:H:453:ALA:C	2.44	0.43
1:D:510:ARG:NH2	4:D:7443:HOH:O	2.52	0.43
4:A:7336:HOH:O	1:B:84:LEU:CD2	2.48	0.42
1:A:418:GLN:CG	4:A:7330:HOH:O	2.43	0.42
1:A:457:GLY:HA3	4:A:7285:HOH:O	2.19	0.42
1:E:121[A]:LEU:CD2	1:H:121[A]:LEU:HD23	2.48	0.42
1:G:167:HIS:NE2	2:G:801:FAD:C8	2.72	0.42
1:H:218:ARG:HD2	4:H:7077:HOH:O	2.19	0.42
1:A:47:TYR:O	1:A:313:ALA:HA	2.19	0.42
1:B:100:ILE:HG12	4:B:7296:HOH:O	2.17	0.42
1:E:173:PRO:HG2	1:E:592:ALA:HB1	2.01	0.42
1:F:194:GLU:HG2	4:F:7320:HOH:O	2.18	0.42
1:D:47:TYR:O	1:D:313:ALA:HA	2.19	0.42
1:D:81:ASP:C	1:D:81:ASP:OD1	2.60	0.42
1:D:347:GLU:HG3	4:D:7423:HOH:O	2.20	0.42
1:E:121[B]:LEU:CD2	1:F:459:VAL:CA	2.90	0.42
1:F:214:LYS:HB2	4:F:7455:HOH:O	2.20	0.42
1:D:459:VAL:HA	1:C:121[B]:LEU:HD23	2.02	0.42
1:B:132:GLN:NE2	3:B:7006:MES:C3	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:GLN:HE21	1:D:132:GLN:HA	1.85	0.42
1:F:542:GLU:HB3	4:F:7392:HOH:O	2.19	0.42
1:A:281:VAL:CG1	1:A:300:ILE:HB	2.50	0.42
1:C:471:TRP:CH2	1:C:526:SER:HA	2.55	0.42
1:A:538:PRO:HG2	1:C:538:PRO:CG	2.50	0.42
1:B:157:VAL:HG21	1:B:324:HIS:HE1	1.85	0.42
1:D:218:ARG:HG3	1:D:430:ASP:OD2	2.20	0.42
1:E:81:ASP:HB2	4:F:7266:HOH:O	2.19	0.42
1:G:132:GLN:NE2	3:G:7008:MES:C3	2.83	0.42
1:G:296:GLU:O	1:G:312:LYS:HD3	2.20	0.42
1:D:619:THR:HG22	4:D:7311:HOH:O	2.20	0.41
1:G:432:GLU:HB2	1:G:433:PRO:HD2	2.01	0.41
3:G:7008:MES:H51	3:G:7008:MES:O1S	2.19	0.41
1:H:404:HIS:HE1	4:H:7279:HOH:O	2.02	0.41
1:A:398:GLY:O	1:A:399:ALA:C	2.62	0.41
1:A:496:ASN:ND2	4:A:7509:HOH:O	2.51	0.41
1:B:413:LYS:NZ	1:B:414:ASN:OD1	2.51	0.41
1:G:167:HIS:CD2	1:G:167:HIS:C	2.98	0.41
1:A:312:LYS:CD	4:A:7560:HOH:O	2.67	0.41
1:F:433:PRO:O	1:F:450:HIS:HA	2.20	0.41
1:G:471:TRP:CH2	1:G:526:SER:HA	2.55	0.41
1:B:385:THR:OG1	1:B:388:GLU:HG3	2.20	0.41
1:C:159:ARG:HA	2:C:801:FAD:O2B	2.19	0.41
1:E:505:ARG:HD2	4:E:7360:HOH:O	2.20	0.41
1:F:167:HIS:CD2	1:F:167:HIS:C	2.97	0.41
1:H:104:VAL:HG21	1:H:454:PHE:C	2.46	0.41
1:A:159:ARG:HA	2:A:801:FAD:O2B	2.21	0.41
1:D:454:PHE:N	4:D:7484:HOH:O	2.53	0.41
1:E:618:PHE:C	1:E:618:PHE:HD1	2.28	0.41
1:F:341:ASN:HD21	1:F:343:ALA:HB3	1.86	0.41
1:F:618:PHE:CD1	1:F:618:PHE:C	2.97	0.41
1:F:56:PRO:HD3	1:F:165:SER:HB3	2.02	0.41
1:F:547:LEU:CD1	2:F:801:FAD:HM83	2.50	0.41
1:B:570:SER:HB3	1:B:580:LEU:O	2.20	0.41
1:C:158:THR:HG22	1:C:160:VAL:HG22	2.03	0.41
1:G:101:ASP:O	1:G:104[B]:VAL:HG22	2.20	0.41
1:G:385:THR:O	1:G:391:TYR:HB2	2.20	0.41
1:A:265:ARG:HA	1:A:266:PRO:C	2.45	0.41
1:A:471:TRP:CH2	1:A:526:SER:HA	2.56	0.41
1:F:214:LYS:HG3	4:F:7451:HOH:O	2.19	0.41
1:F:606:CYS:O	1:F:610:LYS:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:459:VAL:HG11	4:H:7380:HOH:O	2.21	0.41
1:B:285:ARG:NH1	1:B:299:HIS:HD2	2.18	0.41
1:D:576:LYS:HD3	4:D:7295:HOH:O	2.18	0.41
1:C:444:PRO:HD2	1:C:445:TRP:CZ3	2.56	0.41
1:E:157:VAL:HG21	1:E:324:HIS:HE1	1.86	0.41
1:E:45:ILE:HG23	1:E:310:GLU:O	2.20	0.41
1:E:252:GLU:HB3	4:E:7477:HOH:O	2.21	0.41
1:F:216:SER:HB3	1:F:219:HIS:HB3	2.03	0.41
1:H:47:TYR:O	1:H:313:ALA:HA	2.21	0.41
1:A:215:GLU:O	1:A:411:LYS:NZ	2.53	0.40
1:B:108:GLN:HG2	4:B:7505:HOH:O	2.22	0.40
1:F:444:PRO:HD2	1:F:445:TRP:CZ3	2.56	0.40
1:G:355:TYR:HA	1:G:480:LYS:O	2.20	0.40
1:A:293:SER:HA	1:A:574:GLY:O	2.21	0.40
1:D:510:ARG:CZ	4:D:7443:HOH:O	2.69	0.40
1:C:284:GLU:C	1:C:328:LEU:CD1	2.94	0.40
1:E:81:ASP:OD1	1:E:81:ASP:C	2.63	0.40
1:H:167:HIS:CD2	1:H:167:HIS:C	2.99	0.40
1:D:167:HIS:CD2	1:D:167:HIS:C	3.00	0.40
1:C:121[B]:LEU:HD12	1:C:122:VAL:N	2.37	0.40
1:C:347:GLU:HG2	1:C:348:LEU:HG	2.02	0.40
1:F:478:GLU:CD	4:F:7387:HOH:O	2.65	0.40
1:G:459:VAL:CG1	1:H:123:VAL:HG22	2.52	0.40
1:H:452:ASP:CB	4:H:7281:HOH:O	2.20	0.40
1:D:558:ASP:HB3	1:D:561:GLU:HB2	2.02	0.40
1:F:214:LYS:HE2	4:F:7415:HOH:O	2.21	0.40
1:F:505:ARG:NH2	4:F:7223:HOH:O	2.53	0.40
1:F:570:SER:HB3	1:F:580:LEU:O	2.21	0.40
1:G:159:ARG:HA	2:G:801:FAD:O2B	2.22	0.40
1:A:542:GLU:HA	1:A:543:PRO:HD3	1.97	0.40
1:B:233:GLN:HG2	4:B:7569:HOH:O	2.21	0.40
1:B:607:GLU:HG3	4:B:7364:HOH:O	2.21	0.40
1:D:70:TYR:OH	1:D:610:LYS:HA	2.22	0.40
1:D:336:GLN:HB2	1:D:346:PRO:HG3	2.04	0.40
1:C:100:ILE:HD13	1:C:453:ALA:HA	2.02	0.40
1:G:363:PHE:HA	1:G:471:TRP:O	2.21	0.40
1:H:490:LYS:HD3	1:H:491:ILE:HD13	2.04	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	577/623 (93%)	557 (96%)	20 (4%)	0	100	100
1	B	577/623 (93%)	564 (98%)	13 (2%)	0	100	100
1	C	576/623 (92%)	561 (97%)	14 (2%)	1 (0%)	43	36
1	D	578/623 (93%)	564 (98%)	14 (2%)	0	100	100
1	E	577/623 (93%)	562 (97%)	14 (2%)	1 (0%)	43	36
1	F	576/623 (92%)	560 (97%)	16 (3%)	0	100	100
1	G	577/623 (93%)	561 (97%)	15 (3%)	1 (0%)	43	36
1	H	576/623 (92%)	559 (97%)	17 (3%)	0	100	100
All	All	4614/4984 (93%)	4488 (97%)	123 (3%)	3 (0%)	48	40

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	344	ASN
1	G	399	ALA
1	C	344	ASN

5.3.2 Protein sidechains [i](#)

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	507/542 (94%)	494 (97%)	13 (3%)	40	35
1	B	507/542 (94%)	496 (98%)	11 (2%)	45	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	506/542 (93%)	493 (97%)	13 (3%)	40	35
1	D	508/542 (94%)	499 (98%)	9 (2%)	51	50
1	E	507/542 (94%)	493 (97%)	14 (3%)	38	32
1	F	506/542 (93%)	495 (98%)	11 (2%)	45	42
1	G	507/542 (94%)	494 (97%)	13 (3%)	40	35
1	H	506/542 (93%)	495 (98%)	11 (2%)	45	42
All	All	4054/4336 (94%)	3959 (98%)	95 (2%)	44	40

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	MET
1	A	100	ILE
1	A	185	LYS
1	A	206	PHE
1	A	231	LYS
1	A	312	LYS
1	A	328	LEU
1	A	347	GLU
1	A	389	LEU
1	A	390	THR
1	A	401	THR
1	A	490	LYS
1	A	593	ASN
1	B	45	ILE
1	B	100	ILE
1	B	178	GLU
1	B	185	LYS
1	B	206	PHE
1	B	312	LYS
1	B	328	LEU
1	B	344	ASN
1	B	388	GLU
1	B	490	LYS
1	B	496	ASN
1	D	45	ILE
1	D	100	ILE
1	D	104	VAL
1	D	132	GLN
1	D	383	ARG

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Mol	Chain	Res	Type
1	D	389	LEU
1	D	390	THR
1	D	403	LYS
1	D	496	ASN
1	C	45	ILE
1	C	95	GLU
1	C	100	ILE
1	C	204	SER
1	C	206	PHE
1	C	231	LYS
1	C	385	THR
1	C	389	LEU
1	C	490	LYS
1	C	496	ASN
1	C	593	ASN
1	C	618	PHE
1	C	619	THR
1	E	91	LYS
1	E	100	ILE
1	E	194	GLU
1	E	206	PHE
1	E	228	GLU
1	E	385	THR
1	E	388	GLU
1	E	418	GLN
1	E	452	ASP
1	E	455	SER
1	E	490	LYS
1	E	496	ASN
1	E	542	GLU
1	E	593	ASN
1	F	100	ILE
1	F	206	PHE
1	F	228	GLU
1	F	294	GLU
1	F	328	LEU
1	F	389	LEU
1	F	413	LYS
1	F	465	SER
1	F	496	ASN
1	F	576	LYS
1	F	593	ASN

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Mol	Chain	Res	Type
1	G	45	ILE
1	G	95	GLU
1	G	100	ILE
1	G	104[A]	VAL
1	G	104[B]	VAL
1	G	185	LYS
1	G	206	PHE
1	G	228	GLU
1	G	385	THR
1	G	413	LYS
1	G	490	LYS
1	G	496	ASN
1	G	619	THR
1	H	100	ILE
1	H	185	LYS
1	H	194	GLU
1	H	206	PHE
1	H	328	LEU
1	H	385	THR
1	H	389	LEU
1	H	421	GLU
1	H	459	VAL
1	H	496	ASN
1	H	593	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	GLN
1	A	257	ASN
1	A	263	GLN
1	A	276	ASN
1	A	336	GLN
1	A	341	ASN
1	A	419	HIS
1	A	460	GLN
1	B	132	GLN
1	B	224	ASN
1	B	257	ASN
1	B	263	GLN
1	B	299	HIS
1	B	341	ASN

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Mol	Chain	Res	Type
1	B	418	GLN
1	B	461	GLN
1	D	263	GLN
1	D	276	ASN
1	D	336	GLN
1	D	419	HIS
1	D	460	GLN
1	C	105	ASN
1	C	132	GLN
1	C	233	GLN
1	C	257	ASN
1	C	263	GLN
1	C	276	ASN
1	C	341	ASN
1	C	461	GLN
1	E	105	ASN
1	E	108	GLN
1	E	257	ASN
1	E	263	GLN
1	E	299	HIS
1	E	341	ASN
1	E	344	ASN
1	E	418	GLN
1	E	419	HIS
1	E	448	GLN
1	E	460	GLN
1	E	461	GLN
1	E	563	ASN
1	E	593	ASN
1	E	611	GLN
1	F	105	ASN
1	F	108	GLN
1	F	238	GLN
1	F	257	ASN
1	F	263	GLN
1	F	276	ASN
1	F	341	ASN
1	F	419	HIS
1	F	460	GLN
1	G	132	GLN
1	G	257	ASN
1	G	263	GLN

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Mol	Chain	Res	Type
1	G	299	HIS
1	G	341	ASN
1	G	419	HIS
1	G	460	GLN
1	G	461	GLN
1	G	611	GLN
1	H	224	ASN
1	H	257	ASN
1	H	263	GLN
1	H	341	ASN
1	H	419	HIS
1	H	440	GLN
1	H	460	GLN
1	H	461	GLN
1	H	611	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
3	MES	B	7006	-	12,12,12	1.66	1 (8%)	15,16,16	3.81	7 (46%)
2	FAD	H	801	1	58,58,58	1.21	5 (8%)	85,89,89	2.51	33 (38%)
2	FAD	D	801	1	58,58,58	1.47	10 (17%)	85,89,89	2.28	32 (37%)
2	FAD	G	801	1	58,58,58	1.33	9 (15%)	85,89,89	2.48	29 (34%)
2	FAD	B	801	1	58,58,58	1.36	7 (12%)	85,89,89	2.29	29 (34%)
3	MES	A	7003	-	12,12,12	1.87	1 (8%)	15,16,16	4.04	8 (53%)
3	MES	C	7005	-	12,12,12	1.60	1 (8%)	15,16,16	4.11	9 (60%)
2	FAD	F	801	1	58,58,58	1.30	8 (13%)	85,89,89	2.30	28 (32%)
3	MES	D	7007	-	12,12,12	1.69	1 (8%)	15,16,16	4.69	8 (53%)
3	MES	H	7002	-	12,12,12	2.17	1 (8%)	15,16,16	3.71	8 (53%)
2	FAD	A	801	1	58,58,58	1.38	9 (15%)	85,89,89	2.51	33 (38%)
3	MES	E	7004	-	12,12,12	2.11	1 (8%)	15,16,16	5.02	9 (60%)
2	FAD	E	801	1	58,58,58	1.45	7 (12%)	85,89,89	2.42	33 (38%)
3	MES	F	7001	-	12,12,12	1.50	1 (8%)	15,16,16	3.67	7 (46%)
2	FAD	C	801	1	58,58,58	1.39	10 (17%)	85,89,89	2.36	28 (32%)
3	MES	G	7008	-	12,12,12	1.91	1 (8%)	15,16,16	4.08	6 (40%)

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. ^{1,2} means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MES	B	7006	-	-	2/6/14/14	0/1/1/1
2	FAD	H	801	1	-	2/34/50/50	0/6/6/6
2	FAD	D	801	1	-	3/34/50/50	0/6/6/6
2	FAD	G	801	1	-	2/34/50/50	0/6/6/6
2	FAD	B	801	1	-	3/34/50/50	0/6/6/6
3	MES	A	7003	-	-	2/6/14/14	0/1/1/1
3	MES	C	7005	-	-	2/6/14/14	0/1/1/1
2	FAD	F	801	1	-	1/34/50/50	0/6/6/6
3	MES	D	7007	-	-	2/6/14/14	0/1/1/1
3	MES	H	7002	-	-	2/6/14/14	0/1/1/1
2	FAD	A	801	1	-	2/34/50/50	0/6/6/6
3	MES	E	7004	-	-	2/6/14/14	0/1/1/1
2	FAD	E	801	1	-	3/34/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MES	F	7001	-	-	2/6/14/14	0/1/1/1
2	FAD	C	801	1	-	1/34/50/50	0/6/6/6
3	MES	G	7008	-	-	2/6/14/14	0/1/1/1

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	7002	MES	C8-S	-7.14	1.67	1.77
3	E	7004	MES	C8-S	-6.93	1.67	1.77
3	G	7008	MES	C8-S	-6.29	1.68	1.77
2	D	801	FAD	PA-O3P	6.16	1.66	1.59
3	A	7003	MES	C8-S	-6.14	1.69	1.77
3	D	7007	MES	C8-S	-5.46	1.69	1.77
3	B	7006	MES	C8-S	-5.28	1.70	1.77
3	C	7005	MES	C8-S	-5.19	1.70	1.77
2	B	801	FAD	PA-O3P	4.88	1.64	1.59
3	F	7001	MES	C8-S	-4.84	1.70	1.77
2	E	801	FAD	P-O3P	4.30	1.64	1.59
2	E	801	FAD	PA-O3P	3.77	1.63	1.59
2	A	801	FAD	C6-C5X	3.55	1.45	1.40
2	A	801	FAD	P-O3P	3.48	1.63	1.59
2	E	801	FAD	C10-N1	3.33	1.39	1.33
2	C	801	FAD	O4B-C4B	-3.29	1.37	1.45
2	E	801	FAD	C8A-N9A	-3.28	1.32	1.37
2	F	801	FAD	PA-O3P	3.20	1.63	1.59
2	G	801	FAD	C8A-N9A	-3.07	1.32	1.37
2	D	801	FAD	P-O3P	2.98	1.62	1.59
2	H	801	FAD	P-O3P	2.95	1.62	1.59
2	C	801	FAD	C6-C7	2.91	1.43	1.39
2	G	801	FAD	C10-N1	2.87	1.39	1.33
2	H	801	FAD	C5X-N5	-2.86	1.34	1.39
2	A	801	FAD	PA-O3P	2.85	1.62	1.59
2	C	801	FAD	C8A-N9A	-2.85	1.32	1.37
2	F	801	FAD	C4X-N5	2.84	1.36	1.30
2	F	801	FAD	C10-N1	2.71	1.38	1.33
2	G	801	FAD	C6-C5X	2.69	1.44	1.40
2	C	801	FAD	O3B-C3B	-2.69	1.36	1.43
2	G	801	FAD	C5'-C4'	2.66	1.55	1.51
2	G	801	FAD	PA-O3P	2.62	1.62	1.59
2	F	801	FAD	C4A-N9A	-2.62	1.32	1.37
2	D	801	FAD	O3B-C3B	-2.57	1.36	1.43
2	B	801	FAD	C10-N1	2.53	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	FAD	C10-N1	2.52	1.38	1.33
2	B	801	FAD	O4B-C4B	-2.51	1.39	1.45
2	D	801	FAD	O4B-C4B	-2.50	1.39	1.45
2	B	801	FAD	C5A-N7A	-2.46	1.34	1.39
2	A	801	FAD	C8A-N7A	2.44	1.36	1.31
2	B	801	FAD	O2B-C2B	-2.44	1.36	1.43
2	C	801	FAD	C4X-N5	2.41	1.36	1.30
2	F	801	FAD	O3B-C3B	-2.40	1.37	1.43
2	B	801	FAD	C8A-N9A	-2.40	1.33	1.37
2	G	801	FAD	O4B-C4B	-2.40	1.39	1.45
2	C	801	FAD	PA-O3P	2.38	1.62	1.59
2	G	801	FAD	C4X-N5	2.35	1.35	1.30
2	C	801	FAD	C6-C5X	2.31	1.43	1.40
2	A	801	FAD	C2B-C3B	-2.30	1.47	1.53
2	A	801	FAD	C4X-N5	2.29	1.35	1.30
2	C	801	FAD	P-O3P	2.29	1.62	1.59
2	A	801	FAD	C8A-N9A	-2.26	1.33	1.37
2	D	801	FAD	O2B-C2B	-2.25	1.37	1.43
2	D	801	FAD	C4X-N5	2.25	1.35	1.30
2	F	801	FAD	O4B-C4B	-2.24	1.40	1.45
2	E	801	FAD	O3B-C3B	-2.23	1.37	1.43
2	C	801	FAD	C10-N1	2.23	1.37	1.33
2	E	801	FAD	O2-C2	2.21	1.28	1.24
2	G	801	FAD	C5X-N5	-2.20	1.35	1.39
2	D	801	FAD	C2A-N3A	2.19	1.37	1.33
2	F	801	FAD	C6-C5X	2.13	1.43	1.40
2	A	801	FAD	O3B-C3B	-2.11	1.37	1.43
2	B	801	FAD	C2B-C3B	-2.10	1.47	1.53
2	H	801	FAD	C2A-N1A	2.09	1.37	1.33
2	G	801	FAD	C7M-C7	2.09	1.54	1.51
2	E	801	FAD	C5X-N5	-2.06	1.35	1.39
2	D	801	FAD	C6-C5X	2.04	1.43	1.40
2	H	801	FAD	C8A-N9A	-2.03	1.34	1.37
2	D	801	FAD	C2B-C3B	-2.03	1.47	1.53
2	C	801	FAD	C2-N3	-2.02	1.34	1.39
2	F	801	FAD	C2A-N1A	2.02	1.37	1.33
2	H	801	FAD	C6-C5X	2.01	1.43	1.40
2	D	801	FAD	C10-N1	2.01	1.37	1.33

All (307) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	7004	MES	O2S-S-C8	-13.35	86.55	106.73
3	D	7007	MES	O2S-S-C8	-12.71	87.53	106.73
3	G	7008	MES	O1S-S-C8	-11.12	89.92	106.73
3	A	7003	MES	O1S-S-C8	-10.33	91.11	106.73
3	C	7005	MES	O2S-S-C8	-9.65	92.15	106.73
3	B	7006	MES	O1S-S-C8	-9.30	92.68	106.73
3	F	7001	MES	O2S-S-C8	-8.83	93.38	106.73
2	H	801	FAD	C4A-N9A-C8A	8.72	114.89	105.74
2	E	801	FAD	C4A-N9A-C8A	8.30	114.46	105.74
2	A	801	FAD	C4A-N9A-C8A	8.03	114.17	105.74
3	H	7002	MES	O1S-S-C8	-8.02	94.61	106.73
2	C	801	FAD	C4A-N9A-C8A	7.93	114.06	105.74
2	D	801	FAD	C4A-N9A-C8A	7.74	113.87	105.74
2	F	801	FAD	C4A-N9A-C8A	7.48	113.59	105.74
2	G	801	FAD	C4A-N9A-C8A	7.34	113.44	105.74
2	A	801	FAD	N9A-C8A-N7A	-7.31	103.57	113.94
3	D	7007	MES	O1S-S-C8	-7.23	95.81	106.73
3	E	7004	MES	O1S-S-C8	-7.21	95.83	106.73
3	B	7006	MES	O2S-S-C8	-7.11	95.99	106.73
2	C	801	FAD	N3A-C2A-N1A	-6.63	118.54	128.58
3	E	7004	MES	O3S-S-C8	-6.54	93.21	106.00
3	G	7008	MES	C5-N4-C3	6.53	122.91	108.84
2	H	801	FAD	N3A-C2A-N1A	-6.49	118.76	128.58
2	G	801	FAD	N3A-C2A-N1A	-6.39	118.91	128.58
3	D	7007	MES	C5-N4-C3	6.33	122.48	108.84
2	B	801	FAD	C4A-N9A-C8A	6.21	112.26	105.74
3	E	7004	MES	C5-N4-C3	6.19	122.16	108.84
2	A	801	FAD	N3A-C2A-N1A	-6.16	119.25	128.58
2	C	801	FAD	O4-C4-N3	6.10	131.58	120.11
3	G	7008	MES	O2S-S-C8	-6.03	97.62	106.73
2	G	801	FAD	N9A-C8A-N7A	-5.96	105.48	113.94
3	A	7003	MES	C5-N4-C3	5.94	121.64	108.84
3	H	7002	MES	C5-N4-C3	5.93	121.60	108.84
2	E	801	FAD	N3A-C2A-N1A	-5.92	119.62	128.58
2	H	801	FAD	C4-N3-C2	5.89	136.11	125.64
2	E	801	FAD	N9A-C8A-N7A	-5.89	105.58	113.94
2	A	801	FAD	C4-N3-C2	5.85	136.04	125.64
2	G	801	FAD	C2B-C1B-N9A	5.84	127.80	113.30
2	G	801	FAD	O4-C4-N3	5.82	131.05	120.11
2	H	801	FAD	N9A-C8A-N7A	-5.77	105.75	113.94
2	F	801	FAD	N3A-C2A-N1A	-5.75	119.88	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	FAD	N3A-C2A-N1A	-5.72	119.92	128.58
2	B	801	FAD	C2B-C1B-N9A	5.61	127.25	113.30
3	A	7003	MES	O2S-S-C8	-5.59	98.28	106.73
2	B	801	FAD	N3A-C2A-N1A	-5.55	120.19	128.58
3	B	7006	MES	C5-N4-C3	5.52	120.74	108.84
2	D	801	FAD	N9A-C8A-N7A	-5.44	106.21	113.94
2	F	801	FAD	O4B-C1B-N9A	5.44	118.54	108.09
3	C	7005	MES	C5-N4-C3	5.42	120.52	108.84
3	C	7005	MES	O3S-S-C8	-5.35	95.54	106.00
2	E	801	FAD	C2B-C1B-N9A	5.34	126.58	113.30
2	E	801	FAD	O4-C4-N3	5.30	130.08	120.11
2	E	801	FAD	O3B-C3B-C4B	5.29	126.28	111.08
2	H	801	FAD	C2B-C1B-N9A	5.27	126.40	113.30
3	H	7002	MES	O2S-S-C8	-5.27	98.77	106.73
3	C	7005	MES	O3S-S-O2S	5.24	124.51	111.40
2	C	801	FAD	O4B-C1B-N9A	5.22	118.11	108.09
3	H	7002	MES	O3S-S-C8	-5.21	95.81	106.00
2	B	801	FAD	O4B-C1B-N9A	5.17	118.03	108.09
2	C	801	FAD	N9A-C8A-N7A	-5.16	106.61	113.94
2	D	801	FAD	O3B-C3B-C4B	5.16	125.90	111.08
3	F	7001	MES	C5-N4-C3	5.15	119.94	108.84
2	D	801	FAD	O4B-C1B-N9A	5.04	117.77	108.09
3	C	7005	MES	O1S-S-C8	-4.97	99.21	106.73
2	F	801	FAD	N9A-C8A-N7A	-4.93	106.94	113.94
2	B	801	FAD	N9A-C8A-N7A	-4.87	107.03	113.94
3	A	7003	MES	C7-N4-C5	4.83	124.11	111.24
2	C	801	FAD	O4-C4-C4X	-4.82	113.80	126.53
2	F	801	FAD	O3B-C3B-C4B	4.81	124.89	111.08
2	H	801	FAD	O3B-C3B-C4B	4.80	124.86	111.08
3	C	7005	MES	C7-N4-C5	4.79	124.00	111.24
2	F	801	FAD	C2B-C1B-N9A	4.78	125.18	113.30
2	G	801	FAD	O4B-C1B-N9A	4.71	117.14	108.09
3	D	7007	MES	O3S-S-O2S	4.70	123.15	111.40
2	H	801	FAD	N3A-C4A-N9A	4.69	135.15	127.17
3	F	7001	MES	C7-N4-C5	4.68	123.71	111.24
2	G	801	FAD	C4-C4X-N5	4.64	124.62	118.21
2	B	801	FAD	O2B-C2B-C1B	4.62	126.01	110.10
2	G	801	FAD	O4-C4-C4X	-4.61	114.37	126.53
2	A	801	FAD	C5A-N7A-C8A	4.58	110.65	103.45
2	F	801	FAD	C4-C4X-N5	4.56	124.51	118.21
2	F	801	FAD	O2B-C2B-C3B	4.53	126.33	111.82
2	B	801	FAD	O3B-C3B-C4B	4.52	124.06	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	FAD	O2B-C2B-C1B	4.52	125.66	110.10
2	C	801	FAD	C2B-C1B-N9A	4.51	124.50	113.30
2	D	801	FAD	C2B-C1B-N9A	4.50	124.48	113.30
2	G	801	FAD	N3A-C4A-N9A	4.49	134.79	127.17
3	F	7001	MES	O3S-S-O2S	4.37	122.34	111.40
2	B	801	FAD	N3A-C4A-N9A	4.35	134.56	127.17
2	G	801	FAD	C1B-N9A-C8A	-4.33	117.47	127.09
2	G	801	FAD	O3B-C3B-C4B	4.29	123.41	111.08
2	A	801	FAD	C2B-C1B-N9A	4.25	123.86	113.30
2	H	801	FAD	O2B-C2B-C3B	4.22	125.33	111.82
3	E	7004	MES	O1-C2-C3	-4.20	102.72	111.77
3	B	7006	MES	C7-N4-C5	4.14	122.26	111.24
2	C	801	FAD	O3B-C3B-C4B	4.08	122.80	111.08
2	A	801	FAD	O2B-C2B-C3B	4.07	124.85	111.82
3	F	7001	MES	O3S-S-C8	-4.06	98.06	106.00
2	B	801	FAD	C1B-N9A-C8A	-4.06	118.09	127.09
3	E	7004	MES	C7-N4-C5	4.05	122.02	111.24
3	D	7007	MES	C7-N4-C3	4.04	122.00	111.24
3	H	7002	MES	C7-N4-C5	4.01	121.92	111.24
3	F	7001	MES	O1S-S-C8	-4.01	100.67	106.73
2	A	801	FAD	N3-C2-N1	-4.00	111.00	119.50
3	A	7003	MES	O3S-S-C8	-3.98	98.21	106.00
2	A	801	FAD	O4-C4-N3	3.97	127.59	120.11
2	C	801	FAD	N3A-C4A-N9A	3.95	133.88	127.17
3	A	7003	MES	O3S-S-O2S	3.93	121.23	111.40
3	G	7008	MES	O3S-S-O2S	3.93	121.22	111.40
2	B	801	FAD	C4-C4X-N5	3.92	123.63	118.21
3	E	7004	MES	O3S-S-O2S	3.92	121.21	111.40
2	D	801	FAD	N3A-C4A-N9A	3.92	133.83	127.17
2	H	801	FAD	C5A-C4A-N9A	-3.91	101.56	105.81
2	D	801	FAD	O2B-C2B-C1B	3.87	123.44	110.10
2	E	801	FAD	O4B-C1B-N9A	3.87	115.51	108.09
2	D	801	FAD	O4-C4-N3	3.86	127.36	120.11
2	H	801	FAD	C1B-N9A-C8A	-3.85	118.55	127.09
3	H	7002	MES	O3S-S-O1S	3.82	120.95	111.40
3	F	7001	MES	C6-C5-N4	3.78	115.87	110.12
2	H	801	FAD	N3-C2-N1	-3.77	111.48	119.50
2	E	801	FAD	O2B-C2B-C1B	3.76	123.07	110.10
3	D	7007	MES	O3S-S-C8	-3.75	98.68	106.00
2	F	801	FAD	C9A-C5X-N5	-3.73	118.50	122.45
3	G	7008	MES	C7-N4-C5	3.73	121.17	111.24
2	H	801	FAD	O4-C4-N3	3.71	127.10	120.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	801	FAD	O4B-C1B-N9A	3.70	115.20	108.09
2	E	801	FAD	N3A-C4A-N9A	3.67	133.40	127.17
2	F	801	FAD	N3A-C4A-N9A	3.65	133.37	127.17
2	C	801	FAD	C1B-N9A-C8A	-3.61	119.08	127.09
2	C	801	FAD	C2A-N1A-C6A	3.61	124.66	118.73
2	E	801	FAD	O4B-C4B-C5B	3.61	120.90	109.33
2	G	801	FAD	C5A-N7A-C8A	3.59	109.10	103.45
2	H	801	FAD	O2B-C2B-C1B	3.57	122.40	110.10
2	F	801	FAD	C1B-N9A-C8A	-3.57	119.18	127.09
2	E	801	FAD	O2B-C2B-C3B	3.56	123.23	111.82
2	G	801	FAD	C5A-C4A-N3A	-3.55	121.82	126.72
2	A	801	FAD	O4B-C4B-C5B	3.54	120.69	109.33
2	E	801	FAD	C4-N3-C2	3.54	131.93	125.64
2	D	801	FAD	O4B-C4B-C5B	3.50	120.53	109.33
2	E	801	FAD	C5A-C4A-N9A	-3.49	102.01	105.81
2	F	801	FAD	C2A-N1A-C6A	3.46	124.42	118.73
2	A	801	FAD	N3A-C4A-N9A	3.42	132.99	127.17
2	B	801	FAD	O4B-C4B-C5B	3.41	120.27	109.33
2	A	801	FAD	O4B-C1B-C2B	3.41	113.91	106.62
2	A	801	FAD	C1B-N9A-C8A	-3.39	119.57	127.09
2	E	801	FAD	O4-C4-C4X	-3.39	117.59	126.53
2	F	801	FAD	O2B-C2B-C1B	3.38	121.74	110.10
3	B	7006	MES	O3S-S-O2S	3.33	119.73	111.40
3	C	7005	MES	O3S-S-O1S	3.30	119.67	111.40
2	G	801	FAD	O2B-C2B-C1B	3.29	121.43	110.10
2	F	801	FAD	O2A-PA-O3P	3.25	116.07	107.27
2	E	801	FAD	O4B-C4B-C3B	3.24	111.58	105.15
2	A	801	FAD	O2-C2-N3	3.23	124.78	118.58
2	H	801	FAD	O2-C2-N3	3.22	124.75	118.58
2	E	801	FAD	C2A-N1A-C6A	3.19	123.97	118.73
2	A	801	FAD	O3B-C3B-C4B	3.18	120.22	111.08
2	D	801	FAD	O2B-C2B-C3B	3.17	121.98	111.82
2	G	801	FAD	O4B-C4B-C5B	3.17	119.47	109.33
2	C	801	FAD	C5A-C4A-N9A	-3.16	102.37	105.81
2	B	801	FAD	C5A-C4A-N3A	-3.15	122.38	126.72
2	H	801	FAD	C5X-N5-C4X	3.15	123.19	118.09
2	G	801	FAD	C2A-N3A-C4A	3.15	119.52	111.83
2	F	801	FAD	O3P-PA-O1A	-3.15	101.23	110.70
2	E	801	FAD	C5A-N7A-C8A	3.11	108.34	103.45
2	D	801	FAD	O2-C2-N3	3.09	124.51	118.58
2	G	801	FAD	C5B-C4B-C3B	3.08	126.31	115.21
2	C	801	FAD	O2B-C2B-C3B	3.07	121.65	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	FAD	C1B-N9A-C8A	-3.06	120.30	127.09
3	H	7002	MES	O3S-S-O2S	3.04	119.00	111.40
2	C	801	FAD	C5A-N7A-C8A	3.04	108.22	103.45
2	A	801	FAD	O2P-P-O3P	-3.04	99.07	107.27
2	H	801	FAD	C2A-N1A-C6A	3.04	123.72	118.73
2	B	801	FAD	O2A-PA-O3P	3.02	115.44	107.27
2	F	801	FAD	C5A-C4A-N9A	-3.02	102.52	105.81
2	H	801	FAD	C5B-C4B-C3B	3.01	126.06	115.21
2	B	801	FAD	C2A-N1A-C6A	3.01	123.67	118.73
2	A	801	FAD	C5B-C4B-C3B	3.01	126.04	115.21
2	C	801	FAD	C5B-C4B-C3B	3.01	126.03	115.21
2	B	801	FAD	C8M-C8-C9	-3.01	114.28	119.57
2	A	801	FAD	C9A-C5X-N5	-3.00	119.27	122.45
2	B	801	FAD	C5A-N7A-C8A	3.00	108.17	103.45
2	H	801	FAD	O4B-C1B-C2B	3.00	113.05	106.62
2	A	801	FAD	O2B-C2B-C1B	2.99	120.40	110.10
2	G	801	FAD	C5'-C4'-C3'	-2.98	106.59	112.22
2	A	801	FAD	C8M-C8-C9	-2.97	114.34	119.57
2	E	801	FAD	C1B-N9A-C8A	-2.95	120.55	127.09
3	D	7007	MES	O1-C6-C5	-2.93	105.45	111.77
2	D	801	FAD	C5A-C4A-N9A	-2.93	102.62	105.81
2	D	801	FAD	C5A-N7A-C8A	2.91	108.02	103.45
2	G	801	FAD	O2A-PA-O3P	2.91	115.13	107.27
2	B	801	FAD	O2P-P-O3P	-2.89	99.46	107.27
2	E	801	FAD	O2A-PA-O3P	2.88	115.06	107.27
2	G	801	FAD	C9A-C5X-N5	-2.87	119.41	122.45
2	A	801	FAD	C2A-N1A-C6A	2.86	123.44	118.73
2	A	801	FAD	C2A-N3A-C4A	2.84	118.76	111.83
2	F	801	FAD	O4-C4-N3	2.79	125.35	120.11
2	G	801	FAD	O2B-C2B-C3B	2.77	120.70	111.82
2	G	801	FAD	O3P-PA-O1A	-2.76	102.39	110.70
2	A	801	FAD	C5A-C4A-N3A	-2.74	122.95	126.72
2	B	801	FAD	O4B-C4B-C3B	2.72	110.56	105.15
2	D	801	FAD	C4-C4X-N5	2.72	121.96	118.21
2	H	801	FAD	C10-C4X-N5	-2.70	119.29	124.81
2	E	801	FAD	N3-C2-N1	-2.70	113.77	119.50
2	B	801	FAD	C9A-C5X-N5	-2.69	119.60	122.45
2	A	801	FAD	C10-N1-C2	2.69	122.67	116.85
2	G	801	FAD	C4-N3-C2	2.68	130.41	125.64
2	D	801	FAD	O2A-PA-O3P	2.68	114.51	107.27
2	A	801	FAD	O2A-PA-O3P	2.68	114.51	107.27
2	G	801	FAD	C2A-N1A-C6A	2.65	123.09	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	7003	MES	C6-C5-N4	2.65	114.15	110.12
2	H	801	FAD	C4X-C4-N3	-2.65	106.52	113.25
2	D	801	FAD	O4-C4-C4X	-2.63	119.58	126.53
2	F	801	FAD	O2-C2-N3	2.63	123.63	118.58
2	E	801	FAD	O2A-PA-O1A	2.63	124.67	112.44
2	H	801	FAD	C9A-C5X-N5	-2.63	119.67	122.45
2	A	801	FAD	C4A-C5A-N7A	-2.61	107.59	110.58
3	C	7005	MES	C6-C5-N4	2.61	114.09	110.12
2	G	801	FAD	O2P-P-O1P	2.61	124.58	112.44
2	H	801	FAD	C2A-N3A-C4A	2.60	118.18	111.83
3	E	7004	MES	O3S-S-O1S	2.59	117.88	111.40
3	H	7002	MES	C6-C5-N4	2.59	114.06	110.12
2	D	801	FAD	C2A-N1A-C6A	2.58	122.97	118.73
2	H	801	FAD	C5A-N7A-C8A	2.58	107.50	103.45
2	D	801	FAD	O4B-C4B-C3B	2.57	110.26	105.15
2	C	801	FAD	C9A-C5X-N5	-2.57	119.73	122.45
3	G	7008	MES	C6-C5-N4	2.57	114.02	110.12
2	H	801	FAD	C5'-C4'-C3'	-2.55	107.41	112.22
2	B	801	FAD	C5A-C4A-N9A	-2.55	103.04	105.81
2	C	801	FAD	C2A-N3A-C4A	2.54	118.04	111.83
2	H	801	FAD	O4B-C4B-C5B	2.54	117.48	109.33
2	H	801	FAD	O4B-C4B-C3B	2.54	110.19	105.15
2	H	801	FAD	C5A-C4A-N3A	-2.52	123.25	126.72
2	E	801	FAD	O3P-PA-O1A	-2.51	103.14	110.70
2	B	801	FAD	C2A-N3A-C4A	2.49	117.92	111.83
2	B	801	FAD	C7M-C7-C8	2.49	125.84	120.76
2	G	801	FAD	C8M-C8-C9	-2.48	115.21	119.57
2	B	801	FAD	C10-C4X-N5	-2.47	119.76	124.81
2	C	801	FAD	C2B-C3B-C4B	2.44	107.32	102.61
2	E	801	FAD	C5B-C4B-C3B	2.42	123.94	115.21
2	E	801	FAD	O4B-C1B-C2B	2.42	111.80	106.62
2	E	801	FAD	C4-C4X-N5	2.42	121.55	118.21
2	F	801	FAD	C2B-C3B-C4B	2.39	107.23	102.61
2	E	801	FAD	O2P-P-O1P	2.39	123.56	112.44
3	B	7006	MES	O2S-S-O1S	2.39	121.59	113.82
2	F	801	FAD	C10-C4X-N5	-2.39	119.94	124.81
2	A	801	FAD	O4B-C1B-N9A	2.38	112.67	108.09
2	B	801	FAD	O2B-C2B-C3B	2.37	119.42	111.82
2	D	801	FAD	C4-N3-C2	2.37	129.85	125.64
2	C	801	FAD	C8M-C8-C9	-2.37	115.40	119.57
2	G	801	FAD	C5A-C4A-N9A	-2.36	103.24	105.81
2	H	801	FAD	C10-N1-C2	2.35	121.94	116.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	FAD	O2P-P-O1P	2.35	123.36	112.44
2	F	801	FAD	O4-C4-C4X	-2.35	120.34	126.53
2	G	801	FAD	N3-C2-N1	-2.35	114.52	119.50
2	F	801	FAD	O2A-PA-O1A	2.34	123.33	112.44
3	C	7005	MES	O1-C2-C3	-2.33	106.75	111.77
2	D	801	FAD	C2A-N3A-C4A	2.32	117.51	111.83
2	E	801	FAD	C10-N1-C2	2.32	121.87	116.85
2	D	801	FAD	C10-N1-C2	2.32	121.86	116.85
2	E	801	FAD	O5'-P-O1P	-2.31	99.79	108.94
2	F	801	FAD	O4B-C4B-C5B	2.31	116.72	109.33
2	B	801	FAD	C5X-N5-C4X	2.30	121.81	118.09
2	D	801	FAD	C5A-C4A-N3A	-2.29	123.56	126.72
2	F	801	FAD	C5X-N5-C4X	2.29	121.80	118.09
2	E	801	FAD	C5'-C4'-C3'	-2.27	107.93	112.22
2	C	801	FAD	C9-C8-C7	2.27	123.02	119.69
2	D	801	FAD	N3-C2-N1	-2.26	114.69	119.50
2	D	801	FAD	O2P-P-O3P	-2.26	101.17	107.27
2	B	801	FAD	C4X-C10-N10	2.25	119.71	116.48
3	A	7003	MES	O2S-S-O1S	2.24	121.10	113.82
2	D	801	FAD	C4X-C10-N10	2.22	119.66	116.48
2	C	801	FAD	O2A-PA-O1A	2.21	122.73	112.44
2	D	801	FAD	C8M-C8-C9	-2.20	115.69	119.57
2	F	801	FAD	C10-N1-C2	2.20	121.61	116.85
2	A	801	FAD	C7M-C7-C8	2.19	125.24	120.76
2	C	801	FAD	C5A-C4A-N3A	-2.18	123.71	126.72
2	H	801	FAD	O2'-C2'-C3'	2.18	114.34	109.25
2	F	801	FAD	C5B-C4B-C3B	2.16	122.99	115.21
2	F	801	FAD	O4B-C1B-C2B	2.16	111.24	106.62
2	E	801	FAD	C2A-N3A-C4A	2.16	117.10	111.83
2	C	801	FAD	O4B-C1B-C2B	2.14	111.20	106.62
2	D	801	FAD	O4'-C4'-C3'	2.13	114.23	109.25
2	B	801	FAD	C5B-C4B-C3B	2.12	122.83	115.21
2	G	801	FAD	C10-C4X-N5	-2.11	120.49	124.81
2	C	801	FAD	O3P-PA-O1A	-2.11	104.36	110.70
2	E	801	FAD	O2-C2-N3	2.11	122.63	118.58
2	C	801	FAD	C10-C4X-N5	-2.11	120.50	124.81
2	D	801	FAD	O4B-C1B-C2B	2.11	111.13	106.62
2	B	801	FAD	O4-C4-C4X	-2.10	120.98	126.53
2	H	801	FAD	O2A-PA-O1A	2.10	122.21	112.44
3	E	7004	MES	O2S-S-O1S	2.09	120.61	113.82
2	C	801	FAD	C4-N3-C2	2.08	129.34	125.64
2	C	801	FAD	O4B-C4B-C3B	2.06	109.25	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	801	FAD	O5'-P-O1P	-2.06	100.78	108.94
2	H	801	FAD	C4'-C3'-C2'	-2.06	110.15	113.57
2	A	801	FAD	C4X-C4-N3	-2.05	108.03	113.25
2	E	801	FAD	O2P-P-O3P	-2.05	101.73	107.27
2	B	801	FAD	C3B-C2B-C1B	2.05	105.34	101.46
2	A	801	FAD	C5'-C4'-C3'	-2.04	108.36	112.22
2	D	801	FAD	O2P-P-O1P	2.04	121.93	112.44
3	D	7007	MES	O3S-S-O1S	2.04	116.49	111.40
3	B	7006	MES	C2-C3-N4	2.03	113.21	110.12
2	A	801	FAD	C4B-O4B-C1B	-2.03	104.99	109.47
2	A	801	FAD	C4X-C10-N10	2.02	119.38	116.48
2	D	801	FAD	O3P-PA-O1A	-2.01	104.65	110.70
2	H	801	FAD	C4-C4X-N5	2.00	120.97	118.21
2	E	801	FAD	C4B-O4B-C1B	-2.00	105.04	109.47

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	FAD	PA-O3P-P-O5'
2	D	801	FAD	PA-O3P-P-O5'
2	E	801	FAD	PA-O3P-P-O5'
3	A	7003	MES	C8-C7-N4-C5
3	B	7006	MES	C8-C7-N4-C5
3	B	7006	MES	N4-C7-C8-S
3	D	7007	MES	C8-C7-N4-C3
3	D	7007	MES	N4-C7-C8-S
3	C	7005	MES	C8-C7-N4-C5
3	C	7005	MES	N4-C7-C8-S
3	E	7004	MES	C8-C7-N4-C5
3	E	7004	MES	N4-C7-C8-S
3	F	7001	MES	C8-C7-N4-C5
3	G	7008	MES	C8-C7-N4-C5
3	H	7002	MES	C8-C7-N4-C5
3	H	7002	MES	N4-C7-C8-S
3	A	7003	MES	N4-C7-C8-S
3	F	7001	MES	N4-C7-C8-S
3	G	7008	MES	N4-C7-C8-S
2	B	801	FAD	O4B-C4B-C5B-O5B
2	B	801	FAD	PA-O3P-P-O5'
2	F	801	FAD	PA-O3P-P-O5'
2	G	801	FAD	PA-O3P-P-O5'

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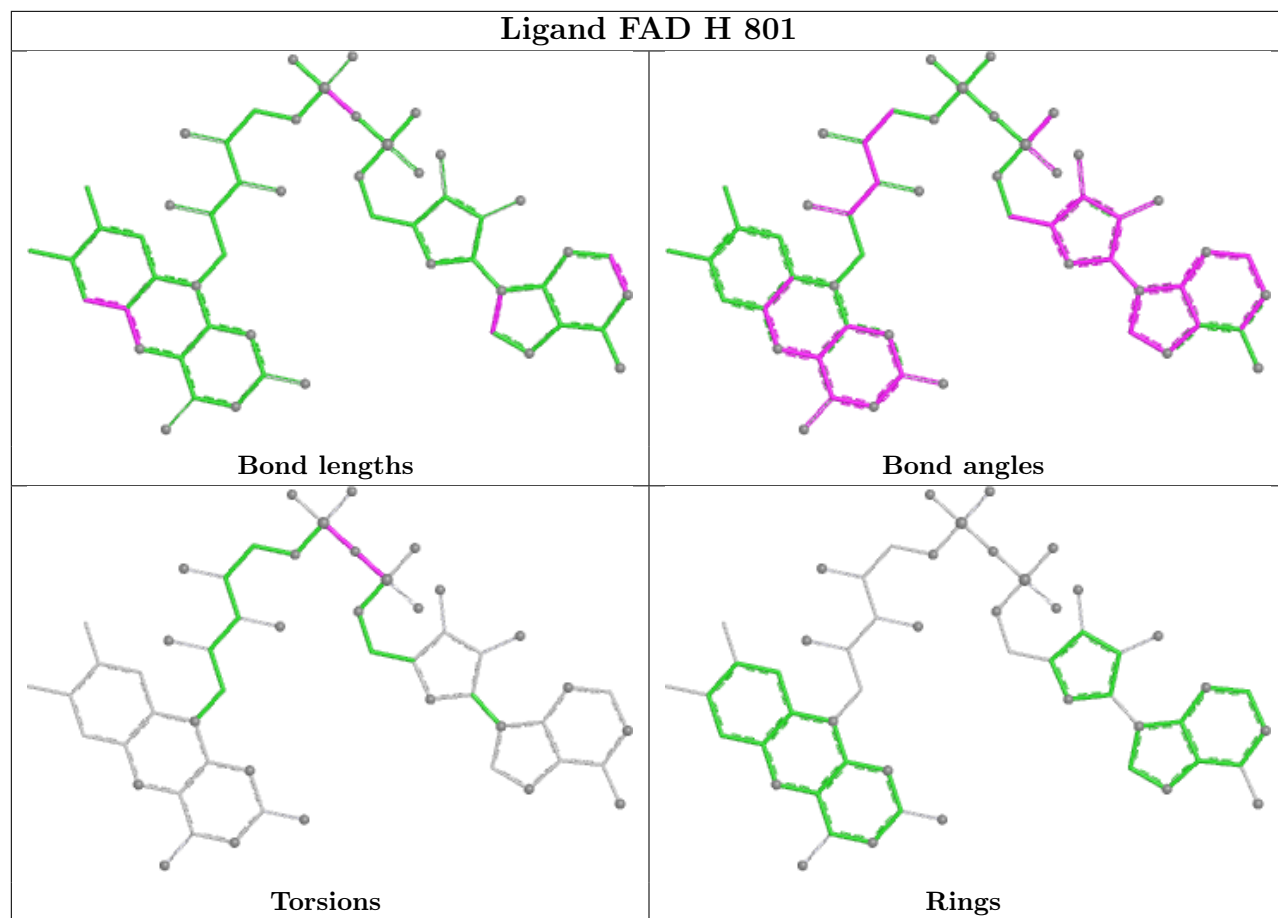
Mol	Chain	Res	Type	Atoms
2	C	801	FAD	O4B-C4B-C5B-O5B
2	E	801	FAD	P-O3P-PA-O2A
2	H	801	FAD	PA-O3P-P-O5'
2	A	801	FAD	P-O3P-PA-O2A
2	B	801	FAD	P-O3P-PA-O2A
2	D	801	FAD	P-O3P-PA-O2A
2	G	801	FAD	P-O3P-PA-O2A
2	D	801	FAD	O4B-C4B-C5B-O5B
2	E	801	FAD	O4B-C4B-C5B-O5B
2	H	801	FAD	P-O3P-PA-O2A

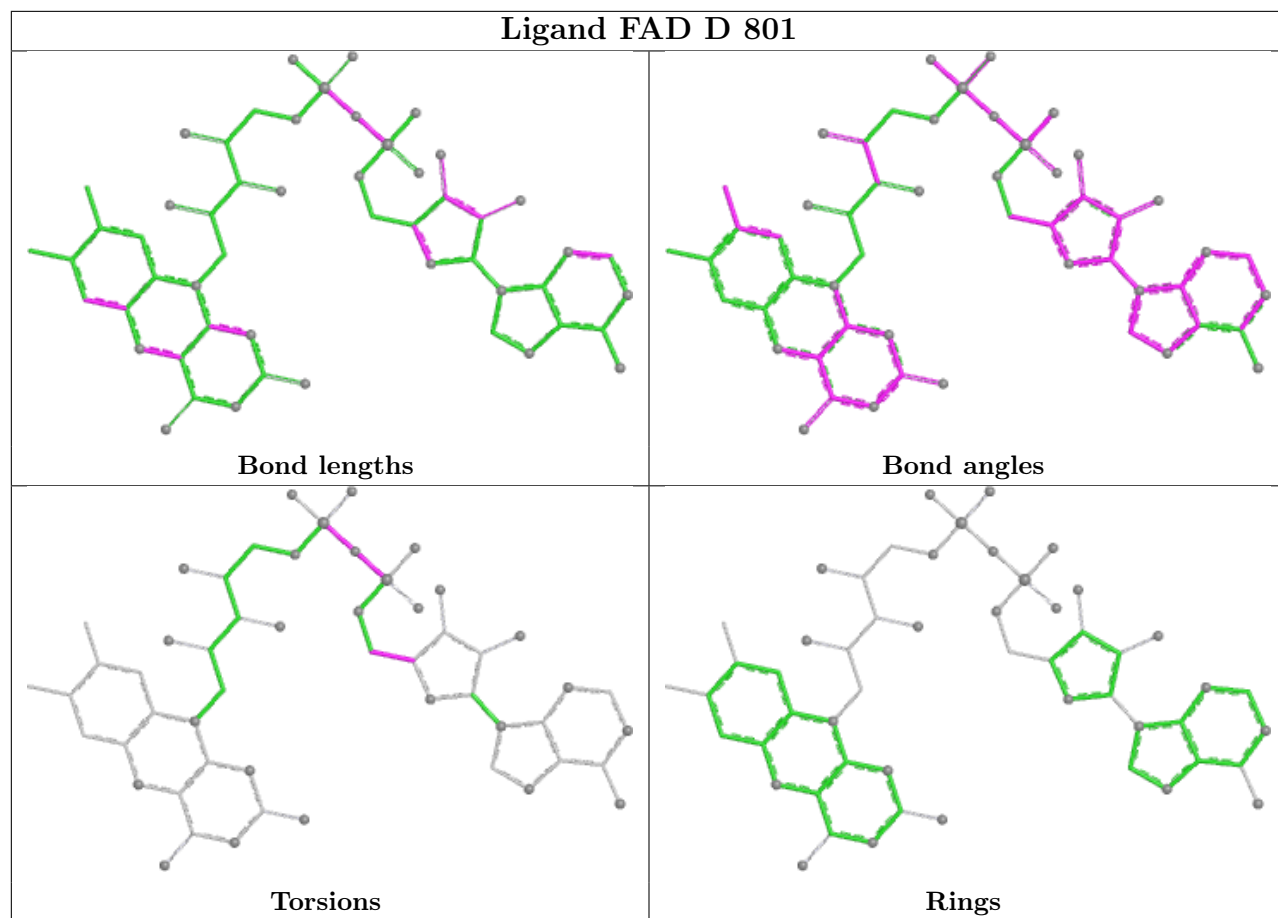
There are no ring outliers.

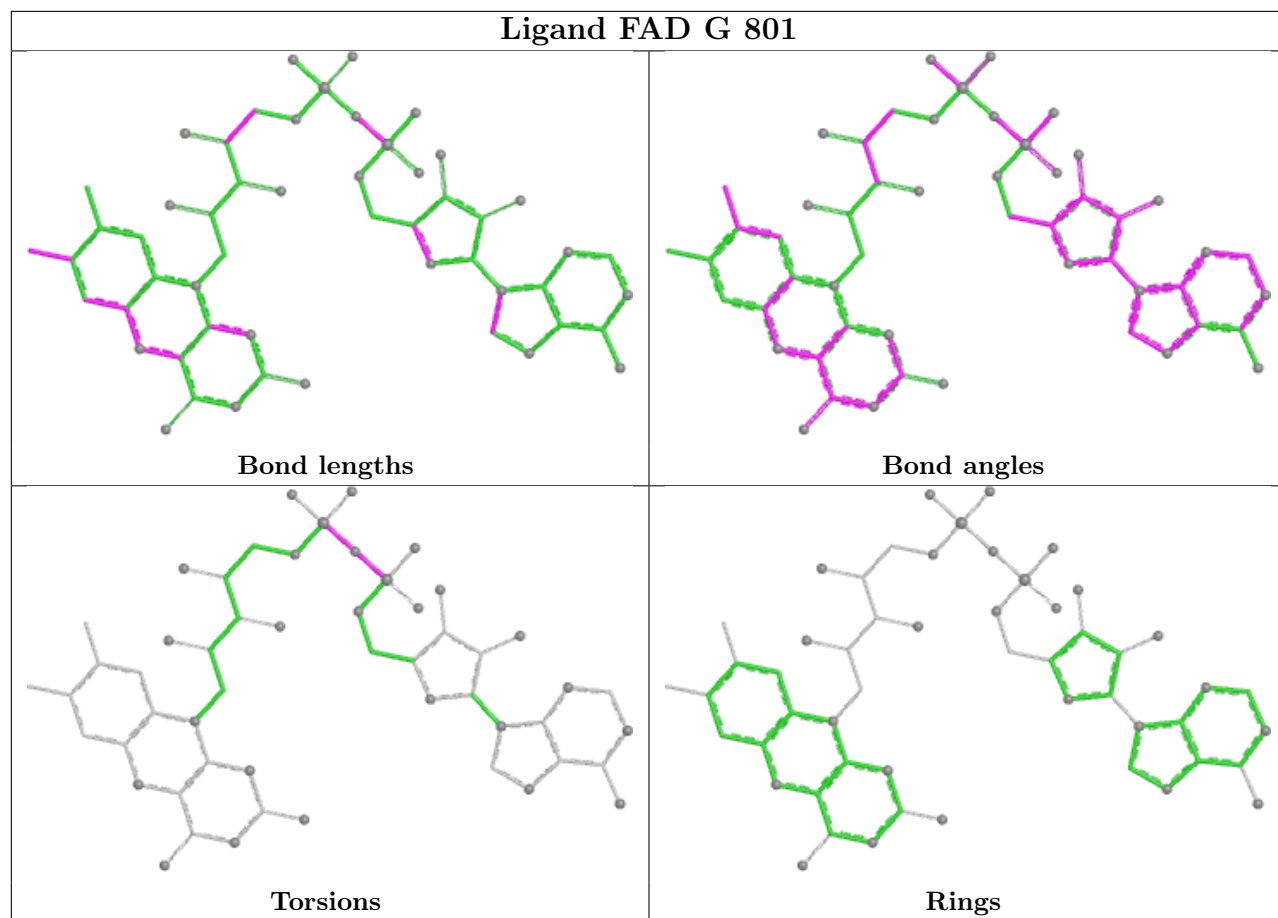
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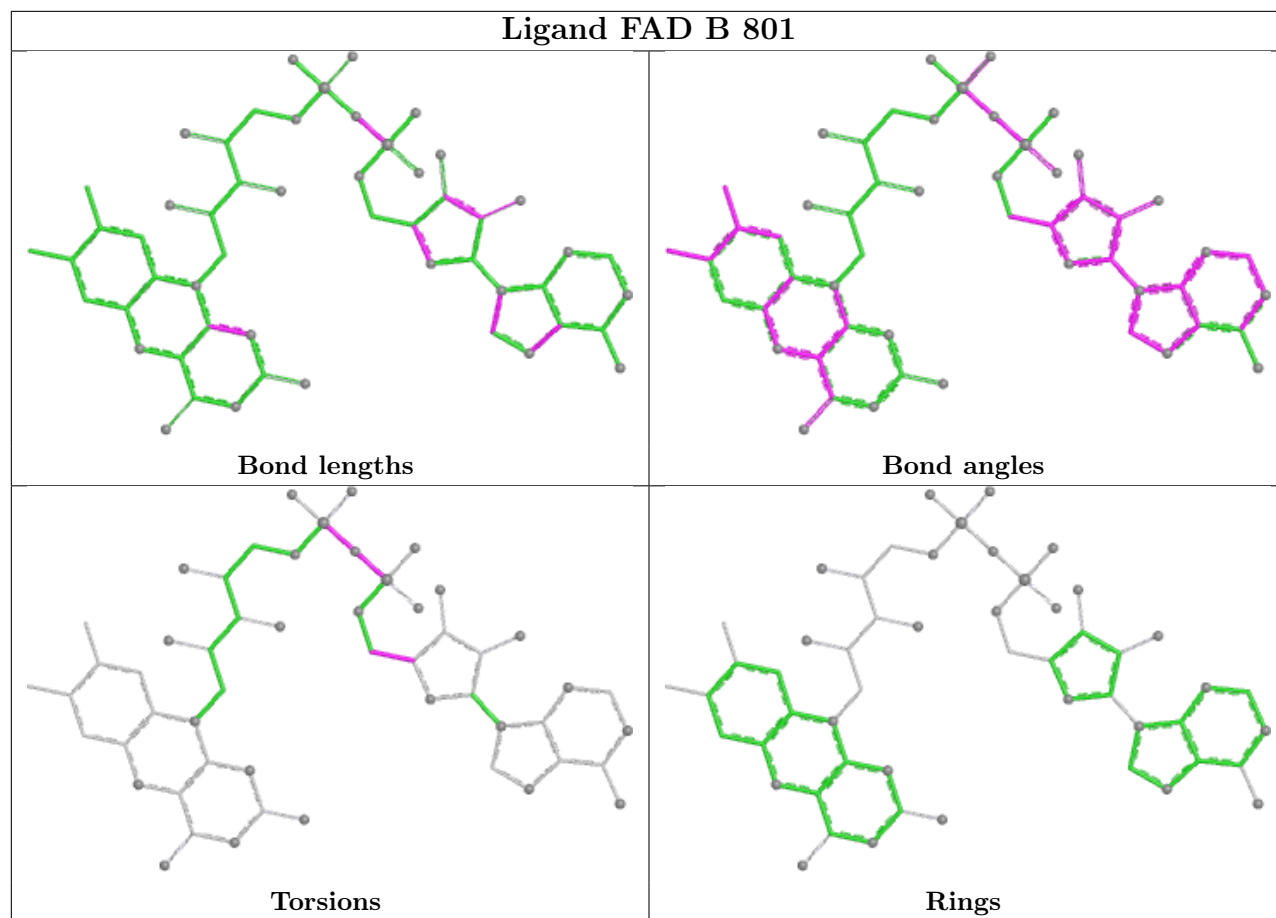
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	7006	MES	1	0
2	H	801	FAD	6	0
2	D	801	FAD	8	0
2	G	801	FAD	10	0
2	B	801	FAD	13	0
3	A	7003	MES	1	0
2	F	801	FAD	9	0
3	D	7007	MES	2	0
3	H	7002	MES	1	0
2	A	801	FAD	6	0
3	E	7004	MES	4	0
2	E	801	FAD	11	0
2	C	801	FAD	8	0
3	G	7008	MES	2	0

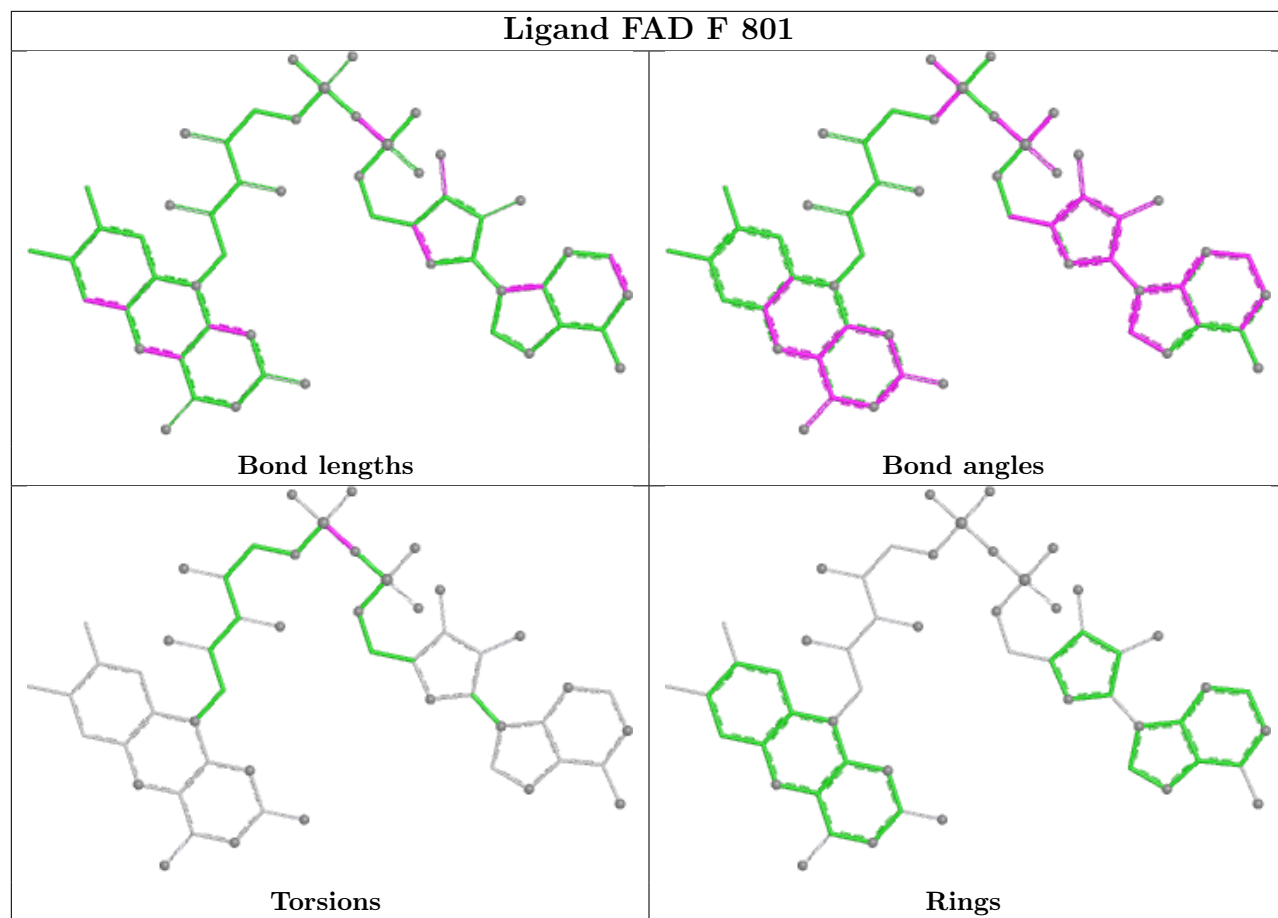
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

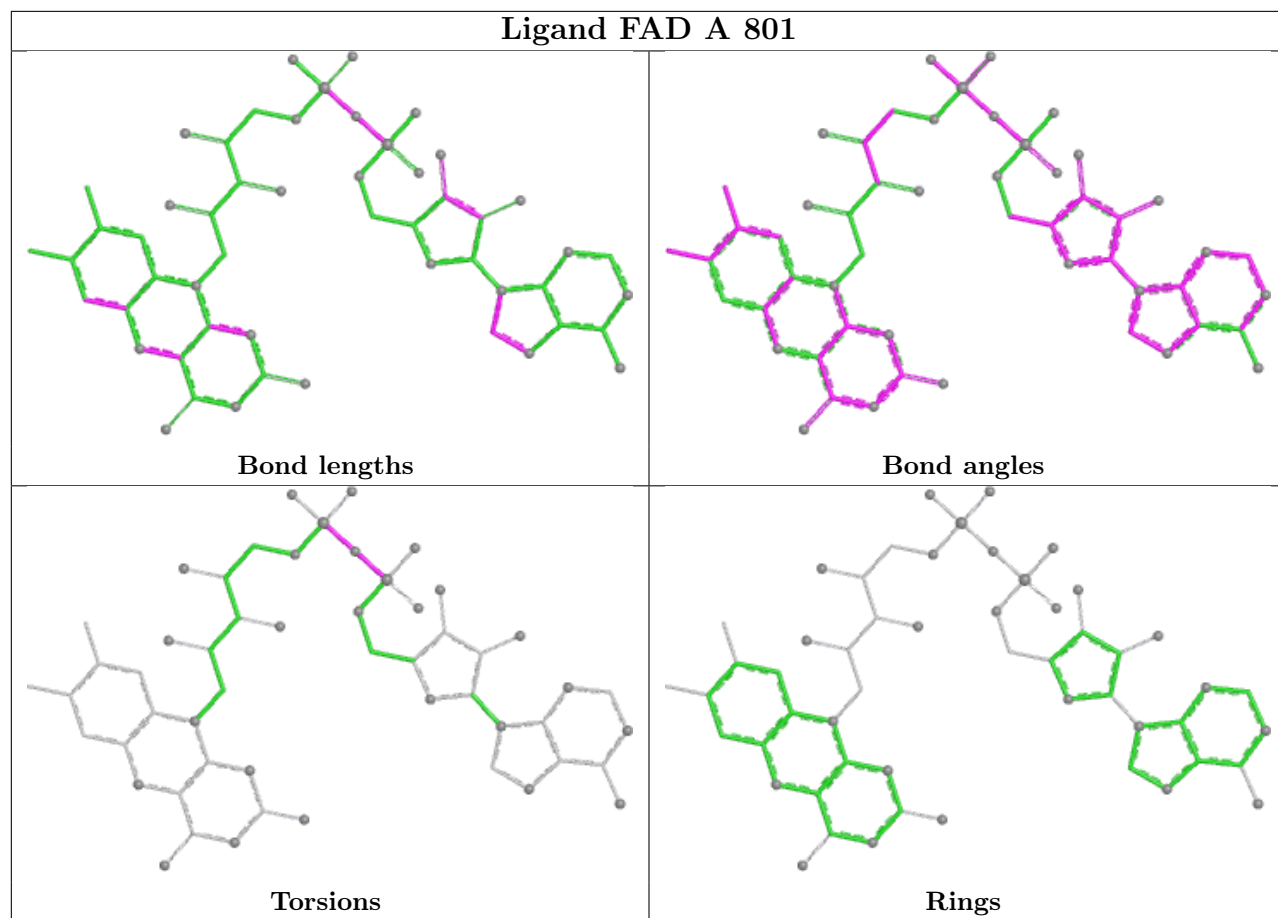


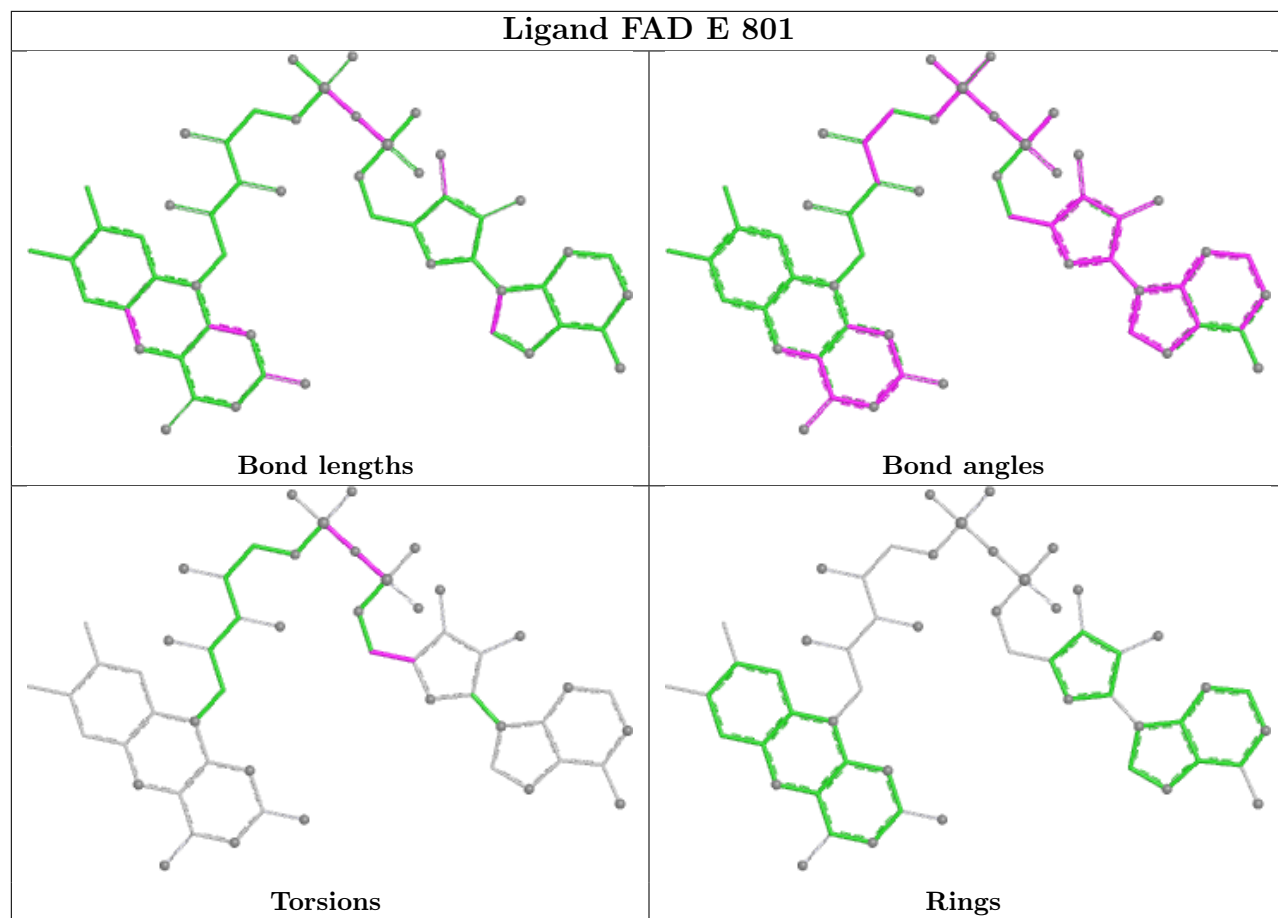


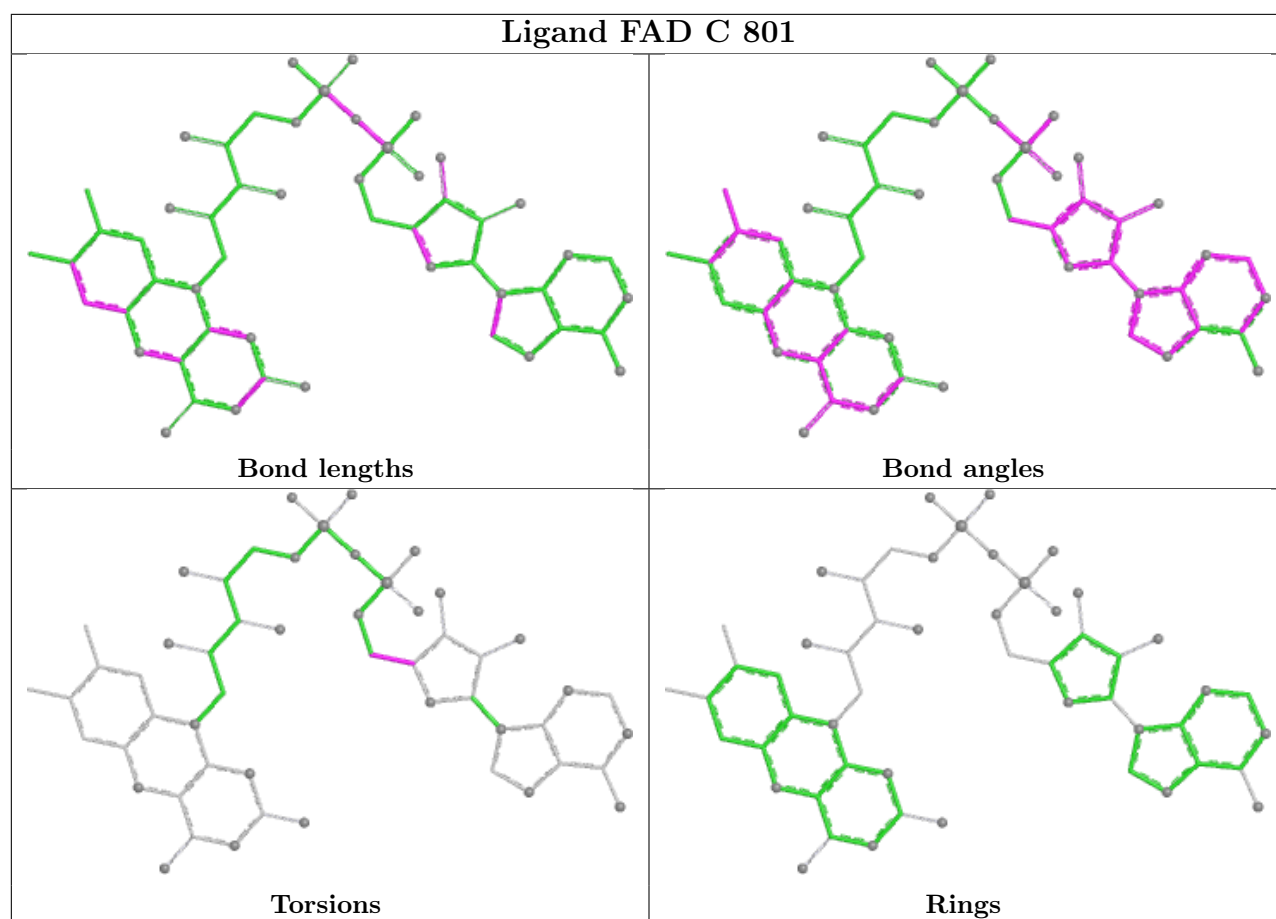












5.7 Other polymers [i](#)

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	577/623 (92%)	-0.45	10 (1%) 69 72	6, 13, 36, 57	2 (0%)
1	B	577/623 (92%)	-0.48	6 (1%) 79 82	5, 14, 31, 49	2 (0%)
1	C	577/623 (92%)	-0.32	11 (1%) 66 70	7, 17, 37, 54	1 (0%)
1	D	577/623 (92%)	-0.41	7 (1%) 76 79	6, 15, 34, 54	3 (0%)
1	E	577/623 (92%)	-0.35	9 (1%) 70 74	6, 17, 34, 53	2 (0%)
1	F	577/623 (92%)	-0.31	12 (2%) 63 67	8, 18, 37, 53	1 (0%)
1	G	577/623 (92%)	-0.31	17 (2%) 53 57	7, 16, 39, 52	2 (0%)
1	H	577/623 (92%)	-0.42	9 (1%) 70 74	8, 15, 31, 53	1 (0%)
All	All	4616/4984 (92%)	-0.38	81 (1%) 67 71	5, 16, 35, 57	14 (0%)

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	619	THR	5.7
1	A	619	THR	5.1
1	C	619	THR	5.1
1	D	619	THR	5.0
1	B	619	THR	4.6
1	G	619	THR	4.5
1	F	44	ASP	4.3
1	B	618	PHE	4.0
1	A	389	LEU	3.9
1	D	45	ILE	3.9
1	C	343	ALA	3.9
1	F	619	THR	3.8
1	C	384	GLY	3.7
1	C	45	ILE	3.7
1	H	343	ALA	3.7
1	H	45	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	619	THR	3.6
1	C	389	LEU	3.6
1	F	45	ILE	3.5
1	C	44	ASP	3.4
1	B	389	LEU	3.4
1	C	390	THR	3.2
1	A	343	ALA	3.2
1	C	385	THR	3.1
1	G	45	ILE	3.1
1	G	309	PHE	3.0
1	D	389	LEU	3.0
1	G	389	LEU	3.0
1	E	45	ILE	3.0
1	D	618	PHE	2.9
1	E	232	GLY	2.9
1	A	390	THR	2.8
1	H	44	ASP	2.8
1	E	618	PHE	2.7
1	G	82	SER	2.7
1	F	343	ALA	2.7
1	H	342	PRO	2.6
1	A	459	VAL	2.6
1	G	618	PHE	2.6
1	D	390	THR	2.6
1	H	618	PHE	2.6
1	F	43	MET	2.6
1	G	343	ALA	2.6
1	E	385	THR	2.6
1	F	342	PRO	2.5
1	A	341	ASN	2.5
1	H	611	GLN	2.5
1	F	561	GLU	2.5
1	B	342	PRO	2.5
1	G	342	PRO	2.4
1	G	400	SER	2.4
1	C	618	PHE	2.4
1	G	397	PRO	2.4
1	A	44	ASP	2.3
1	D	81	ASP	2.3
1	G	81	ASP	2.3
1	F	341	ASN	2.3
1	F	390	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	388	GLU	2.2
1	G	388	GLU	2.2
1	G	100	ILE	2.2
1	A	618	PHE	2.2
1	H	459	VAL	2.2
1	A	397	PRO	2.2
1	H	344	ASN	2.1
1	E	387	GLY	2.1
1	E	342	PRO	2.1
1	D	344	ASN	2.1
1	F	344	ASN	2.1
1	G	341	ASN	2.1
1	B	383	ARG	2.1
1	G	390	THR	2.1
1	G	418	GLN	2.1
1	A	385	THR	2.0
1	F	299	HIS	2.0
1	C	383	ARG	2.0
1	E	343	ALA	2.0
1	C	43	MET	2.0
1	B	344	ASN	2.0
1	E	341	ASN	2.0
1	G	344	ASN	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.

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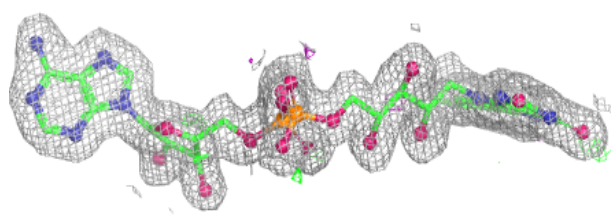
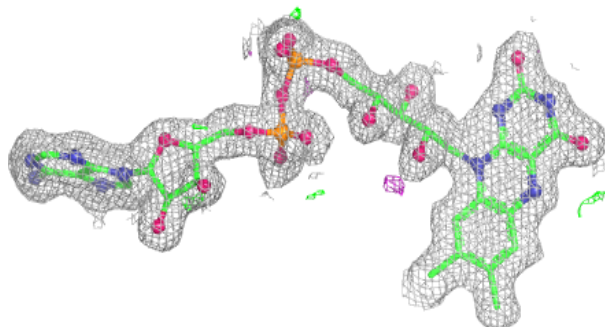
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MES	C	7005	12/12	0.95	0.09	17,20,22,23	0
3	MES	G	7008	12/12	0.95	0.08	19,22,24,24	0
3	MES	B	7006	12/12	0.96	0.07	22,23,26,26	0
3	MES	E	7004	12/12	0.96	0.07	19,22,25,27	0
3	MES	D	7007	12/12	0.96	0.07	20,24,25,25	0
3	MES	H	7002	12/12	0.96	0.08	18,20,21,22	0
3	MES	F	7001	12/12	0.97	0.07	14,18,19,19	0
3	MES	A	7003	12/12	0.98	0.06	16,17,19,20	0
2	FAD	B	801	53/53	0.98	0.04	8,11,13,19	0
2	FAD	D	801	53/53	0.98	0.04	10,12,14,16	0
2	FAD	C	801	53/53	0.98	0.05	9,13,16,19	0
2	FAD	E	801	53/53	0.98	0.04	9,13,15,18	0
2	FAD	F	801	53/53	0.98	0.04	10,13,15,17	0
2	FAD	G	801	53/53	0.98	0.04	10,12,15,17	0
2	FAD	H	801	53/53	0.98	0.04	9,13,15,17	0
2	FAD	A	801	53/53	0.99	0.04	7,10,14,16	0

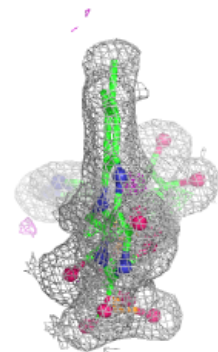
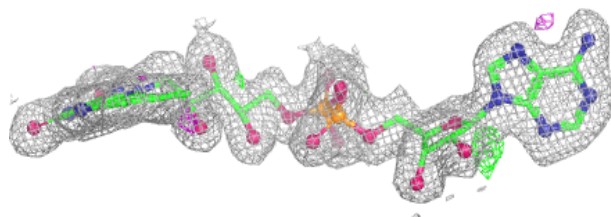
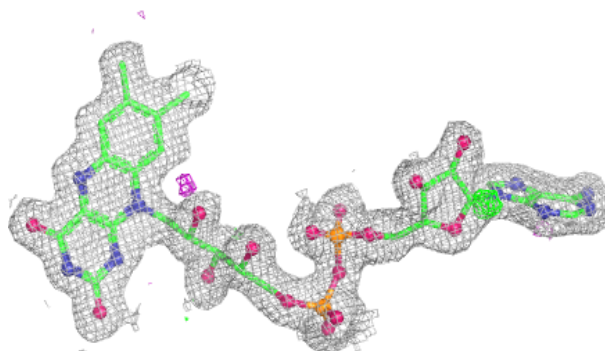
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FAD B 801:

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

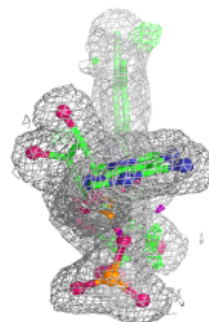
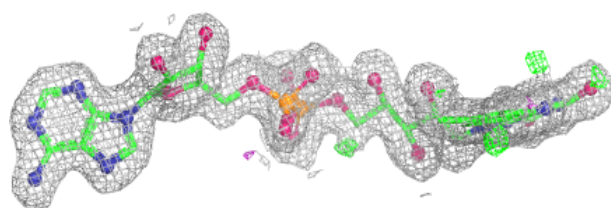
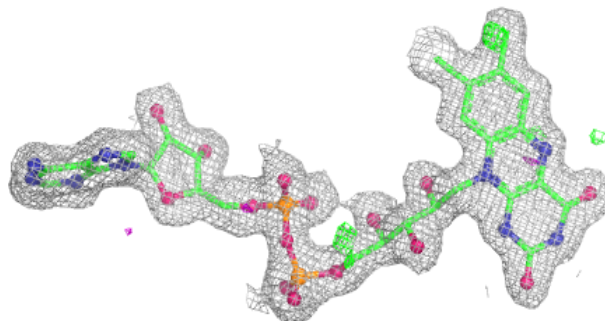
**Electron density around FAD D 801:**

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

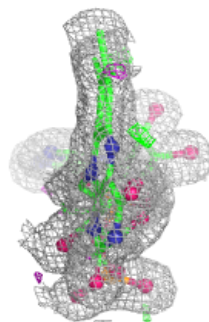
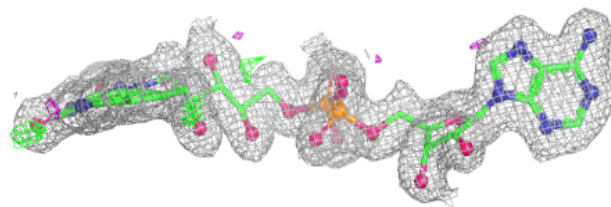
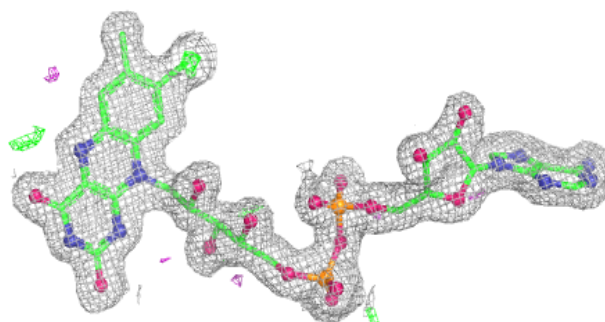


Electron density around FAD C 801:

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

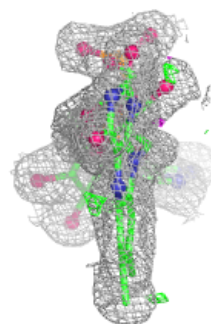
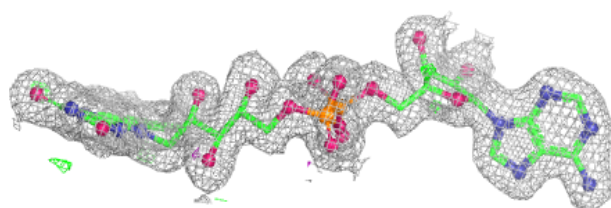
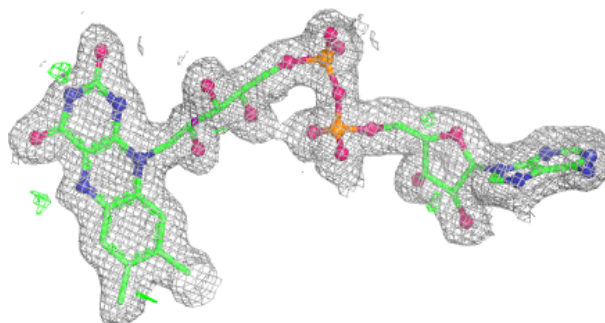
**Electron density around FAD E 801:**

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

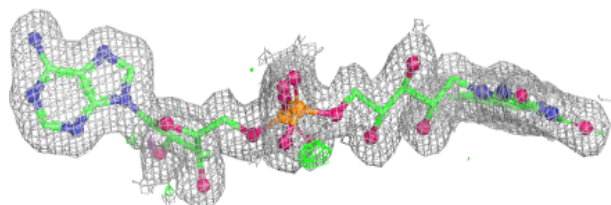
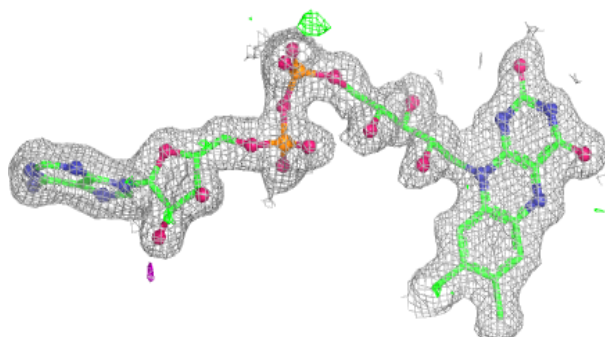


Electron density around FAD F 801:

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

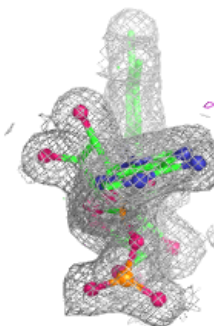
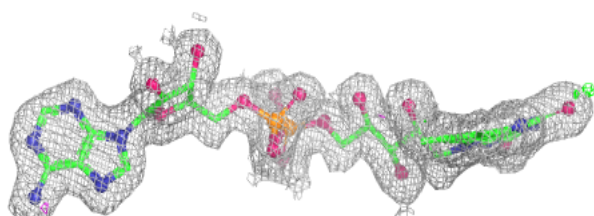
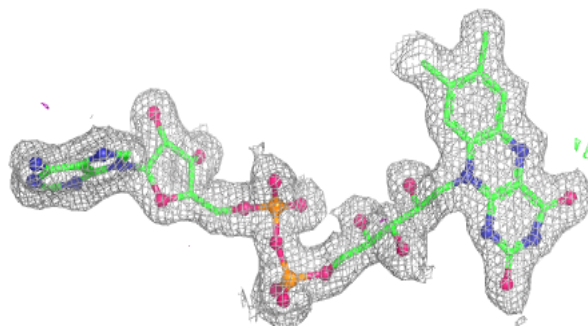
**Electron density around FAD G 801:**

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

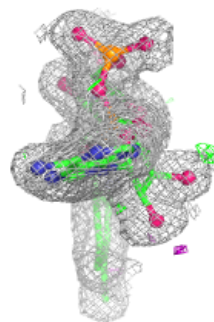
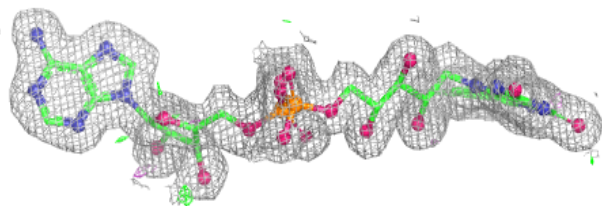
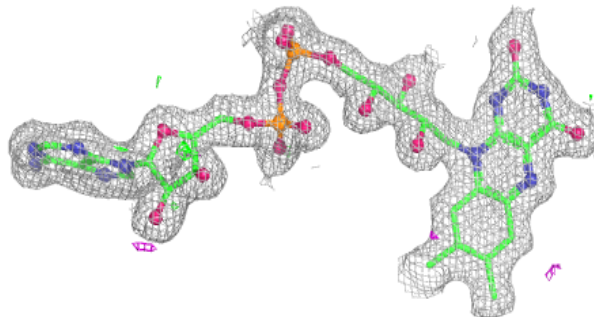


Electron density around FAD H 801:

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

**Electron density around FAD A 801:**

$2mF_o-DF_c$ (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.