Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 02:54 PM EDT

PDB ID	:	2IGN
Title	:	Crystal structure of recombinant pyranose 2-oxidase H167A mutant
Authors	:	Divne, C.
Deposited on	:	2006-09-22
Resolution	:	1.65 Å(reported)

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

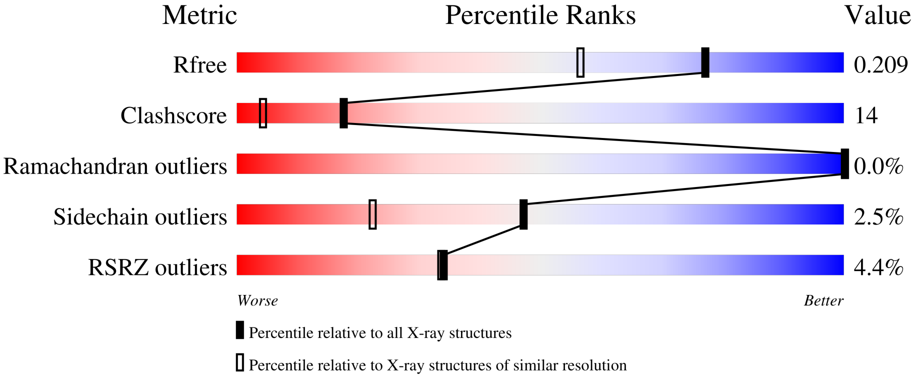
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

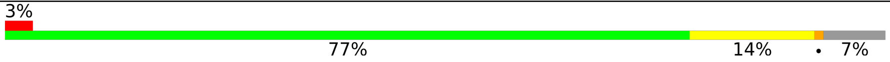
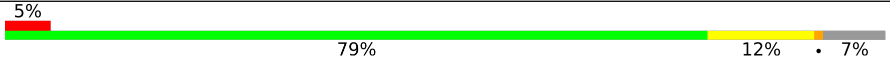
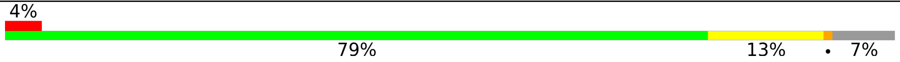
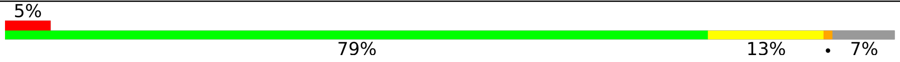
The reported resolution of this entry is 1.65 Å.

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}	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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 <=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	 4% 78% 13% • 7%
1	B	623	 3% 77% 14% • 7%
1	C	623	 5% 79% 12% • 7%
1	D	623	 4% 79% 13% • 7%
1	E	623	 5% 79% 13% • 7%

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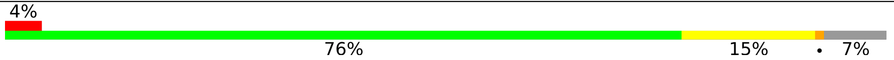
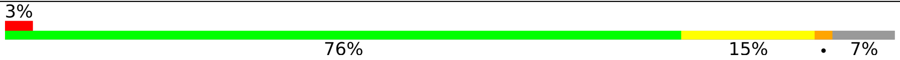
Mol	Chain	Length	Quality of chain
1	F	623	
1	G	623	
1	H	623	

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	MES	B	8003	-	-	X	-
3	MES	C	8008	-	-	X	-
3	MES	D	8005	-	-	X	-
3	MES	E	8007	-	-	X	-
3	MES	G	8006	-	-	X	-
3	MES	H	8004	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 41758 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.

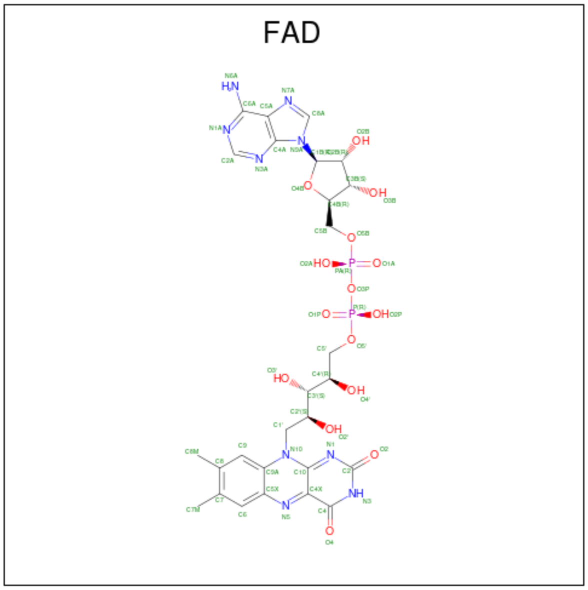
- Molecule 1 is a protein called Pyranose oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	577	Total 4551	C 2874	N 777	O 875	S 25	0	1	0
1	B	577	Total 4560	C 2879	N 779	O 877	S 25	0	2	0
1	D	577	Total 4560	C 2879	N 779	O 877	S 25	0	2	0
1	C	577	Total 4560	C 2879	N 779	O 877	S 25	0	2	0
1	E	577	Total 4560	C 2879	N 779	O 877	S 25	0	2	0
1	F	577	Total 4551	C 2874	N 777	O 875	S 25	0	1	0
1	H	577	Total 4568	C 2884	N 780	O 878	S 26	0	3	0
1	G	577	Total 4570	C 2885	N 782	O 878	S 25	0	3	0

There are 8 discrepancies between the modelled and reference sequences:

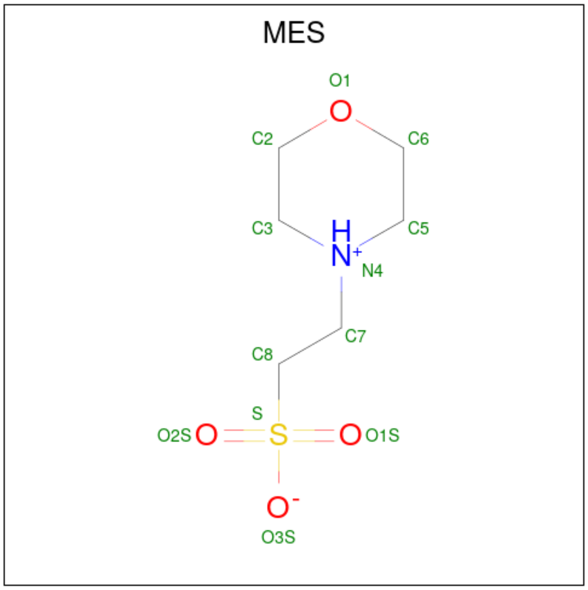
Chain	Residue	Modelled	Actual	Comment	Reference
A	167	ALA	HIS	engineered mutation	UNP Q7ZA32
B	167	ALA	HIS	engineered mutation	UNP Q7ZA32
C	167	ALA	HIS	engineered mutation	UNP Q7ZA32
D	167	ALA	HIS	engineered mutation	UNP Q7ZA32
E	167	ALA	HIS	engineered mutation	UNP Q7ZA32
F	167	ALA	HIS	engineered mutation	UNP Q7ZA32
G	167	ALA	HIS	engineered mutation	UNP Q7ZA32
H	167	ALA	HIS	engineered mutation	UNP Q7ZA32

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



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

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



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	705	Total O 705 705	0	0
4	B	670	Total O 670 670	0	0
4	D	577	Total O 577 577	0	0
4	C	528	Total O 528 528	0	0

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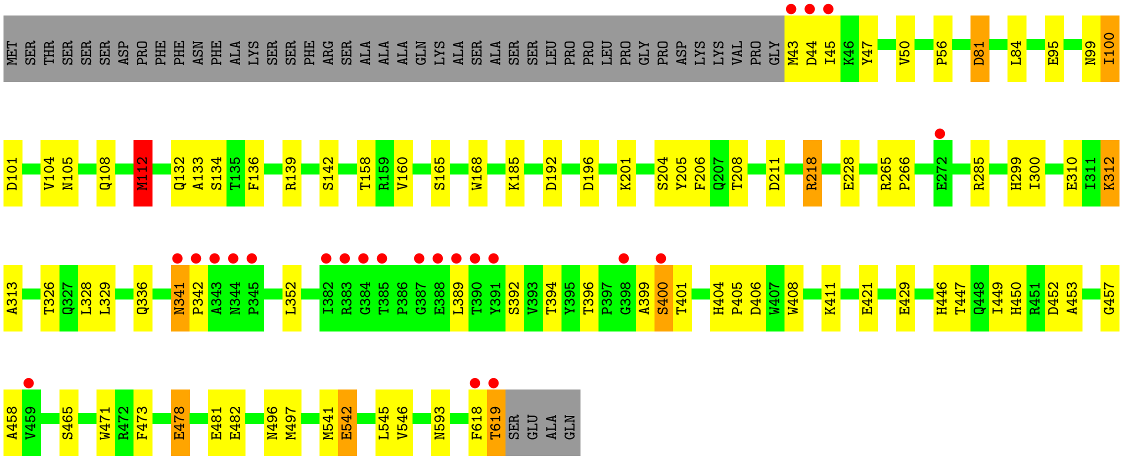
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	565	Total O 565 565	0	0
4	F	498	Total O 498 498	0	0
4	H	611	Total O 611 611	0	0
4	G	604	Total O 604 604	0	0

3 Residue-property plots ⓘ

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

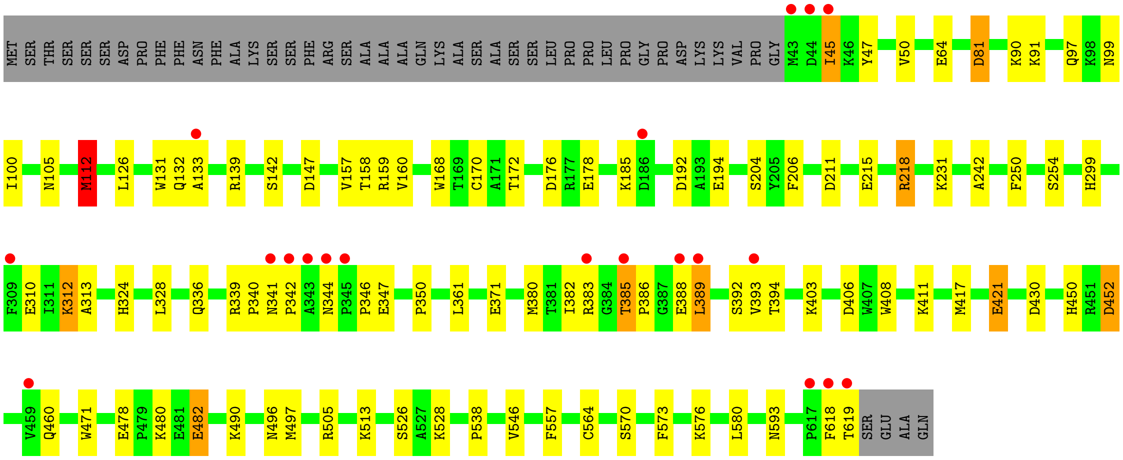
- Molecule 1: Pyranose oxidase

Chain A:



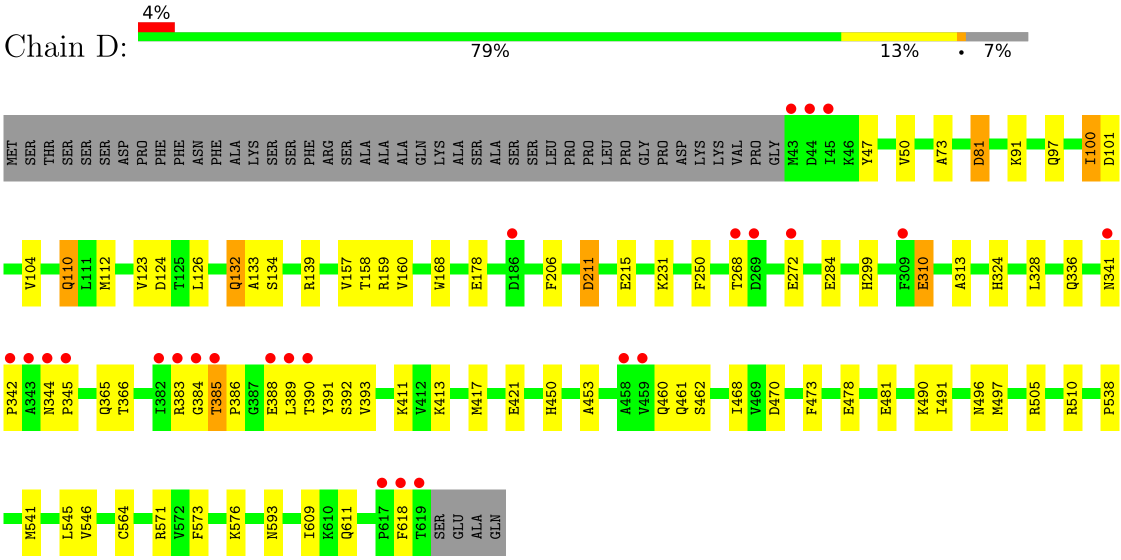
- Molecule 1: Pyranose oxidase

Chain B:



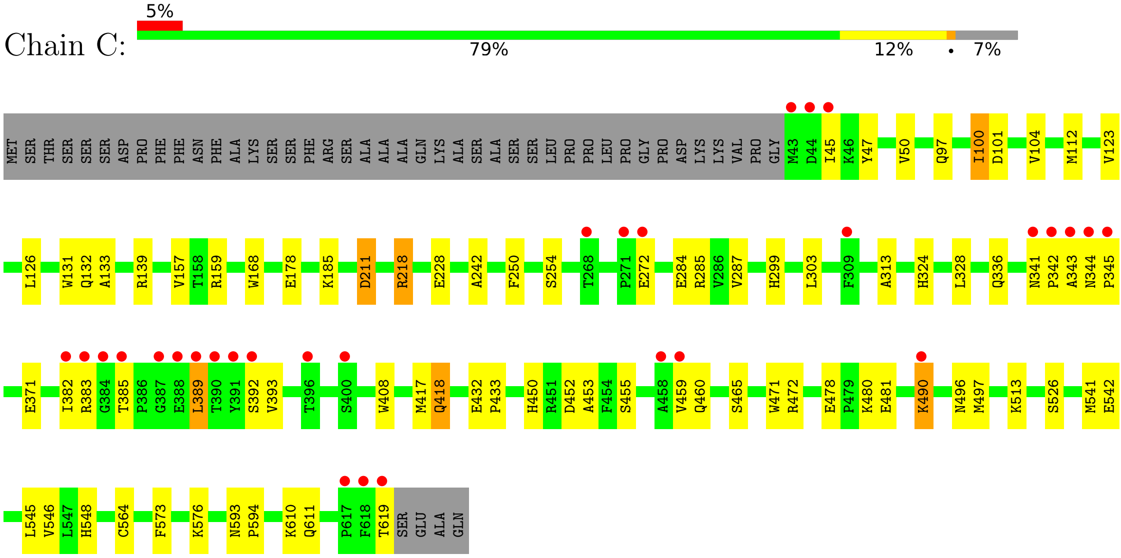
- Molecule 1: Pyranose oxidase

Chain D:



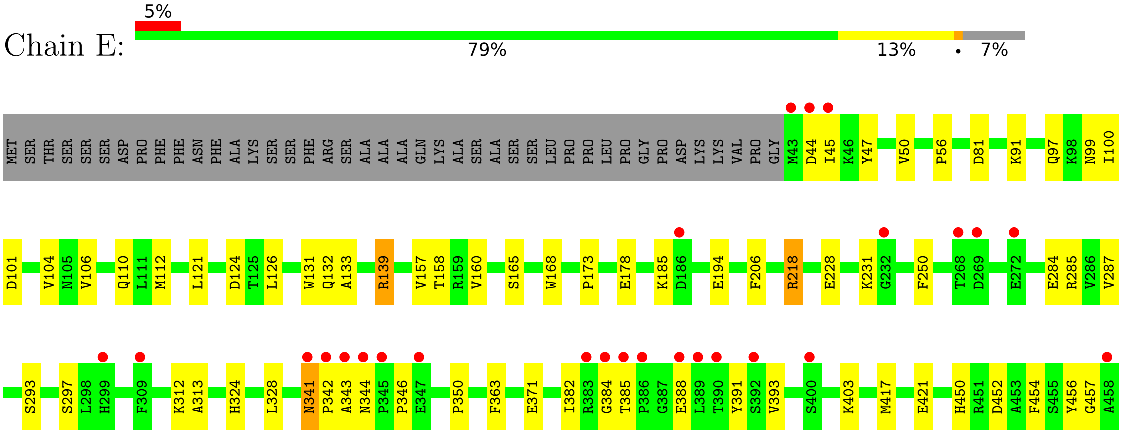
- Molecule 1: Pyranose oxidase

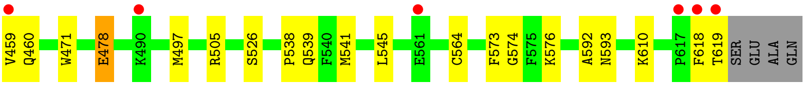
Chain C:



- Molecule 1: Pyranose oxidase

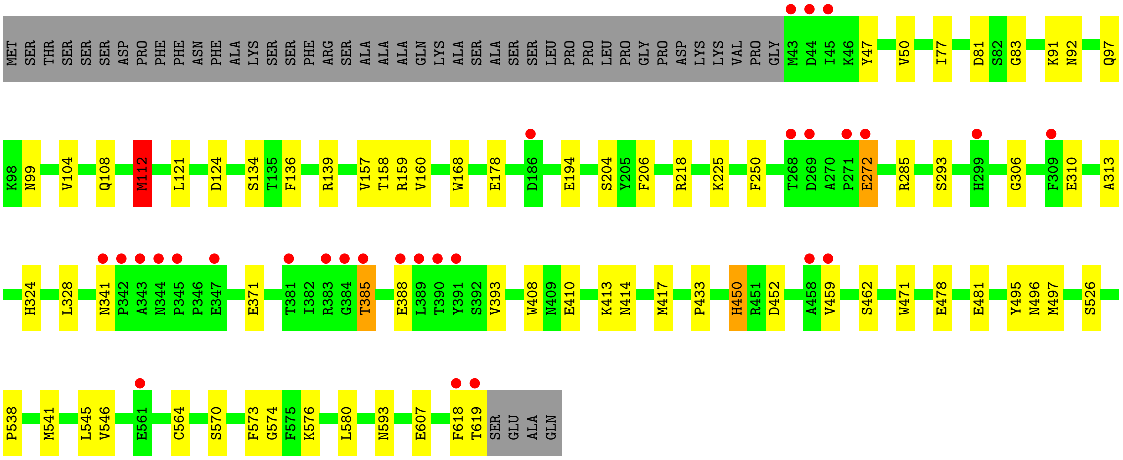
Chain E:





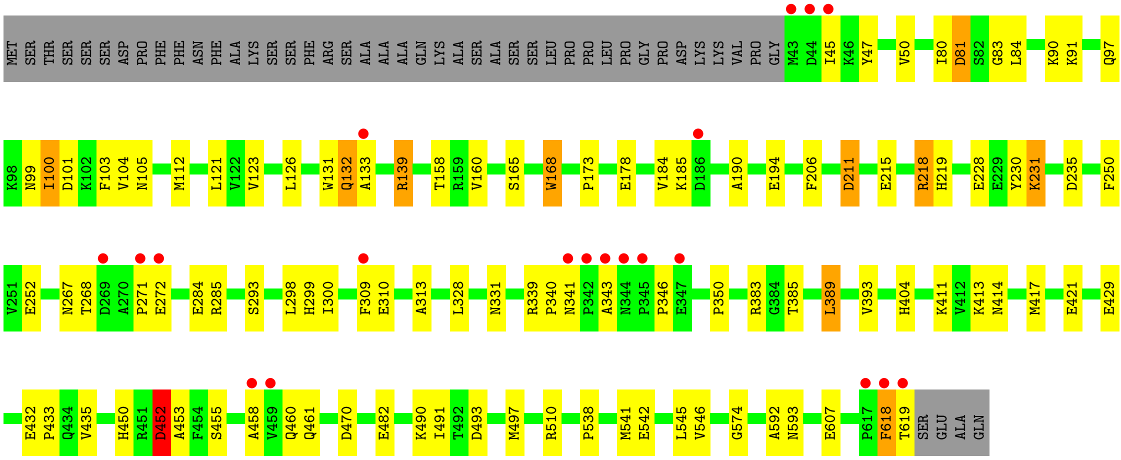
- Molecule 1: Pyranose oxidase

Chain F:



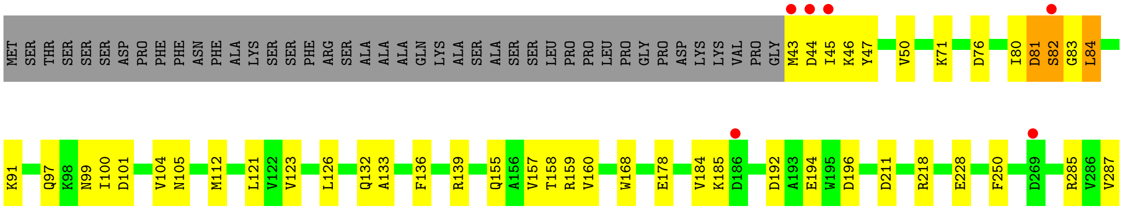
- Molecule 1: Pyranose oxidase

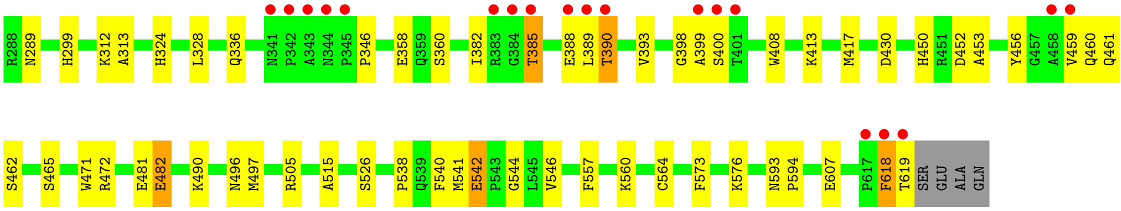
Chain H:



- Molecule 1: Pyranose oxidase

Chain G:




R288
N289
H299
K312
A313
H324
L328
Q336
N341
P342
A343
N344
P345
P346
E358
Q359
S360
I382
R383
G384
T385
E388
L389
T390
V393
G398
A399
S400
T401
W408
K413
M417
D430
H450
R451
D452
A453
Y456
G457
A458
V459
Q460
Q461
S462
S465
W471
R472
E481
E482
K490
N496
M497
R505
A515
S526
P538
Q539
F540
M541
E542
P543
G544
L545
V546
F557
K560
C564
F573
K576
N593
P594
E607
P617
F618
T619
SER
GLU
ALA
GLN

4 Data and refinement statistics (i)

Property	**Value**	**Source**
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	168.07Å 103.00Å 168.56Å 90.00° 106.43° 90.00°	Depositor
Resolution (Å)	39.00 – 1.65 38.98 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.00-1.65) 99.9 (38.98-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.172 , 0.205 0.179 , 0.209	Depositor DCC
R_{free} test set	6563 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å^2)	18.8	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 48.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.014 for l,-k,h	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	41758	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 19.82 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.9631e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.94	5/4666 (0.1%)	0.92	11/6345 (0.2%)
1	B	0.90	2/4675 (0.0%)	0.92	13/6357 (0.2%)
1	C	0.84	0/4675	0.86	7/6357 (0.1%)
1	D	0.82	2/4675 (0.0%)	0.87	11/6357 (0.2%)
1	E	0.81	1/4675 (0.0%)	0.84	5/6357 (0.1%)
1	F	0.81	2/4666 (0.0%)	0.84	5/6345 (0.1%)
1	G	0.89	5/4686 (0.1%)	0.90	11/6372 (0.2%)
1	H	0.89	2/4683 (0.0%)	0.92	12/6367 (0.2%)
All	All	0.86	19/37401 (0.1%)	0.88	75/50857 (0.1%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	310	GLU	CG-CD	7.49	1.63	1.51
1	D	310	GLU	CB-CG	7.16	1.65	1.52
1	B	482	GLU	CG-CD	6.94	1.62	1.51
1	G	81	ASP	CA-C	6.58	1.70	1.52
1	B	421	GLU	CB-CG	5.97	1.63	1.52
1	G	228	GLU	CG-CD	5.84	1.60	1.51
1	F	310	GLU	CG-CD	5.78	1.60	1.51
1	A	310	GLU	CB-CG	5.71	1.63	1.52
1	G	482	GLU	CG-CD	5.62	1.60	1.51
1	A	478	GLU	CD-OE1	5.41	1.31	1.25
1	A	310	GLU	CG-CD	5.41	1.60	1.51
1	G	542	GLU	CB-CG	-5.37	1.42	1.52
1	H	81	ASP	CB-CG	-5.35	1.40	1.51
1	F	478	GLU	CD-OE1	5.33	1.31	1.25
1	A	482	GLU	CG-CD	5.31	1.59	1.51
1	A	542	GLU	CG-CD	5.25	1.59	1.51
1	H	310	GLU	CG-CD	5.23	1.59	1.51
1	E	478	GLU	CD-OE1	5.15	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	82	SER	C-O	5.01	1.32	1.23

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	139	ARG	NE-CZ-NH2	-19.15	110.72	120.30
1	G	139	ARG	NE-CZ-NH2	-18.35	111.12	120.30
1	E	139	ARG	NE-CZ-NH2	-17.48	111.56	120.30
1	G	139	ARG	NE-CZ-NH1	17.45	129.03	120.30
1	F	139	ARG	NE-CZ-NH2	-17.08	111.76	120.30
1	B	139	ARG	NE-CZ-NH2	-16.83	111.89	120.30
1	A	139	ARG	NE-CZ-NH2	-15.57	112.52	120.30
1	H	139	ARG	NE-CZ-NH2	-15.53	112.54	120.30
1	C	139	ARG	NE-CZ-NH2	-14.82	112.89	120.30
1	D	139	ARG	NE-CZ-NH1	14.72	127.66	120.30
1	E	139	ARG	NE-CZ-NH1	14.47	127.54	120.30
1	C	139	ARG	NE-CZ-NH1	14.26	127.43	120.30
1	B	139	ARG	NE-CZ-NH1	14.05	127.33	120.30
1	F	139	ARG	NE-CZ-NH1	12.14	126.37	120.30
1	H	139	ARG	NE-CZ-NH1	11.52	126.06	120.30
1	H	389	LEU	CA-CB-CG	10.72	139.96	115.30
1	A	139	ARG	NE-CZ-NH1	9.73	125.16	120.30
1	B	81	ASP	CB-CG-OD1	-9.13	110.08	118.30
1	B	218	ARG	NE-CZ-NH1	8.43	124.52	120.30
1	B	81	ASP	CB-CG-OD2	8.35	125.81	118.30
1	H	218	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	A	211	ASP	CB-CG-OD1	8.11	125.59	118.30
1	G	81	ASP	CB-CG-OD1	-7.52	111.53	118.30
1	H	211	ASP	CB-CG-OD1	7.33	124.89	118.30
1	A	81	ASP	CB-CG-OD1	-7.18	111.84	118.30
1	D	211	ASP	CB-CG-OD1	6.83	124.44	118.30
1	C	472	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	B	211	ASP	CB-CG-OD1	6.70	124.33	118.30
1	H	493	ASP	CB-CG-OD1	6.40	124.06	118.30
1	E	81	ASP	CB-CG-OD1	-6.25	112.67	118.30
1	A	211	ASP	CB-CG-OD2	-6.24	112.68	118.30
1	C	218	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	A	192	ASP	CB-CG-OD1	6.12	123.80	118.30
1	G	76	ASP	CB-CG-OD2	6.09	123.78	118.30
1	C	211	ASP	CB-CG-OD1	6.02	123.72	118.30
1	A	112	MET	CG-SD-CE	5.95	109.72	100.20
1	A	218	ARG	NE-CZ-NH1	5.94	123.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	139	ARG	CD-NE-CZ	5.93	131.91	123.60
1	E	218	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	D	81	ASP	CB-CG-OD1	-5.78	113.10	118.30
1	C	139	ARG	CD-NE-CZ	5.75	131.65	123.60
1	B	406	ASP	CB-CG-OD1	5.73	123.46	118.30
1	H	452	ASP	CB-CA-C	5.72	121.84	110.40
1	B	218	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	G	472	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	F	218	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	H	470	ASP	CB-CG-OD1	5.56	123.31	118.30
1	B	139	ARG	CD-NE-CZ	5.55	131.38	123.60
1	G	196	ASP	CB-CG-OD1	5.47	123.23	118.30
1	B	192	ASP	CB-CG-OD1	5.47	123.22	118.30
1	D	139	ARG	CG-CD-NE	-5.46	100.33	111.80
1	G	139	ARG	CD-NE-CZ	5.46	131.24	123.60
1	A	196	ASP	CB-CG-OD1	5.44	123.19	118.30
1	C	472	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	H	211	ASP	CB-CG-OD2	-5.38	113.45	118.30
1	G	81	ASP	CB-CG-OD2	5.37	123.13	118.30
1	D	571	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	D	81	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	218	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	G	192	ASP	CB-CG-OD1	5.23	123.01	118.30
1	D	470	ASP	CB-CG-OD1	5.22	123.00	118.30
1	B	112	MET	CA-CB-CG	5.21	122.16	113.30
1	H	389	LEU	N-CA-CB	-5.21	99.99	110.40
1	H	81	ASP	CB-CG-OD1	-5.14	113.67	118.30
1	F	139	ARG	CD-NE-CZ	5.13	130.78	123.60
1	A	473	PHE	CB-CG-CD2	-5.12	117.22	120.80
1	B	147	ASP	CB-CG-OD1	5.10	122.89	118.30
1	E	139	ARG	CD-NE-CZ	5.10	130.74	123.60
1	B	452	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	D	473	PHE	CB-CG-CD1	5.09	124.36	120.80
1	F	112	MET	CG-SD-CE	5.09	108.34	100.20
1	G	472	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	G	211	ASP	CB-CG-OD1	5.05	122.85	118.30
1	D	473	PHE	CB-CG-CD2	-5.04	117.27	120.80
1	H	383	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4551	0	4401	126	0
1	B	4560	0	4408	152	0
1	C	4560	0	4408	107	0
1	D	4560	0	4408	93	0
1	E	4560	0	4408	98	0
1	F	4551	0	4401	74	0
1	G	4570	0	4414	170	0
1	H	4568	0	4416	163	1
2	A	53	0	31	0	0
2	B	53	0	30	2	0
2	C	53	0	28	1	0
2	D	53	0	30	1	0
2	E	53	0	29	0	0
2	F	53	0	30	1	0
2	G	53	0	30	1	0
2	H	53	0	29	0	0
3	A	12	0	12	4	0
3	B	12	0	12	9	0
3	C	12	0	12	10	0
3	D	12	0	12	14	0
3	E	12	0	12	11	0
3	F	12	0	12	4	0
3	G	12	0	12	9	0
3	H	12	0	12	17	0
4	A	705	0	0	100	2
4	B	670	0	0	111	1
4	C	528	0	0	73	0
4	D	577	0	0	56	0
4	E	565	0	0	64	0
4	F	498	0	0	48	0
4	G	604	0	0	110	3
4	H	611	0	0	122	1
All	All	41758	0	35597	993	4

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 14.

All (993) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:528:LYS:HE3	4:B:8620:HOH:O	1.23	1.38
1:B:452:ASP:HB2	4:B:8464:HOH:O	1.26	1.34
1:G:104[A]:VAL:HG23	4:G:8521:HOH:O	1.28	1.33
1:B:142:SER:HB3	4:B:8632:HOH:O	1.28	1.33
1:A:204:SER:HB2	4:A:8479:HOH:O	1.16	1.31
1:D:546:VAL:HG12	4:D:8527:HOH:O	1.15	1.30
1:C:328:LEU:HG	4:C:8437:HOH:O	1.28	1.29
1:A:208:THR:HG21	4:A:8588:HOH:O	1.16	1.27
1:C:546:VAL:HA	4:C:8472:HOH:O	1.10	1.27
1:D:328:LEU:HG	4:D:8462:HOH:O	1.34	1.27
1:H:413:LYS:HD2	4:H:8507:HOH:O	1.24	1.26
1:A:546:VAL:HA	4:A:8473:HOH:O	1.09	1.25
1:A:133:ALA:HB1	4:A:8381:HOH:O	1.36	1.25
1:G:546:VAL:HA	4:G:8455:HOH:O	1.25	1.25
1:B:328:LEU:HG	4:B:8525:HOH:O	1.37	1.25
1:F:546:VAL:HA	4:F:8436:HOH:O	1.21	1.25
1:B:133:ALA:HA	4:B:8607:HOH:O	1.38	1.23
1:F:204:SER:HB2	4:F:8421:HOH:O	1.28	1.23
1:A:204:SER:CB	4:A:8479:HOH:O	1.70	1.23
1:F:134:SER:HB2	4:F:8441:HOH:O	1.35	1.23
1:E:371:GLU:HB3	4:E:8522:HOH:O	1.38	1.22
4:H:8528:HOH:O	1:G:121:LEU:HD12	1.33	1.22
1:F:452:ASP:HB2	4:F:8405:HOH:O	1.32	1.21
1:A:160:VAL:HB	4:A:8654:HOH:O	1.04	1.20
1:C:104[A]:VAL:HG23	4:C:8397:HOH:O	1.41	1.19
1:C:452:ASP:HB2	4:C:8432:HOH:O	1.39	1.18
1:G:328:LEU:HG	4:G:8550:HOH:O	1.38	1.18
1:A:108:GLN:HG2	4:A:8376:HOH:O	1.43	1.18
1:A:142:SER:HB3	4:A:8535:HOH:O	1.42	1.17
1:G:465:SER:HB2	4:G:8570:HOH:O	1.01	1.17
1:B:204:SER:HB2	4:B:8547:HOH:O	0.99	1.16
1:B:478:GLU:HB2	4:B:8610:HOH:O	1.45	1.15
1:B:45:ILE:HD12	4:B:8338:HOH:O	1.47	1.15
1:H:133:ALA:HA	4:H:8544:HOH:O	1.45	1.14
1:E:459:VAL:HG22	4:E:8545:HOH:O	1.48	1.13
1:D:133:ALA:HB3	3:D:8005:MES:C7	1.77	1.13
1:D:609:ILE:HG22	4:D:8536:HOH:O	1.49	1.13
1:H:331:ASN:HB3	4:H:8576:HOH:O	1.48	1.13
1:H:546:VAL:HA	4:H:8375:HOH:O	0.94	1.12
1:D:546:VAL:HA	4:D:8470:HOH:O	0.98	1.12
1:E:454:PHE:HE2	4:E:8500:HOH:O	1.32	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:SER:HB2	4:A:8630:HOH:O	1.46	1.12
1:A:465:SER:HB2	4:A:8522:HOH:O	0.96	1.10
1:E:497:MET:CE	4:E:8276:HOH:O	1.99	1.08
1:A:399:ALA:HB1	4:A:8622:HOH:O	1.53	1.08
1:A:545:LEU:HD13	4:A:8649:HOH:O	1.53	1.07
1:B:371:GLU:HB3	4:B:8526:HOH:O	1.52	1.07
1:C:465:SER:HB2	4:C:8393:HOH:O	0.89	1.06
1:F:112:MET:CG	4:F:8442:HOH:O	2.02	1.06
1:H:104[A]:VAL:HG23	4:H:8555:HOH:O	1.55	1.06
1:H:435:VAL:HG23	4:H:8587:HOH:O	1.56	1.05
1:H:452:ASP:HB2	4:H:8499:HOH:O	1.54	1.05
1:D:468:ILE:HG23	4:D:8526:HOH:O	1.56	1.05
1:G:155:GLN:HG2	4:G:8530:HOH:O	1.53	1.04
1:A:44:ASP:HB3	4:A:8394:HOH:O	1.57	1.04
1:G:452:ASP:HB2	4:G:8460:HOH:O	1.56	1.03
1:B:340:PRO:HD2	4:B:8553:HOH:O	1.57	1.03
1:C:545:LEU:HD13	4:C:8502:HOH:O	1.56	1.03
1:F:459:VAL:HG13	4:F:8302:HOH:O	1.57	1.02
1:G:453:ALA:HB1	4:G:8521:HOH:O	1.60	1.02
1:E:497:MET:HE2	4:E:8276:HOH:O	1.56	1.01
1:A:542:GLU:HB3	4:A:8649:HOH:O	1.59	1.01
1:B:133:ALA:HB3	3:B:8003:MES:C7	1.91	1.00
1:G:497:MET:CE	4:G:8374:HOH:O	2.09	1.00
1:H:393:VAL:H	1:H:417[B]:MET:HE1	1.26	1.00
1:G:312:LYS:HB2	4:G:8555:HOH:O	1.62	0.99
3:D:8005:MES:H72	4:D:8310:HOH:O	1.62	0.99
1:C:453:ALA:HB1	4:C:8397:HOH:O	1.60	0.99
1:A:312:LYS:HB3	4:A:8623:HOH:O	1.61	0.99
1:D:133:ALA:HB3	3:D:8005:MES:H72	1.42	0.99
1:G:594:PRO:HG3	4:G:8572:HOH:O	1.62	0.99
1:D:133:ALA:HB3	3:D:8005:MES:H71	1.42	0.98
4:B:8469:HOH:O	1:C:542:GLU:HB2	1.62	0.98
1:H:97:GLN:HB2	4:H:8480:HOH:O	1.63	0.98
1:H:298:LEU:HB3	4:H:8578:HOH:O	1.63	0.98
1:A:112:MET:HB2	4:B:8609:HOH:O	1.62	0.98
1:B:172:THR:HG23	4:B:8594:HOH:O	1.61	0.98
1:H:298:LEU:CD1	4:H:8520:HOH:O	2.10	0.97
1:E:459:VAL:HG13	4:E:8503:HOH:O	1.64	0.97
1:H:104[B]:VAL:HG13	4:H:8555:HOH:O	1.64	0.97
1:B:204:SER:CB	4:B:8547:HOH:O	1.68	0.97
1:B:133:ALA:CA	4:B:8607:HOH:O	2.03	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:454:PHE:CE2	4:E:8500:HOH:O	2.10	0.97
4:H:8615:HOH:O	1:G:84:LEU:HG	1.64	0.97
1:A:405:PRO:C	4:A:8625:HOH:O	2.02	0.96
1:D:133:ALA:CB	3:D:8005:MES:C7	2.42	0.96
1:A:352:LEU:HD21	4:A:8656:HOH:O	1.63	0.96
1:H:453:ALA:HB1	4:H:8555:HOH:O	1.66	0.96
1:C:541:MET:CE	4:C:8146:HOH:O	2.12	0.96
1:G:465:SER:CB	4:G:8570:HOH:O	1.67	0.95
1:C:541:MET:HE3	4:C:8146:HOH:O	1.67	0.95
1:E:541:MET:SD	4:E:8502:HOH:O	2.24	0.95
1:H:211:ASP:HB3	4:H:8421:HOH:O	1.66	0.95
1:C:542:GLU:HB3	4:C:8502:HOH:O	1.66	0.95
1:D:272:GLU:HG2	4:D:8433:HOH:O	1.65	0.94
1:F:92:ASN:C	4:F:8419:HOH:O	2.05	0.94
1:H:84:LEU:HD21	4:G:8586:HOH:O	1.65	0.94
1:E:393:VAL:H	1:E:417:MET:HE2	1.32	0.93
1:D:100:ILE:HG12	4:D:8425:HOH:O	1.68	0.93
1:H:300:ILE:HG13	4:H:8590:HOH:O	1.69	0.92
1:D:133:ALA:CB	3:D:8005:MES:H71	1.98	0.92
3:B:8003:MES:H72	4:B:8503:HOH:O	1.70	0.92
1:H:81:ASP:HB2	4:H:8304:HOH:O	1.69	0.92
1:G:389:LEU:HD13	4:G:8577:HOH:O	1.68	0.92
1:C:619:THR:HG22	4:C:8291:HOH:O	1.68	0.92
1:B:112:MET:HE2	4:B:8592:HOH:O	1.69	0.91
1:A:542:GLU:HG3	4:D:8339:HOH:O	1.69	0.91
1:E:133:ALA:HB2	3:E:8007:MES:O1S	1.70	0.91
1:D:133:ALA:HB2	3:D:8005:MES:O3S	1.71	0.91
1:E:126:LEU:CD1	1:E:132[B]:GLN:HG3	2.00	0.91
1:H:230:TYR:C	4:H:8510:HOH:O	2.08	0.91
1:A:112:MET:CB	4:B:8609:HOH:O	2.18	0.90
1:D:126:LEU:HD12	1:D:132[B]:GLN:HG3	1.51	0.90
1:H:541:MET:HG3	4:H:8603:HOH:O	1.70	0.90
1:H:458:ALA:O	4:H:8528:HOH:O	1.90	0.90
1:B:178:GLU:HG3	4:B:8262:HOH:O	1.72	0.90
1:G:101:ASP:O	4:G:8521:HOH:O	1.89	0.90
1:C:285:ARG:HD3	4:C:8385:HOH:O	1.70	0.90
1:H:458:ALA:C	4:H:8528:HOH:O	2.10	0.90
1:B:178:GLU:HB2	4:B:8626:HOH:O	1.70	0.89
1:B:385:THR:HG23	1:B:388:GLU:OE1	1.72	0.89
1:C:611:GLN:HG2	4:C:8423:HOH:O	1.73	0.89
1:C:126:LEU:HD12	1:C:132[B]:GLN:HG3	1.51	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:HIS:CD2	4:B:8612:HOH:O	2.25	0.89
1:B:112:MET:CE	4:B:8592:HOH:O	2.18	0.89
1:G:360:SER:HB3	4:G:8588:HOH:O	1.74	0.88
1:B:250:PHE:HD2	4:B:8670:HOH:O	1.55	0.88
1:B:133:ALA:HB3	3:B:8003:MES:H71	1.54	0.88
1:B:133:ALA:HB3	3:B:8003:MES:H72	1.56	0.88
1:E:121:LEU:HB3	4:F:8302:HOH:O	1.74	0.88
1:H:298:LEU:HD11	4:H:8520:HOH:O	1.68	0.88
3:H:8004:MES:H72	1:G:462:SER:O	1.73	0.87
1:D:126:LEU:CD1	1:D:132[B]:GLN:HG3	2.03	0.87
1:F:112:MET:SD	4:F:8442:HOH:O	2.31	0.87
1:D:126:LEU:CD1	1:D:132[B]:GLN:CG	2.54	0.85
1:A:43:MET:HE1	4:A:8342:HOH:O	1.75	0.85
1:B:393:VAL:H	1:B:417:MET:HE2	1.38	0.85
3:C:8008:MES:H72	4:C:8251:HOH:O	1.76	0.84
1:A:545:LEU:HB2	4:A:8649:HOH:O	1.77	0.84
1:C:594:PRO:HG3	4:C:8370:HOH:O	1.76	0.84
1:A:112:MET:SD	4:B:8609:HOH:O	2.35	0.84
1:C:303:LEU:HD21	4:C:8361:HOH:O	1.77	0.83
1:A:312:LYS:HE2	4:A:8623:HOH:O	1.78	0.83
1:A:618:PHE:HB3	4:A:8553:HOH:O	1.79	0.83
1:A:112:MET:CG	4:B:8609:HOH:O	2.26	0.83
1:A:447:THR:HG22	4:A:8655:HOH:O	1.77	0.83
1:G:312:LYS:HD2	4:G:8555:HOH:O	1.79	0.83
1:C:126:LEU:CD1	1:C:132[B]:GLN:HG3	2.08	0.83
1:C:287:VAL:CG2	4:C:8497:HOH:O	2.26	0.83
1:B:133:ALA:HB2	3:B:8003:MES:O2S	1.79	0.82
1:B:497:MET:CE	4:B:8369:HOH:O	2.26	0.82
1:F:112:MET:HG2	4:F:8442:HOH:O	1.71	0.82
1:A:404:HIS:O	4:A:8625:HOH:O	1.97	0.82
1:F:417:MET:HE3	4:F:8415:HOH:O	1.78	0.82
1:H:132[B]:GLN:OE1	3:H:8004:MES:H52	1.80	0.82
1:B:393:VAL:H	1:B:417:MET:CE	1.93	0.82
1:B:126:LEU:CD1	1:B:132[B]:GLN:HG3	2.09	0.82
1:E:459:VAL:CG2	4:E:8545:HOH:O	2.14	0.82
1:H:618:PHE:HB3	4:H:8344:HOH:O	1.79	0.82
1:G:497:MET:HE2	4:G:8374:HOH:O	1.72	0.82
1:H:133:ALA:CB	3:H:8004:MES:H81	2.09	0.81
1:G:312:LYS:CB	4:G:8555:HOH:O	2.24	0.81
1:D:541:MET:HE3	4:D:8191:HOH:O	1.79	0.81
1:H:228:GLU:OE1	4:H:8446:HOH:O	1.96	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:126:LEU:CD1	1:G:132[B]:GLN:HG3	2.10	0.81
1:A:541:MET:SD	4:A:8689:HOH:O	2.38	0.81
4:H:8279:HOH:O	1:G:81:ASP:HA	1.79	0.81
3:A:8002:MES:H72	4:A:8414:HOH:O	1.80	0.81
1:G:133:ALA:HB3	3:G:8006:MES:C7	2.11	0.81
1:G:497:MET:HE1	4:G:8374:HOH:O	1.72	0.80
1:H:100:ILE:HG12	4:H:8387:HOH:O	1.80	0.80
1:G:299[A]:HIS:CE1	4:G:8370:HOH:O	2.34	0.80
1:B:126:LEU:HD12	1:B:132[B]:GLN:HG3	1.63	0.80
1:B:250:PHE:CD2	4:B:8670:HOH:O	2.31	0.80
1:H:133:ALA:CA	4:H:8544:HOH:O	2.15	0.80
1:B:172:THR:CG2	4:B:8594:HOH:O	2.25	0.80
1:A:133:ALA:CB	4:A:8381:HOH:O	2.07	0.79
1:B:112:MET:SD	4:B:8592:HOH:O	2.39	0.79
1:D:541:MET:CE	4:D:8191:HOH:O	2.29	0.79
3:G:8006:MES:H72	4:G:8371:HOH:O	1.82	0.79
1:B:170:CYS:O	4:B:8594:HOH:O	1.99	0.79
1:A:389:LEU:HA	4:A:8611:HOH:O	1.83	0.79
1:H:250:PHE:CD2	4:H:8480:HOH:O	2.34	0.79
1:B:482:GLU:HG3	4:B:8564:HOH:O	1.82	0.79
1:B:328:LEU:CD1	4:B:8525:HOH:O	2.30	0.78
1:C:610:LYS:O	4:C:8494:HOH:O	2.01	0.78
4:E:8545:HOH:O	1:F:121:LEU:HD22	1.82	0.78
1:G:184:VAL:HG12	4:G:8589:HOH:O	1.83	0.78
1:D:478:GLU:HB2	4:D:8535:HOH:O	1.83	0.78
1:A:545:LEU:HD22	4:A:8649:HOH:O	1.82	0.78
1:A:619:THR:HG22	4:A:8659:HOH:O	1.83	0.78
1:F:204:SER:CB	4:F:8421:HOH:O	2.00	0.78
1:A:228:GLU:HG3	4:A:8362:HOH:O	1.83	0.77
1:G:456:TYR:HB3	4:G:8463:HOH:O	1.85	0.77
1:H:123:VAL:H	3:H:8004:MES:H22	1.49	0.77
1:A:133:ALA:N	4:A:8633:HOH:O	2.18	0.77
1:A:452:ASP:CB	4:A:8367:HOH:O	2.33	0.77
1:D:341:ASN:ND2	4:D:8533:HOH:O	2.15	0.77
1:E:228:GLU:OE1	4:E:8412:HOH:O	2.02	0.77
1:F:341:ASN:ND2	4:F:8423:HOH:O	2.16	0.77
1:A:133:ALA:O	4:A:8679:HOH:O	2.04	0.76
1:A:452:ASP:HB2	4:A:8367:HOH:O	1.84	0.76
1:G:413:LYS:HD2	4:G:8496:HOH:O	1.85	0.76
1:E:619:THR:HG23	4:E:8531:HOH:O	1.86	0.76
1:C:133:ALA:HB3	3:C:8008:MES:H72	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:MET:CE	4:A:8380:HOH:O	2.33	0.76
1:G:619:THR:HG21	4:G:8569:HOH:O	1.84	0.76
1:F:393:VAL:H	1:F:417:MET:CE	1.98	0.76
1:C:45:ILE:HG23	4:C:8400:HOH:O	1.86	0.75
1:C:133:ALA:HB3	3:C:8008:MES:C7	2.15	0.75
1:H:133:ALA:HB3	3:H:8004:MES:H51	1.68	0.75
1:G:81:ASP:CA	4:G:8299:HOH:O	2.32	0.75
1:G:133:ALA:HB3	3:G:8006:MES:H71	1.67	0.75
1:C:465:SER:CB	4:C:8393:HOH:O	1.68	0.75
1:B:131:TRP:CZ3	4:B:8607:HOH:O	2.38	0.75
1:D:384:GLY:HA3	4:D:8483:HOH:O	1.87	0.75
1:D:391:TYR:HB3	4:D:8401:HOH:O	1.86	0.75
1:D:611:GLN:HG2	4:D:8393:HOH:O	1.87	0.75
1:C:393:VAL:H	1:C:417:MET:HE2	1.51	0.75
1:G:132[A]:GLN:HG2	4:G:8290:HOH:O	1.86	0.74
1:G:285:ARG:HD3	4:G:8414:HOH:O	1.85	0.74
1:C:104[B]:VAL:HG13	4:C:8397:HOH:O	1.87	0.74
1:E:126:LEU:HD13	1:E:132[B]:GLN:CG	2.17	0.74
1:A:299:HIS:NE2	4:A:8599:HOH:O	2.20	0.74
1:C:132[A]:GLN:HG2	4:C:8244:HOH:O	1.86	0.74
1:C:101:ASP:HA	4:C:8397:HOH:O	1.87	0.74
1:B:176:ASP:OD1	4:B:8626:HOH:O	2.05	0.74
1:E:126:LEU:CD1	1:E:132[B]:GLN:CG	2.65	0.73
1:G:360:SER:CB	4:G:8588:HOH:O	2.34	0.73
1:B:100:ILE:HD13	4:B:8444:HOH:O	1.87	0.73
1:B:528:LYS:NZ	4:B:8620:HOH:O	2.14	0.73
1:D:133:ALA:CB	3:D:8005:MES:H72	2.11	0.73
3:D:8005:MES:C7	4:D:8310:HOH:O	2.23	0.73
1:F:462:SER:OG	4:F:8327:HOH:O	2.05	0.73
1:G:126:LEU:HD13	1:G:132[B]:GLN:CG	2.19	0.73
1:E:460:GLN:NE2	4:E:8500:HOH:O	2.21	0.73
1:A:100:ILE:HG12	4:A:8662:HOH:O	1.88	0.73
1:B:133:ALA:CB	3:B:8003:MES:C7	2.67	0.73
3:B:8003:MES:C7	4:B:8503:HOH:O	2.29	0.73
1:F:92:ASN:O	4:F:8419:HOH:O	2.03	0.73
1:F:124:ASP:OD1	4:F:8449:HOH:O	2.07	0.73
1:G:133:ALA:HB2	3:G:8006:MES:O3S	1.87	0.73
1:G:393:VAL:H	1:G:417:MET:CE	2.02	0.73
1:A:399:ALA:CB	4:A:8622:HOH:O	2.20	0.72
1:D:178:GLU:OE1	4:D:8307:HOH:O	2.05	0.72
1:B:341:ASN:HB3	4:B:8604:HOH:O	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:133:ALA:HA	4:E:8271:HOH:O	1.88	0.72
1:F:410:GLU:HB3	4:F:8476:HOH:O	1.89	0.72
1:H:393:VAL:H	1:H:417[B]:MET:CE	2.00	0.72
1:G:541:MET:SD	4:G:8540:HOH:O	2.46	0.72
1:B:421:GLU:OE2	4:B:8672:HOH:O	2.07	0.72
1:F:538:PRO:HG2	1:H:538:PRO:HG2	1.70	0.72
1:B:361:LEU:HB2	4:B:8629:HOH:O	1.90	0.72
1:B:45:ILE:HD12	1:B:45:ILE:H	1.55	0.72
1:H:133:ALA:HB2	3:H:8004:MES:H81	1.72	0.72
1:B:385:THR:HB	4:B:8392:HOH:O	1.89	0.72
1:E:126:LEU:HD12	1:E:132[B]:GLN:HG3	1.71	0.72
1:C:126:LEU:CD1	1:C:132[B]:GLN:CG	2.67	0.72
1:E:297:SER:HB2	4:E:8536:HOH:O	1.87	0.72
1:H:393:VAL:N	1:H:417[B]:MET:HE1	2.04	0.72
1:G:81:ASP:HB2	4:G:8299:HOH:O	1.90	0.72
1:A:329:LEU:HB2	4:A:8656:HOH:O	1.89	0.72
1:A:545:LEU:CG	4:A:8649:HOH:O	2.38	0.72
1:H:460:GLN:O	4:H:8562:HOH:O	2.06	0.72
1:A:133:ALA:O	4:A:8633:HOH:O	2.08	0.71
1:B:126:LEU:CD1	1:B:132[B]:GLN:CG	2.66	0.71
1:B:133:ALA:CB	3:B:8003:MES:H71	2.19	0.71
1:G:460:GLN:C	4:G:8463:HOH:O	2.27	0.71
1:B:497:MET:HE2	4:B:8369:HOH:O	1.86	0.71
1:E:178:GLU:OE1	4:E:8277:HOH:O	2.07	0.71
1:F:413:LYS:HE2	4:F:8470:HOH:O	1.89	0.71
1:A:394:THR:HG23	4:A:8486:HOH:O	1.90	0.71
1:G:100:ILE:HG13	4:G:8331:HOH:O	1.89	0.71
1:D:211:ASP:HB3	4:D:8348:HOH:O	1.89	0.70
1:E:421:GLU:OE2	4:E:8571:HOH:O	2.08	0.70
1:A:300:ILE:O	4:A:8599:HOH:O	2.10	0.70
1:D:299:HIS:HB2	1:D:310:GLU:OE1	1.91	0.70
1:D:393:VAL:H	1:D:417:MET:CE	2.04	0.70
1:H:126:LEU:CD1	1:H:132[B]:GLN:HG3	2.21	0.70
1:B:312:LYS:HE2	4:B:8573:HOH:O	1.91	0.70
1:B:385:THR:HG23	1:B:388:GLU:CD	2.11	0.70
1:B:45:ILE:HB	4:B:8568:HOH:O	1.92	0.70
4:E:8545:HOH:O	1:F:121:LEU:HD13	1.92	0.69
1:A:396:THR:HG22	4:A:8593:HOH:O	1.91	0.69
1:D:126:LEU:HD13	1:D:132[B]:GLN:HG2	1.73	0.69
1:D:546:VAL:CG1	4:D:8527:HOH:O	1.92	0.69
1:G:390:THR:CB	4:G:8559:HOH:O	2.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:LEU:HD13	4:B:8639:HOH:O	1.93	0.69
1:B:528:LYS:CE	4:B:8620:HOH:O	1.94	0.69
1:H:126:LEU:HD13	1:H:132[B]:GLN:CG	2.23	0.69
1:C:133:ALA:HB2	3:C:8008:MES:O1S	1.93	0.69
1:A:396:THR:HB	4:A:8640:HOH:O	1.91	0.68
1:H:298:LEU:HD12	4:H:8520:HOH:O	1.86	0.68
1:G:126:LEU:CD1	1:G:132[B]:GLN:CG	2.71	0.68
1:D:366:THR:O	4:D:8526:HOH:O	2.11	0.68
1:E:91:LYS:CE	4:E:8307:HOH:O	2.42	0.68
1:C:497:MET:CE	4:C:8350:HOH:O	2.40	0.68
1:G:453:ALA:HB3	4:G:8552:HOH:O	1.92	0.68
1:G:393:VAL:H	1:G:417:MET:HE2	1.58	0.68
1:A:101:ASP:O	1:A:104[A]:VAL:HG23	1.94	0.68
1:C:178:GLU:OE1	4:C:8276:HOH:O	2.12	0.68
1:A:465:SER:CB	4:A:8522:HOH:O	1.74	0.67
1:D:421:GLU:HG3	4:D:8542:HOH:O	1.93	0.67
1:H:97:GLN:CB	4:H:8480:HOH:O	2.25	0.67
1:C:545:LEU:CG	4:C:8502:HOH:O	2.42	0.67
1:H:194:GLU:HG2	4:H:8356:HOH:O	1.92	0.67
1:H:131:TRP:CH2	4:H:8544:HOH:O	2.47	0.67
1:G:44:ASP:HB3	4:G:8492:HOH:O	1.95	0.67
1:B:64:GLU:OE1	4:B:8366:HOH:O	2.12	0.67
1:F:413:LYS:NZ	1:F:414:ASN:OD1	2.27	0.67
1:H:267:ASN:O	4:H:8596:HOH:O	2.12	0.67
1:G:178:GLU:OE1	4:G:8332:HOH:O	2.12	0.67
1:G:461:GLN:N	4:G:8463:HOH:O	2.26	0.67
1:E:194:GLU:HG2	4:E:8441:HOH:O	1.94	0.67
4:F:8449:HOH:O	1:G:542:GLU:HG3	1.93	0.67
1:G:289:ASN:N	4:G:8562:HOH:O	2.28	0.67
1:G:389:LEU:HD12	4:G:8491:HOH:O	1.93	0.67
1:D:124:ASP:OD1	4:D:8339:HOH:O	2.12	0.67
1:D:462:SER:OG	4:D:8439:HOH:O	2.13	0.67
1:C:371:GLU:HB3	4:C:8492:HOH:O	1.94	0.67
1:F:272:GLU:HG2	4:F:8328:HOH:O	1.93	0.67
1:G:44:ASP:CB	4:G:8492:HOH:O	2.43	0.67
1:A:458:ALA:HA	4:A:8638:HOH:O	1.93	0.66
1:C:576:LYS:HD3	4:C:8260:HOH:O	1.94	0.66
1:B:131:TRP:CH2	4:B:8607:HOH:O	2.47	0.66
1:D:497:MET:CE	4:D:8282:HOH:O	2.42	0.66
4:H:8279:HOH:O	1:G:81:ASP:CA	2.41	0.66
1:A:446:HIS:O	4:A:8655:HOH:O	2.12	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:497:MET:HE1	4:B:8369:HOH:O	1.93	0.66
1:H:461:GLN:HA	4:H:8562:HOH:O	1.94	0.66
1:G:44:ASP:HB3	4:G:8305:HOH:O	1.94	0.66
1:A:100:ILE:HD13	1:A:100:ILE:O	1.95	0.66
1:E:133:ALA:HB2	3:E:8007:MES:H81	1.78	0.66
1:H:331:ASN:CB	4:H:8576:HOH:O	2.22	0.66
4:H:8528:HOH:O	1:G:121:LEU:CD1	2.12	0.66
1:C:393:VAL:H	1:C:417:MET:CE	2.07	0.66
1:A:497:MET:HE1	4:A:8380:HOH:O	1.95	0.66
1:B:194:GLU:CG	4:B:8505:HOH:O	2.43	0.66
1:E:297:SER:CB	4:E:8536:HOH:O	2.43	0.66
1:A:497:MET:HE2	4:A:8380:HOH:O	1.93	0.65
1:C:545:LEU:CD1	4:C:8502:HOH:O	2.27	0.65
1:B:194:GLU:CD	4:B:8505:HOH:O	2.34	0.65
1:C:481:GLU:HG2	4:C:8336:HOH:O	1.96	0.65
1:G:80:ILE:HD13	4:G:8586:HOH:O	1.95	0.65
1:C:460:GLN:O	4:C:8263:HOH:O	2.14	0.65
1:H:131:TRP:CZ3	4:H:8544:HOH:O	2.49	0.65
1:A:285:ARG:HA	1:A:328:LEU:CD1	2.27	0.65
1:C:389:LEU:HD22	1:C:389:LEU:H	1.61	0.65
1:A:100:ILE:HD12	4:A:8505:HOH:O	1.96	0.65
1:A:132:GLN:HB3	4:A:8633:HOH:O	1.97	0.65
1:F:481:GLU:HG2	4:F:8289:HOH:O	1.97	0.65
1:E:539:GLN:HG3	4:E:8502:HOH:O	1.94	0.65
1:F:306:GLY:O	4:F:8466:HOH:O	2.14	0.65
1:F:50:VAL:HG13	1:F:313:ALA:HB2	1.79	0.65
1:H:126:LEU:CD1	1:H:132[B]:GLN:CG	2.75	0.65
1:G:312:LYS:HE3	4:G:8468:HOH:O	1.96	0.65
1:E:538:PRO:HG2	1:G:538:PRO:HG2	1.78	0.65
1:H:178:GLU:OE1	4:H:8329:HOH:O	2.14	0.64
1:G:83:GLY:N	4:G:8288:HOH:O	2.16	0.64
1:D:97:GLN:HG3	1:D:250:PHE:CE2	2.32	0.64
3:A:8002:MES:C7	4:A:8414:HOH:O	2.41	0.64
1:F:393:VAL:H	1:F:417:MET:HE1	1.62	0.64
1:G:81:ASP:CB	4:G:8299:HOH:O	2.45	0.64
1:A:545:LEU:CD1	4:A:8649:HOH:O	2.24	0.64
1:E:133:ALA:CB	4:E:8271:HOH:O	2.45	0.64
1:G:104[B]:VAL:HG13	4:G:8521:HOH:O	1.98	0.64
1:G:385:THR:HG22	1:G:388:GLU:OE2	1.96	0.64
1:D:100:ILE:HD13	1:D:453:ALA:HA	1.80	0.64
1:A:43:MET:HG2	4:A:8636:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:133:ALA:HB2	3:H:8004:MES:O3S	1.98	0.64
1:E:126:LEU:HD13	1:E:132[B]:GLN:HG3	1.76	0.64
1:H:126:LEU:HD12	1:H:132[B]:GLN:HG3	1.80	0.64
1:G:540:PHE:CE1	4:G:8588:HOH:O	2.50	0.64
1:C:545:LEU:HD22	4:C:8502:HOH:O	1.98	0.64
4:E:8371:HOH:O	1:H:542:GLU:HG3	1.98	0.64
1:B:194:GLU:HG2	4:B:8505:HOH:O	1.98	0.63
1:G:126:LEU:HD12	1:G:132[B]:GLN:HG3	1.80	0.63
1:H:101:ASP:O	4:H:8555:HOH:O	2.15	0.63
1:F:121:LEU:CD2	1:G:121:LEU:HD21	2.28	0.63
1:F:607:GLU:HG3	4:F:8394:HOH:O	1.96	0.63
1:F:393:VAL:H	1:F:417:MET:HE2	1.63	0.63
1:A:411:LYS:NZ	4:A:8518:HOH:O	2.14	0.63
1:G:400:SER:HA	4:G:8493:HOH:O	1.99	0.63
1:B:339:ARG:HG3	4:B:8553:HOH:O	1.98	0.62
1:C:287:VAL:HG23	4:C:8497:HOH:O	1.93	0.62
1:A:112:MET:CE	4:B:8609:HOH:O	2.45	0.62
1:H:343:ALA:CB	4:H:8537:HOH:O	2.47	0.62
1:H:97:GLN:HG2	4:H:8488:HOH:O	1.98	0.62
1:B:157:VAL:HG21	1:B:324:HIS:HE1	1.64	0.62
1:C:382:ILE:HD13	4:C:8388:HOH:O	2.00	0.62
1:A:405:PRO:CA	4:A:8625:HOH:O	2.45	0.62
1:F:121:LEU:HD21	1:G:121:LEU:CD2	2.29	0.62
1:H:104[B]:VAL:HG21	1:H:455:SER:OG	2.00	0.62
1:G:388:GLU:CG	4:G:8559:HOH:O	2.47	0.62
1:D:385:THR:OG1	1:D:388:GLU:OE1	2.09	0.62
1:A:545:LEU:CD2	4:A:8649:HOH:O	2.44	0.62
1:H:133:ALA:HB3	3:H:8004:MES:H81	1.80	0.62
1:E:393:VAL:H	1:E:417:MET:CE	2.09	0.62
1:H:271:PRO:CD	4:H:8596:HOH:O	2.47	0.62
1:B:178:GLU:CB	4:B:8626:HOH:O	2.37	0.62
1:G:328:LEU:CG	4:G:8550:HOH:O	2.17	0.61
1:H:250:PHE:HD2	4:H:8480:HOH:O	1.77	0.61
1:B:99:ASN:HB3	4:B:8326:HOH:O	2.00	0.61
1:C:545:LEU:HB2	4:C:8502:HOH:O	2.00	0.61
1:F:121:LEU:CD2	1:G:121:LEU:CD2	2.78	0.61
1:H:343:ALA:HB3	4:H:8537:HOH:O	2.01	0.61
1:A:478:GLU:HB2	4:A:8519:HOH:O	2.00	0.61
1:G:560:LYS:HE2	4:G:8549:HOH:O	1.99	0.61
1:D:126:LEU:CD1	1:D:132[B]:GLN:HG2	2.30	0.61
1:E:132[A]:GLN:CG	4:E:8344:HOH:O	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:132[B]:GLN:C	4:H:8544:HOH:O	2.38	0.61
1:H:339:ARG:HG2	4:H:8511:HOH:O	2.00	0.61
1:G:112:MET:HE1	4:G:8302:HOH:O	2.01	0.61
1:B:312:LYS:CE	4:B:8573:HOH:O	2.48	0.60
1:C:389:LEU:CD2	4:C:8365:HOH:O	2.49	0.60
1:E:312:LYS:HB2	4:E:8565:HOH:O	2.00	0.60
1:E:456:TYR:CD1	4:E:8500:HOH:O	2.51	0.60
1:H:228:GLU:HB2	4:H:8560:HOH:O	2.00	0.60
1:A:411:LYS:HE3	4:A:8590:HOH:O	2.01	0.60
1:D:50:VAL:HG13	1:D:313:ALA:HB2	1.84	0.60
1:G:328:LEU:CD1	4:G:8550:HOH:O	2.45	0.60
1:C:345:PRO:CB	4:C:8443:HOH:O	2.49	0.60
1:C:460:GLN:C	4:C:8263:HOH:O	2.40	0.60
1:G:81:ASP:OD1	1:G:81:ASP:C	2.37	0.60
1:A:545:LEU:CB	4:A:8649:HOH:O	2.41	0.60
1:E:133:ALA:CB	3:E:8007:MES:H81	2.31	0.60
4:A:8679:HOH:O	1:D:505:ARG:NH2	2.34	0.60
1:F:112:MET:CB	4:F:8442:HOH:O	2.40	0.60
1:D:393:VAL:H	1:D:417:MET:HE2	1.66	0.60
1:C:211:ASP:HB3	4:C:8440:HOH:O	2.02	0.60
1:G:133:ALA:HB3	3:G:8006:MES:H72	1.81	0.60
1:A:396:THR:O	4:A:8640:HOH:O	2.17	0.60
1:F:417:MET:CE	4:F:8415:HOH:O	2.42	0.60
1:H:219:HIS:HA	4:H:8587:HOH:O	2.00	0.59
1:G:194:GLU:HG2	4:G:8360:HOH:O	2.02	0.59
1:E:384:GLY:HA3	4:E:8490:HOH:O	2.02	0.59
1:B:339:ARG:CG	4:B:8553:HOH:O	2.50	0.59
1:E:363:PHE:HB3	4:E:8502:HOH:O	2.01	0.59
1:A:326:THR:O	4:A:8656:HOH:O	2.17	0.59
1:D:133:ALA:HB2	3:D:8005:MES:C7	2.32	0.59
1:E:619:THR:HG22	4:E:8169:HOH:O	2.01	0.59
1:H:97:GLN:CG	4:H:8480:HOH:O	2.49	0.59
1:G:358:GLU:OE2	4:G:8530:HOH:O	2.16	0.59
1:C:132[A]:GLN:CD	4:C:8462:HOH:O	2.40	0.59
1:C:490:LYS:HB2	4:C:8450:HOH:O	2.02	0.59
1:H:271:PRO:HD3	4:H:8596:HOH:O	2.02	0.59
1:G:540:PHE:HE1	4:G:8588:HOH:O	1.83	0.59
1:A:285:ARG:HA	1:A:328:LEU:HD11	1.84	0.59
4:H:8279:HOH:O	1:G:82:SER:N	2.36	0.58
1:A:481:GLU:HG2	4:A:8352:HOH:O	2.03	0.58
1:B:126:LEU:HD13	1:B:132[B]:GLN:CG	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:THR:CG2	4:A:8655:HOH:O	2.42	0.58
1:A:452:ASP:HB3	4:A:8367:HOH:O	2.01	0.58
3:C:8008:MES:C7	4:C:8251:HOH:O	2.42	0.58
1:H:429:GLU:HG2	4:H:8571:HOH:O	2.03	0.58
1:A:44:ASP:O	4:A:8572:HOH:O	2.17	0.58
1:F:97:GLN:HG3	1:F:250:PHE:CE2	2.39	0.58
1:F:538:PRO:HG2	1:H:538:PRO:CG	2.34	0.58
1:E:97:GLN:HG3	1:E:250:PHE:CE2	2.38	0.58
1:E:497:MET:HE1	4:E:8276:HOH:O	1.82	0.58
1:H:497:MET:CE	4:H:8307:HOH:O	2.52	0.58
1:D:481:GLU:HG2	4:D:8251:HOH:O	2.04	0.58
1:D:497:MET:HE2	4:D:8282:HOH:O	2.01	0.58
1:H:404:HIS:CE1	4:H:8295:HOH:O	2.57	0.58
1:C:133:ALA:HB3	3:C:8008:MES:H71	1.86	0.57
1:H:101:ASP:HA	4:H:8555:HOH:O	2.03	0.57
1:F:47:TYR:O	1:F:313:ALA:HA	2.04	0.57
1:H:252:GLU:CD	4:H:8565:HOH:O	2.42	0.57
1:H:432:GLU:OE2	4:H:8512:HOH:O	2.17	0.57
1:B:385:THR:HG23	1:B:388:GLU:OE2	2.05	0.57
1:D:541:MET:HE2	1:D:545:LEU:HD23	1.86	0.57
1:C:389:LEU:HD22	4:C:8365:HOH:O	2.04	0.57
1:H:228:GLU:HG3	4:H:8297:HOH:O	2.03	0.57
1:A:341:ASN:HD22	1:A:342:PRO:HD2	1.69	0.57
1:D:496:ASN:CB	4:D:8575:HOH:O	2.53	0.57
1:E:421:GLU:CB	4:E:8513:HOH:O	2.52	0.57
1:E:452:ASP:HB3	4:E:8303:HOH:O	2.05	0.57
1:G:413:LYS:CD	4:G:8496:HOH:O	2.48	0.57
1:B:133:ALA:N	4:B:8607:HOH:O	2.31	0.57
1:D:510:ARG:NH2	4:D:8535:HOH:O	2.37	0.57
1:H:80:ILE:HG21	1:G:84:LEU:HD21	1.87	0.57
1:A:99:ASN:HB3	4:A:8357:HOH:O	2.05	0.57
1:B:100:ILE:HD11	4:B:8252:HOH:O	2.04	0.57
1:B:347:GLU:HG3	4:B:8551:HOH:O	2.05	0.57
1:A:421:GLU:HG3	4:B:8486:HOH:O	2.05	0.57
1:A:429:GLU:HG2	4:A:8644:HOH:O	2.04	0.57
1:H:298:LEU:CB	4:H:8578:HOH:O	2.35	0.57
1:G:112:MET:CE	4:G:8302:HOH:O	2.51	0.57
1:B:310:GLU:CB	4:B:8535:HOH:O	2.52	0.56
1:B:380:MET:HA	4:B:8496:HOH:O	2.06	0.56
1:D:478:GLU:CB	4:D:8535:HOH:O	2.49	0.56
1:E:133:ALA:CA	4:E:8271:HOH:O	2.50	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:497:MET:HE2	4:F:8284:HOH:O	2.03	0.56
3:H:8004:MES:C7	4:H:8306:HOH:O	2.53	0.56
1:G:155:GLN:NE2	4:G:8530:HOH:O	2.12	0.56
1:B:557:PHE:HA	4:B:8477:HOH:O	2.04	0.56
1:C:343:ALA:HB3	4:C:8445:HOH:O	2.06	0.56
1:F:619:THR:HG23	1:F:619:THR:O	2.06	0.56
1:B:81:ASP:HB3	4:B:8572:HOH:O	2.06	0.56
1:E:228:GLU:HG3	4:E:8554:HOH:O	2.06	0.56
1:H:389:LEU:HB3	4:H:8517:HOH:O	2.06	0.56
1:A:394:THR:CG2	4:A:8486:HOH:O	2.52	0.56
1:B:242:ALA:N	4:B:8594:HOH:O	2.38	0.56
1:H:132[A]:GLN:C	4:H:8544:HOH:O	2.43	0.56
1:H:435:VAL:CG2	4:H:8587:HOH:O	2.31	0.56
1:C:611:GLN:CG	4:C:8423:HOH:O	2.39	0.56
3:F:8001:MES:C8	4:F:8407:HOH:O	2.54	0.56
1:A:100:ILE:HG21	4:A:8505:HOH:O	2.06	0.56
1:H:230:TYR:CA	4:H:8510:HOH:O	2.52	0.56
4:E:8250:HOH:O	1:F:81:ASP:HA	2.06	0.55
1:H:299:HIS:CD2	4:H:8526:HOH:O	2.59	0.55
1:D:496:ASN:HB2	4:D:8575:HOH:O	2.06	0.55
1:H:219:HIS:ND1	4:H:8587:HOH:O	2.33	0.55
1:H:619:THR:O	1:H:619:THR:HG23	2.05	0.55
4:H:8279:HOH:O	1:G:81:ASP:C	2.44	0.55
1:G:312:LYS:CD	4:G:8555:HOH:O	2.46	0.55
1:B:385:THR:OG1	1:B:388:GLU:OE2	2.19	0.55
4:E:8503:HOH:O	1:F:121:LEU:HB3	2.06	0.55
1:G:126:LEU:HD13	1:G:132[B]:GLN:HG3	1.83	0.55
1:F:459:VAL:HG22	4:F:8302:HOH:O	2.05	0.55
1:G:459:VAL:HG12	4:G:8563:HOH:O	2.06	0.55
1:G:482:GLU:HG3	4:G:8580:HOH:O	2.05	0.55
1:E:126:LEU:HD13	1:E:132[B]:GLN:HG2	1.89	0.55
1:B:619:THR:HA	4:B:8373:HOH:O	2.05	0.55
1:B:126:LEU:HD13	1:B:132[B]:GLN:HG2	1.89	0.55
1:B:328:LEU:HB2	4:B:8639:HOH:O	2.06	0.55
3:F:8001:MES:C7	4:F:8407:HOH:O	2.55	0.55
1:H:389:LEU:CB	4:H:8514:HOH:O	2.54	0.55
1:A:541:MET:HE3	1:A:545:LEU:HD23	1.89	0.54
1:E:132[B]:GLN:NE2	3:E:8007:MES:O3S	2.35	0.54
1:E:194:GLU:OE2	4:E:8441:HOH:O	2.18	0.54
4:A:8705:HOH:O	1:B:421:GLU:HG3	2.06	0.54
1:E:610:LYS:HE3	4:E:8482:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:497:MET:CE	4:F:8284:HOH:O	2.54	0.54
1:G:83:GLY:CA	4:G:8288:HOH:O	2.54	0.54
1:B:132[A]:GLN:HG2	4:B:8347:HOH:O	2.07	0.54
1:F:99:ASN:HB3	4:F:8219:HOH:O	2.06	0.54
1:H:80:ILE:HG21	1:G:84:LEU:CD2	2.37	0.54
1:H:340:PRO:HD2	4:H:8511:HOH:O	2.06	0.54
1:G:47:TYR:O	1:G:313:ALA:HA	2.07	0.54
1:D:393:VAL:H	1:D:417:MET:HE1	1.70	0.54
1:C:185:LYS:HD3	4:C:8530:HOH:O	2.07	0.54
1:C:497:MET:HE2	4:C:8350:HOH:O	2.02	0.54
1:H:194:GLU:CG	4:H:8356:HOH:O	2.53	0.54
1:G:390:THR:OG1	4:G:8559:HOH:O	1.87	0.54
1:D:461:GLN:HA	4:D:8453:HOH:O	2.08	0.54
1:A:81:ASP:HB3	4:A:8483:HOH:O	2.07	0.54
1:A:542:GLU:CB	4:D:8339:HOH:O	2.55	0.54
1:A:136:PHE:HA	4:A:8414:HOH:O	2.08	0.54
1:D:299:HIS:CB	1:D:310:GLU:OE1	2.55	0.54
1:C:131:TRP:O	1:C:132[B]:GLN:HG2	2.08	0.54
1:G:126:LEU:HD13	1:G:132[B]:GLN:HG2	1.90	0.54
1:A:100:ILE:CG2	4:A:8505:HOH:O	2.57	0.53
1:A:406:ASP:N	4:A:8625:HOH:O	2.34	0.53
1:D:541:MET:HE1	4:D:8191:HOH:O	2.02	0.53
3:A:8002:MES:C8	4:A:8414:HOH:O	2.56	0.53
1:E:460:GLN:C	4:E:8533:HOH:O	2.47	0.53
1:H:411:LYS:HE3	4:H:8436:HOH:O	2.06	0.53
1:G:45:ILE:N	4:G:8305:HOH:O	2.41	0.53
1:E:421:GLU:HB3	4:E:8513:HOH:O	2.09	0.53
1:A:201:LYS:HE2	1:A:205:TYR:OH	2.08	0.53
1:G:50:VAL:HG13	1:G:313:ALA:HB2	1.91	0.53
1:A:95:GLU:HG3	1:B:112:MET:HE3	1.90	0.53
1:E:112:MET:CE	4:E:8332:HOH:O	2.55	0.53
3:E:8007:MES:H51	4:F:8327:HOH:O	2.08	0.53
1:H:230:TYR:HA	4:H:8510:HOH:O	2.08	0.53
1:B:81:ASP:OD1	1:B:81:ASP:C	2.45	0.53
1:C:611:GLN:HA	4:C:8423:HOH:O	2.09	0.53
3:G:8006:MES:C7	4:G:8371:HOH:O	2.49	0.53
1:A:336:GLN:HG3	4:A:8568:HOH:O	2.08	0.53
1:H:458:ALA:HB1	4:H:8528:HOH:O	2.07	0.53
1:H:490:LYS:HD3	1:H:491:ILE:HD13	1.91	0.53
1:A:133:ALA:CA	4:A:8381:HOH:O	2.47	0.53
1:C:343:ALA:CB	4:C:8445:HOH:O	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:ASP:O	1:D:104[B]:VAL:HG22	2.08	0.52
3:H:8004:MES:C8	4:H:8306:HOH:O	2.55	0.52
1:E:194:GLU:CD	4:E:8441:HOH:O	2.47	0.52
1:D:112:MET:CE	4:D:8311:HOH:O	2.57	0.52
1:H:133:ALA:N	4:H:8544:HOH:O	2.35	0.52
1:A:336:GLN:HA	4:A:8568:HOH:O	2.10	0.52
1:D:497:MET:HE1	4:D:8282:HOH:O	2.05	0.52
1:F:385:THR:OG1	1:F:388:GLU:OE1	2.21	0.52
1:D:365:GLN:HB3	4:D:8526:HOH:O	2.09	0.52
1:C:344:ASN:ND2	4:C:8445:HOH:O	2.42	0.52
3:H:8004:MES:H71	4:H:8306:HOH:O	2.10	0.52
1:B:389:LEU:N	1:B:389:LEU:HD22	2.24	0.52
1:H:218:ARG:HD2	4:H:8090:HOH:O	2.10	0.52
1:B:100:ILE:HG13	4:B:8336:HOH:O	2.09	0.52
1:E:139:ARG:HD3	3:E:8007:MES:H82	1.92	0.52
1:B:394:THR:OG1	4:B:8653:HOH:O	2.19	0.52
1:B:157:VAL:HG21	1:B:324:HIS:CE1	2.45	0.51
1:E:158:THR:HG22	1:E:160:VAL:HG22	1.93	0.51
1:H:404:HIS:HE1	4:H:8295:HOH:O	1.91	0.51
1:B:328:LEU:HD22	4:B:8639:HOH:O	2.09	0.51
1:C:497:MET:HE1	4:C:8350:HOH:O	2.07	0.51
1:E:101:ASP:O	1:E:104[B]:VAL:HG22	2.09	0.51
1:D:47:TYR:O	1:D:313:ALA:HA	2.09	0.51
1:C:336:GLN:NE2	1:C:344:ASN:O	2.43	0.51
1:E:173:PRO:HG2	1:E:592:ALA:HB1	1.91	0.51
1:H:158:THR:HG22	1:H:160:VAL:HG22	1.91	0.51
1:B:393:VAL:N	1:B:417:MET:HE2	2.18	0.51
1:E:284:GLU:C	1:E:328:LEU:CD1	2.79	0.51
3:F:8001:MES:H72	4:F:8407:HOH:O	2.10	0.51
1:H:133:ALA:HB2	3:H:8004:MES:C8	2.40	0.51
1:G:515:ALA:HB1	4:G:8588:HOH:O	2.10	0.51
1:E:385:THR:O	4:E:8379:HOH:O	2.18	0.51
1:E:50:VAL:HG13	1:E:313:ALA:HB2	1.92	0.51
3:A:8002:MES:H71	4:A:8633:HOH:O	2.11	0.51
1:D:158:THR:HG22	1:D:160:VAL:HG22	1.93	0.51
1:D:576:LYS:CD	4:D:8297:HOH:O	2.58	0.51
1:C:133:ALA:CB	3:C:8008:MES:C7	2.87	0.51
1:C:285:ARG:HD2	4:C:8522:HOH:O	2.10	0.51
1:C:47:TYR:O	1:C:313:ALA:HA	2.10	0.51
1:C:50:VAL:HG13	1:C:313:ALA:HB2	1.93	0.51
1:H:231:LYS:N	4:H:8510:HOH:O	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:389:LEU:HA	4:G:8491:HOH:O	2.11	0.51
1:A:457:GLY:HA3	4:A:8341:HOH:O	2.11	0.51
1:H:607:GLU:HG3	4:H:8367:HOH:O	2.10	0.51
1:G:576:LYS:HG3	4:G:8579:HOH:O	2.11	0.51
1:B:478:GLU:CG	4:B:8615:HOH:O	2.59	0.50
1:A:95:GLU:OE2	4:A:8460:HOH:O	2.18	0.50
1:B:513:LYS:NZ	4:B:8575:HOH:O	2.43	0.50
1:F:541:MET:CE	1:F:545:LEU:HD23	2.41	0.50
1:B:576:LYS:HG3	4:B:8622:HOH:O	2.10	0.50
1:G:619:THR:HG23	1:G:619:THR:O	2.11	0.50
4:A:8705:HOH:O	1:B:421:GLU:CG	2.59	0.50
1:E:385:THR:O	1:E:388:GLU:HG3	2.11	0.50
1:G:336:GLN:HB2	1:G:346:PRO:HG3	1.92	0.50
1:A:619:THR:HG22	4:A:8645:HOH:O	2.10	0.50
1:B:178:GLU:CG	4:B:8626:HOH:O	2.59	0.50
1:D:268:THR:HG22	4:D:8553:HOH:O	2.12	0.50
1:E:478:GLU:HG2	4:E:8399:HOH:O	2.12	0.50
1:H:541:MET:HE2	4:H:8603:HOH:O	2.10	0.50
1:G:97:GLN:HG3	1:G:250:PHE:CE2	2.47	0.50
1:G:100:ILE:CG1	4:G:8331:HOH:O	2.55	0.50
1:G:133:ALA:CB	3:G:8006:MES:H71	2.40	0.50
1:G:218:ARG:HD2	4:G:8031:HOH:O	2.12	0.50
1:G:101:ASP:C	4:G:8521:HOH:O	2.42	0.50
1:B:342:PRO:HB3	4:B:8576:HOH:O	2.12	0.49
1:C:383:ARG:HB3	1:C:392:SER:HB3	1.93	0.49
1:C:513:LYS:HD3	4:C:8335:HOH:O	2.12	0.49
1:H:45:ILE:C	1:H:45:ILE:HD12	2.32	0.49
1:G:84:LEU:CD2	1:G:84:LEU:N	2.74	0.49
1:C:97:GLN:HG3	1:C:250:PHE:CE2	2.46	0.49
1:E:47:TYR:O	1:E:313:ALA:HA	2.11	0.49
1:E:132[B]:GLN:OE1	3:E:8007:MES:H31	2.12	0.49
1:E:564:CYS:HG	1:E:573:PHE:HE2	1.60	0.49
1:H:50:VAL:HG13	1:H:313:ALA:HB2	1.94	0.49
1:H:339:ARG:CG	4:H:8511:HOH:O	2.59	0.49
1:H:482:GLU:HG3	4:H:8472:HOH:O	2.11	0.49
1:B:505:ARG:HD2	4:C:8462:HOH:O	2.12	0.49
1:C:218:ARG:HD2	4:C:8029:HOH:O	2.11	0.49
1:G:385:THR:CG2	1:G:388:GLU:OE2	2.59	0.49
1:G:576:LYS:HG2	4:G:8295:HOH:O	2.12	0.49
1:F:371:GLU:HB3	4:F:8435:HOH:O	2.12	0.49
1:E:124:ASP:OD1	4:E:8371:HOH:O	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:619:THR:CG2	4:E:8531:HOH:O	2.54	0.49
1:G:81:ASP:HA	4:G:8299:HOH:O	2.02	0.49
1:G:184:VAL:CG1	4:G:8589:HOH:O	2.53	0.49
1:B:380:MET:CA	4:B:8496:HOH:O	2.61	0.49
1:E:619:THR:HG23	4:E:8372:HOH:O	2.11	0.49
1:H:413:LYS:HE3	1:H:414:ASN:OD1	2.13	0.49
1:G:45:ILE:HD12	4:G:8305:HOH:O	2.12	0.49
1:A:158:THR:HG22	1:A:160:VAL:HG22	1.94	0.49
1:B:112:MET:CE	4:B:8328:HOH:O	2.60	0.49
1:B:478:GLU:HG2	4:B:8615:HOH:O	2.12	0.49
1:F:136:PHE:HA	4:F:8407:HOH:O	2.12	0.49
1:B:242:ALA:HB1	1:B:254:SER:HB2	1.95	0.49
1:G:43:MET:CE	4:G:8501:HOH:O	2.60	0.49
1:G:155:GLN:CG	4:G:8530:HOH:O	2.29	0.49
1:B:546:VAL:HG11	4:B:8629:HOH:O	2.13	0.48
1:D:345:PRO:CA	4:D:8484:HOH:O	2.61	0.48
3:D:8005:MES:C8	4:D:8310:HOH:O	2.59	0.48
1:C:299:HIS:HB2	4:C:8497:HOH:O	2.13	0.48
1:C:619:THR:O	1:C:619:THR:HG23	2.13	0.48
1:E:218:ARG:HD2	4:E:8073:HOH:O	2.13	0.48
3:E:8007:MES:H71	1:F:462:SER:O	2.12	0.48
3:F:8001:MES:H32	3:F:8001:MES:O3S	2.13	0.48
1:G:481:GLU:HG2	4:G:8293:HOH:O	2.13	0.48
4:E:8371:HOH:O	1:H:542:GLU:CG	2.61	0.48
1:F:157:VAL:HG21	1:F:324:HIS:HE1	1.77	0.48
1:H:112:MET:CE	4:H:8331:HOH:O	2.61	0.48
1:D:490:LYS:HD3	1:D:491:ILE:HD13	1.95	0.48
1:C:126:LEU:HD13	1:C:132[B]:GLN:CG	2.42	0.48
1:C:389:LEU:CD1	4:C:8365:HOH:O	2.61	0.48
1:C:545:LEU:CD2	4:C:8502:HOH:O	2.56	0.48
1:G:91:LYS:NZ	4:G:8508:HOH:O	2.29	0.48
1:B:389:LEU:HD22	1:B:389:LEU:H	1.76	0.48
1:F:225:LYS:NZ	4:F:8427:HOH:O	2.30	0.48
1:B:218:ARG:HG3	1:B:430:ASP:OD2	2.14	0.48
1:B:336:GLN:NE2	1:B:344:ASN:O	2.46	0.48
1:D:576:LYS:HD3	4:D:8297:HOH:O	2.13	0.48
1:G:400:SER:CA	4:G:8493:HOH:O	2.57	0.48
1:B:158:THR:HG22	1:B:160:VAL:HG22	1.94	0.48
1:A:312:LYS:CD	4:A:8546:HOH:O	2.61	0.48
1:B:231:LYS:HE2	4:B:8482:HOH:O	2.14	0.48
1:D:134:SER:HB2	4:D:8459:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ILE:C	1:A:45:ILE:HD12	2.34	0.48
1:F:121:LEU:HD23	1:G:121:LEU:HD21	1.95	0.48
1:H:346:PRO:HG2	1:H:350:PRO:HA	1.96	0.48
1:H:452:ASP:CB	4:H:8499:HOH:O	2.35	0.48
1:G:184:VAL:C	4:G:8589:HOH:O	2.52	0.48
1:A:299:HIS:CE1	4:A:8599:HOH:O	2.62	0.47
1:F:371:GLU:CG	4:F:8336:HOH:O	2.62	0.47
1:G:158:THR:CG2	1:G:160:VAL:HG22	2.44	0.47
1:G:398:GLY:O	1:G:399:ALA:C	2.52	0.47
1:A:341:ASN:HB3	4:A:8641:HOH:O	2.13	0.47
1:B:382:ILE:HD13	4:B:8420:HOH:O	2.14	0.47
1:B:564:CYS:HG	1:B:573:PHE:HE2	1.63	0.47
1:H:99:ASN:HB3	4:H:8312:HOH:O	2.13	0.47
1:A:541:MET:CE	1:A:545:LEU:HD23	2.44	0.47
1:D:460:GLN:C	4:D:8453:HOH:O	2.52	0.47
1:C:490:LYS:HG3	4:C:8450:HOH:O	2.14	0.47
1:E:284:GLU:O	1:E:328:LEU:HD12	2.14	0.47
1:G:133:ALA:CB	3:G:8006:MES:O3S	2.60	0.47
1:D:564:CYS:HG	1:D:573:PHE:HE2	1.62	0.47
1:H:497:MET:HE1	4:H:8307:HOH:O	2.13	0.47
1:C:185:LYS:CE	4:C:8507:HOH:O	2.63	0.47
1:G:81:ASP:C	4:G:8299:HOH:O	2.52	0.47
1:G:100:ILE:HD11	4:G:8311:HOH:O	2.14	0.47
1:G:389:LEU:HG	4:G:8599:HOH:O	2.14	0.47
1:D:336:GLN:NE2	1:D:344:ASN:O	2.48	0.47
1:C:101:ASP:O	4:C:8397:HOH:O	2.20	0.47
1:C:159:ARG:HA	2:C:7004:FAD:O2B	2.15	0.47
1:E:158:THR:CG2	1:E:160:VAL:HG22	2.44	0.47
1:E:346:PRO:HG2	1:E:350:PRO:HA	1.97	0.47
4:E:8371:HOH:O	1:H:542:GLU:CB	2.62	0.47
1:D:284:GLU:C	1:D:328:LEU:CD1	2.83	0.47
1:C:157:VAL:HG21	1:C:324:HIS:HE1	1.79	0.47
1:H:100:ILE:HD13	1:H:100:ILE:O	2.14	0.47
1:H:497:MET:HE2	4:H:8307:HOH:O	2.13	0.47
1:G:336:GLN:NE2	4:G:8482:HOH:O	2.47	0.47
1:G:388:GLU:HG3	4:G:8559:HOH:O	2.13	0.47
1:G:541:MET:CE	4:G:8540:HOH:O	2.63	0.47
4:D:8439:HOH:O	3:C:8008:MES:H52	2.15	0.47
1:H:184:VAL:HG11	1:H:190:ALA:HB3	1.97	0.47
1:F:459:VAL:HA	4:F:8302:HOH:O	2.13	0.47
1:G:83:GLY:HA2	4:G:8288:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:345:PRO:HA	4:D:8484:HOH:O	2.14	0.47
4:F:8449:HOH:O	1:G:542:GLU:CB	2.63	0.47
1:A:84:LEU:HD23	4:B:8332:HOH:O	2.14	0.46
1:H:417[B]:MET:CE	4:H:8345:HOH:O	2.62	0.46
1:A:541:MET:HE3	1:A:545:LEU:CD2	2.45	0.46
1:D:132[B]:GLN:OE1	3:D:8005:MES:H71	2.15	0.46
1:G:218:ARG:HG3	1:G:430:ASP:OD2	2.15	0.46
1:B:91:LYS:CE	4:B:8327:HOH:O	2.63	0.46
1:C:342:PRO:C	4:C:8466:HOH:O	2.53	0.46
1:H:541:MET:CE	1:H:545:LEU:HD23	2.46	0.46
4:H:8615:HOH:O	1:G:84:LEU:CG	2.42	0.46
1:G:471:TRP:CH2	1:G:526:SER:HA	2.51	0.46
1:A:47:TYR:O	1:A:313:ALA:HA	2.16	0.46
1:A:312:LYS:HD3	4:A:8546:HOH:O	2.15	0.46
1:B:158:THR:CG2	1:B:160:VAL:HG22	2.46	0.46
1:D:110:GLN:NE2	4:D:8488:HOH:O	2.22	0.46
1:G:97:GLN:HG3	1:G:250:PHE:CD2	2.51	0.46
1:G:393:VAL:H	1:G:417:MET:HE1	1.76	0.46
1:B:346:PRO:HG2	1:B:350:PRO:HA	1.98	0.46
1:F:83:GLY:HA2	4:F:8157:HOH:O	2.15	0.46
1:G:388:GLU:CB	4:G:8598:HOH:O	2.63	0.46
1:F:83:GLY:N	4:F:8157:HOH:O	2.42	0.46
1:H:104[A]:VAL:CG2	4:H:8555:HOH:O	2.34	0.46
1:H:139:ARG:HD3	3:H:8004:MES:H82	1.97	0.46
1:B:47:TYR:O	1:B:313:ALA:HA	2.15	0.46
1:B:132[B]:GLN:C	4:B:8607:HOH:O	2.52	0.46
1:F:293:SER:HA	1:F:574:GLY:O	2.15	0.46
3:H:8004:MES:H51	4:H:8306:HOH:O	2.16	0.46
1:G:544:GLY:CA	4:G:8530:HOH:O	2.64	0.46
1:A:100:ILE:HD13	1:A:100:ILE:C	2.35	0.46
1:B:385:THR:CG2	1:B:388:GLU:OE2	2.63	0.46
1:D:389:LEU:HB2	4:D:8465:HOH:O	2.16	0.46
1:C:272:GLU:HG2	4:C:8442:HOH:O	2.16	0.46
1:C:345:PRO:HB3	4:C:8443:HOH:O	2.12	0.46
1:G:285:ARG:NH2	1:G:287:VAL:HG22	2.31	0.46
1:G:619:THR:HA	4:G:8582:HOH:O	2.16	0.46
1:B:460:GLN:HB3	4:B:8558:HOH:O	2.15	0.46
1:H:91:LYS:CG	4:H:8488:HOH:O	2.64	0.46
1:G:46:LYS:N	4:G:8305:HOH:O	2.25	0.46
1:A:81:ASP:C	1:A:81:ASP:OD1	2.54	0.45
1:B:45:ILE:HD13	4:B:8488:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:LYS:HD3	4:B:8528:HOH:O	2.15	0.45
1:E:157:VAL:HG21	1:E:324:HIS:HE1	1.80	0.45
1:A:100:ILE:CD1	1:A:453:ALA:HB2	2.45	0.45
1:F:459:VAL:CG1	4:F:8302:HOH:O	2.37	0.45
3:H:8004:MES:H31	1:G:462:SER:OG	2.15	0.45
1:A:43:MET:HG3	4:A:8572:HOH:O	2.15	0.45
1:B:100:ILE:HA	4:B:8336:HOH:O	2.14	0.45
1:H:417[B]:MET:HE2	4:H:8345:HOH:O	2.16	0.45
1:C:123:VAL:HB	3:C:8008:MES:H62	1.99	0.45
1:C:418:GLN:HE21	1:C:418:GLN:HB3	1.51	0.45
1:C:564:CYS:HG	1:C:573:PHE:HE2	1.64	0.45
1:F:194:GLU:HG2	4:F:8264:HOH:O	2.17	0.45
1:G:123:VAL:HB	3:G:8006:MES:H22	1.98	0.45
1:D:576:LYS:HG3	4:D:8297:HOH:O	2.16	0.45
1:C:432:GLU:HB2	1:C:433:PRO:HD2	1.99	0.45
1:E:342:PRO:C	1:E:344:ASN:H	2.20	0.45
1:H:126:LEU:HD13	1:H:132[B]:GLN:HG2	1.98	0.45
1:H:389:LEU:HB2	4:H:8514:HOH:O	2.16	0.45
1:H:429:GLU:CG	4:H:8571:HOH:O	2.61	0.45
1:A:285:ARG:HA	1:A:328:LEU:HD12	1.98	0.45
1:B:218:ARG:HD2	4:B:8041:HOH:O	2.17	0.45
1:B:310:GLU:HB2	4:B:8535:HOH:O	2.16	0.45
1:H:194:GLU:CD	4:H:8356:HOH:O	2.55	0.45
1:A:285:ARG:CA	1:A:328:LEU:HD11	2.47	0.45
1:A:299:HIS:CD2	4:A:8599:HOH:O	2.66	0.45
1:E:99:ASN:CG	4:E:8537:HOH:O	2.55	0.45
1:D:133:ALA:HB2	3:D:8005:MES:H71	1.88	0.44
1:B:328:LEU:CG	4:B:8525:HOH:O	2.12	0.44
1:B:546:VAL:HB	4:B:8629:HOH:O	2.17	0.44
1:C:576:LYS:CD	4:C:8260:HOH:O	2.57	0.44
1:E:312:LYS:HD3	4:E:8565:HOH:O	2.16	0.44
1:H:231:LYS:CE	4:H:8297:HOH:O	2.66	0.44
1:G:158:THR:HG22	1:G:160:VAL:HG22	1.99	0.44
1:C:133:ALA:CB	3:C:8008:MES:H71	2.47	0.44
1:H:105:ASN:HB3	1:G:105:ASN:O	2.17	0.44
1:H:389:LEU:CA	4:H:8514:HOH:O	2.64	0.44
1:B:392:SER:HA	1:B:417:MET:HE1	1.99	0.44
1:C:185:LYS:CD	4:C:8530:HOH:O	2.64	0.44
1:G:413:LYS:CE	4:G:8496:HOH:O	2.65	0.44
1:A:50:VAL:HG13	1:A:313:ALA:HB2	2.00	0.44
1:B:242:ALA:HB2	4:B:8594:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:132[A]:GLN:HG2	4:E:8344:HOH:O	2.12	0.44
1:G:84:LEU:N	1:G:84:LEU:HD23	2.32	0.44
1:G:618:PHE:CD1	1:G:618:PHE:C	2.89	0.44
1:B:478:GLU:CD	1:B:480:LYS:HE2	2.38	0.44
3:D:8005:MES:H32	3:D:8005:MES:O2S	2.18	0.44
1:C:460:GLN:HB3	4:C:8263:HOH:O	2.18	0.44
1:G:299[A]:HIS:CG	4:G:8370:HOH:O	2.71	0.44
1:D:91:LYS:NZ	4:D:8250:HOH:O	2.49	0.44
1:D:157:VAL:HG21	1:D:324:HIS:HE1	1.83	0.44
1:D:159:ARG:HA	2:D:7003:FAD:O2B	2.18	0.44
1:H:123:VAL:HG22	1:G:459:VAL:CG1	2.48	0.44
1:G:99:ASN:CG	4:G:8551:HOH:O	2.56	0.44
1:C:478:GLU:OE2	1:C:480:LYS:HE2	2.18	0.44
1:G:157:VAL:HG21	1:G:324:HIS:HE1	1.82	0.44
1:G:385:THR:CB	1:G:388:GLU:OE2	2.66	0.44
1:G:385:THR:HB	1:G:388:GLU:OE2	2.18	0.44
1:F:541:MET:HE1	4:F:8480:HOH:O	2.16	0.44
1:H:268:THR:C	4:H:8596:HOH:O	2.57	0.44
1:G:564:CYS:HG	1:G:573:PHE:HE2	1.66	0.44
1:B:383:ARG:HG3	4:B:8514:HOH:O	2.18	0.43
1:B:393:VAL:H	1:B:417:MET:HE1	1.79	0.43
1:C:284:GLU:C	1:C:328:LEU:CD1	2.87	0.43
1:E:541:MET:HE3	1:E:545:LEU:HD23	2.00	0.43
1:H:211:ASP:CB	4:H:8421:HOH:O	2.44	0.43
1:H:541:MET:HE3	4:H:8149:HOH:O	2.18	0.43
1:G:159:ARG:HA	2:G:7008:FAD:O2B	2.18	0.43
1:A:400:SER:CB	4:A:8523:HOH:O	2.66	0.43
1:A:421:GLU:OE2	4:A:8681:HOH:O	2.21	0.43
1:D:123:VAL:HG22	1:C:459:VAL:HG12	1.98	0.43
1:C:100:ILE:HD13	1:C:100:ILE:O	2.17	0.43
1:F:158:THR:HG22	1:F:160:VAL:HG22	2.00	0.43
1:G:544:GLY:HA2	4:G:8530:HOH:O	2.18	0.43
1:D:215:GLU:O	1:D:411:LYS:NZ	2.51	0.43
1:E:45:ILE:HG13	4:E:8442:HOH:O	2.16	0.43
1:H:101:ASP:O	1:H:104[B]:VAL:HG22	2.19	0.43
1:B:112:MET:HE1	4:B:8328:HOH:O	2.18	0.43
1:B:385:THR:CB	1:B:388:GLU:OE2	2.66	0.43
1:D:81:ASP:C	1:D:81:ASP:OD1	2.54	0.43
1:C:471:TRP:CH2	1:C:526:SER:HA	2.54	0.43
1:E:44:ASP:HB3	4:E:8443:HOH:O	2.18	0.43
1:E:91:LYS:HE2	4:E:8307:HOH:O	2.13	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:452:ASP:OD1	1:E:452:ASP:N	2.52	0.43
1:F:159:ARG:HA	2:F:7006:FAD:O2B	2.19	0.43
1:H:309:PHE:HD2	4:H:8590:HOH:O	2.01	0.43
1:A:449:ILE:HG12	1:A:471:TRP:CE3	2.53	0.43
1:B:178:GLU:CD	4:B:8626:HOH:O	2.56	0.43
1:D:158:THR:CG2	1:D:160:VAL:HG22	2.48	0.43
1:C:100:ILE:HD13	1:C:453:ALA:HB2	2.00	0.43
3:E:8007:MES:C8	4:E:8255:HOH:O	2.66	0.43
1:H:293:SER:HA	1:H:574:GLY:O	2.18	0.43
1:H:343:ALA:HB1	4:H:8537:HOH:O	2.15	0.43
1:D:299:HIS:CA	1:D:310:GLU:OE1	2.67	0.43
1:D:342:PRO:HD2	4:D:8533:HOH:O	2.18	0.43
1:E:459:VAL:HA	4:E:8503:HOH:O	2.18	0.43
1:H:105:ASN:O	1:G:105:ASN:HB3	2.19	0.43
1:G:505:ARG:NH1	4:G:8363:HOH:O	2.51	0.43
1:B:538:PRO:HG2	1:D:538:PRO:HG2	2.00	0.43
1:C:242:ALA:HB1	1:C:254:SER:HB2	2.01	0.43
1:H:231:LYS:HD3	4:H:8416:HOH:O	2.19	0.43
1:H:331:ASN:C	4:H:8576:HOH:O	2.56	0.43
1:A:56:PRO:HD3	1:A:165:SER:HB3	2.01	0.43
1:B:97:GLN:HB2	4:B:8633:HOH:O	2.19	0.43
1:E:194:GLU:CG	4:E:8441:HOH:O	2.58	0.43
1:F:541:MET:HE3	1:F:545:LEU:HD23	2.00	0.43
1:A:312:LYS:CE	4:A:8623:HOH:O	2.52	0.43
1:A:542:GLU:CG	4:D:8339:HOH:O	2.43	0.43
1:E:56:PRO:HD3	1:E:165:SER:HB3	2.01	0.43
1:E:133:ALA:HB1	4:E:8271:HOH:O	2.17	0.43
1:H:228:GLU:CD	4:H:8465:HOH:O	2.57	0.43
1:B:45:ILE:CD1	4:B:8488:HOH:O	2.67	0.42
1:B:100:ILE:CD1	4:B:8252:HOH:O	2.64	0.42
1:B:328:LEU:CB	4:B:8639:HOH:O	2.66	0.42
1:A:399:ALA:N	4:A:8593:HOH:O	2.51	0.42
1:D:47:TYR:CD2	1:D:73:ALA:HB2	2.54	0.42
1:D:385:THR:HA	1:D:386:PRO:HD3	1.93	0.42
1:H:91:LYS:HG3	4:H:8488:HOH:O	2.19	0.42
1:C:112:MET:CE	4:C:8372:HOH:O	2.68	0.42
1:C:548:HIS:C	4:C:8370:HOH:O	2.57	0.42
1:H:47:TYR:O	1:H:313:ALA:HA	2.20	0.42
1:H:271:PRO:N	4:H:8596:HOH:O	2.51	0.42
1:H:285:ARG:HG2	4:H:8576:HOH:O	2.19	0.42
1:A:132:GLN:C	4:A:8633:HOH:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:THR:HA	1:B:386:PRO:HD3	1.91	0.42
1:D:496:ASN:CG	4:D:8575:HOH:O	2.57	0.42
3:E:8007:MES:H81	4:E:8255:HOH:O	2.19	0.42
1:F:459:VAL:CB	4:F:8302:HOH:O	2.65	0.42
1:G:312:LYS:CG	4:G:8555:HOH:O	2.58	0.42
1:E:293:SER:HA	1:E:574:GLY:O	2.19	0.42
1:B:204:SER:OG	4:B:8547:HOH:O	2.05	0.42
1:G:136:PHE:HA	4:G:8371:HOH:O	2.20	0.42
1:G:185:LYS:HD2	4:G:8567:HOH:O	2.19	0.42
1:A:104[A]:VAL:HG13	4:A:8551:HOH:O	2.20	0.42
1:B:619:THR:HB	4:B:8625:HOH:O	2.20	0.42
1:E:382:ILE:CG2	1:E:391:TYR:CE1	3.03	0.42
1:E:541:MET:CE	1:E:545:LEU:HD23	2.50	0.42
1:F:83:GLY:CA	4:F:8157:HOH:O	2.67	0.42
1:B:50:VAL:HG13	1:B:313:ALA:HB2	2.02	0.42
1:F:77:ILE:HD11	1:F:495:TYR:CD2	2.55	0.42
1:H:103:PHE:HB2	4:H:8387:HOH:O	2.20	0.42
1:B:341:ASN:HD22	1:B:342:PRO:HD2	1.85	0.42
1:E:341:ASN:C	1:E:341:ASN:HD22	2.24	0.42
1:D:383:ARG:HB3	1:D:392:SER:HB3	2.02	0.41
1:H:81:ASP:O	1:H:90:LYS:HE2	2.19	0.41
1:H:458:ALA:CB	4:H:8528:HOH:O	2.66	0.41
1:G:46:LYS:CE	4:G:8576:HOH:O	2.67	0.41
1:G:388:GLU:CD	4:G:8559:HOH:O	2.58	0.41
1:D:413:LYS:HE3	4:D:8443:HOH:O	2.20	0.41
1:E:285:ARG:HH21	1:E:287:VAL:HG22	1.86	0.41
1:F:91:LYS:HG2	4:F:8296:HOH:O	2.21	0.41
1:H:389:LEU:HA	4:H:8514:HOH:O	2.20	0.41
1:G:101:ASP:O	1:G:104[B]:VAL:HG22	2.19	0.41
2:B:7002:FAD:H8A	4:B:8158:HOH:O	2.20	0.41
1:C:389:LEU:HD13	4:C:8365:HOH:O	2.18	0.41
1:E:505:ARG:NH2	4:E:8354:HOH:O	2.53	0.41
1:H:231:LYS:HE2	4:H:8297:HOH:O	2.20	0.41
1:B:618:PHE:HD1	4:B:8417:HOH:O	2.03	0.41
1:H:83:GLY:N	4:H:8279:HOH:O	2.36	0.41
1:H:101:ASP:O	1:H:104[A]:VAL:HG23	2.20	0.41
1:H:510:ARG:NH2	4:H:8504:HOH:O	2.53	0.41
1:G:43:MET:HE3	4:G:8501:HOH:O	2.20	0.41
1:A:218:ARG:HD2	4:A:8189:HOH:O	2.20	0.41
1:E:106:VAL:O	1:E:110:GLN:HG2	2.21	0.41
1:G:557:PHE:HA	4:G:8584:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:481:GLU:CG	4:F:8289:HOH:O	2.64	0.41
1:H:331:ASN:ND2	4:H:8576:HOH:O	2.52	0.41
1:C:157:VAL:HG21	1:C:324:HIS:CE1	2.54	0.41
1:C:619:THR:CG2	4:C:8291:HOH:O	2.47	0.41
1:E:471:TRP:CH2	1:E:526:SER:HA	2.56	0.41
1:H:123:VAL:N	3:H:8004:MES:H22	2.26	0.41
1:G:607:GLU:HG3	4:G:8317:HOH:O	2.21	0.41
1:A:105:ASN:HB3	1:B:105:ASN:O	2.20	0.41
1:A:265:ARG:HA	1:A:266:PRO:C	2.40	0.41
1:B:388:GLU:HB3	1:B:389:LEU:HD22	2.02	0.41
1:C:228:GLU:HG3	4:C:8249:HOH:O	2.20	0.41
1:E:576:LYS:HD2	4:E:8386:HOH:O	2.20	0.41
1:F:570:SER:HB3	1:F:580:LEU:O	2.20	0.41
1:H:215:GLU:O	1:H:411:LYS:NZ	2.54	0.41
1:A:312:LYS:HD2	4:A:8456:HOH:O	2.21	0.41
1:C:545:LEU:CB	4:C:8502:HOH:O	2.58	0.41
1:E:457:GLY:H	1:E:460:GLN:HE21	1.67	0.41
1:F:433:PRO:O	1:F:450:HIS:HA	2.21	0.41
1:F:564:CYS:HG	1:F:573:PHE:HE2	1.67	0.41
3:H:8004:MES:C7	1:G:462:SER:O	2.56	0.41
1:G:382:ILE:HD13	4:G:8401:HOH:O	2.20	0.41
1:B:159:ARG:HA	2:B:7002:FAD:O2B	2.21	0.41
1:B:383:ARG:HD2	4:B:8485:HOH:O	2.20	0.41
1:D:576:LYS:CG	4:D:8297:HOH:O	2.68	0.41
1:F:104[A]:VAL:HG12	1:F:108:GLN:NE2	2.36	0.41
1:H:81:ASP:CB	4:H:8304:HOH:O	2.48	0.41
1:B:133:ALA:CB	3:B:8003:MES:O2S	2.62	0.40
1:B:389:LEU:H	1:B:389:LEU:HD13	1.86	0.40
1:B:471:TRP:CH2	1:B:526:SER:HA	2.56	0.40
1:C:101:ASP:O	1:C:104[B]:VAL:HG22	2.20	0.40
1:G:619:THR:O	1:G:619:THR:CG2	2.68	0.40
1:B:570:SER:HB3	1:B:580:LEU:O	2.21	0.40
1:H:45:ILE:C	1:H:45:ILE:CD1	2.89	0.40
1:B:132[A]:GLN:C	4:B:8607:HOH:O	2.57	0.40
4:B:8469:HOH:O	1:C:542:GLU:CB	2.42	0.40
1:D:211:ASP:CB	4:D:8348:HOH:O	2.59	0.40
1:E:131:TRP:O	1:E:132[B]:GLN:HG2	2.22	0.40
1:H:173:PRO:HG2	1:H:592:ALA:HB1	2.02	0.40
1:H:284:GLU:C	1:H:328:LEU:CD1	2.90	0.40
1:H:343:ALA:CA	4:H:8588:HOH:O	2.69	0.40
1:B:242:ALA:CB	4:B:8594:HOH:O	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:8007:MES:H51	1:F:462:SER:OG	2.21	0.40
1:F:471:TRP:CH2	1:F:526:SER:HA	2.56	0.40
1:H:165:SER:HA	1:H:168:TRP:CD1	2.57	0.40
1:G:71:LYS:NZ	4:G:8492:HOH:O	2.54	0.40
1:B:215:GLU:O	1:B:411:LYS:NZ	2.55	0.40
1:E:121:LEU:CD2	1:H:121:LEU:CD2	3.00	0.40
1:H:81:ASP:HA	4:G:8288:HOH:O	2.21	0.40
1:H:421:GLU:OE2	4:H:8273:HOH:O	2.22	0.40
1:H:432:GLU:HB2	1:H:433:PRO:HD2	2.04	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:8534:HOH:O	4:G:8089:HOH:O[2_646]	1.69	0.51
4:A:8707:HOH:O	4:G:8089:HOH:O[2_646]	1.73	0.47
4:H:8261:HOH:O	4:G:8557:HOH:O[2_655]	1.81	0.39
1:H:235:ASP:OD2	4:B:8535:HOH:O[2_666]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	576/623 (92%)	563 (98%)	13 (2%)	0	100	100
1	B	577/623 (93%)	564 (98%)	13 (2%)	0	100	100
1	C	577/623 (93%)	558 (97%)	19 (3%)	0	100	100
1	D	577/623 (93%)	564 (98%)	13 (2%)	0	100	100
1	E	577/623 (93%)	561 (97%)	15 (3%)	1 (0%)	47	28
1	F	576/623 (92%)	563 (98%)	13 (2%)	0	100	100
1	G	578/623 (93%)	562 (97%)	16 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	578/623 (93%)	562 (97%)	16 (3%)	0	100	100
All	All	4616/4984 (93%)	4497 (97%)	118 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	343	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	505/541 (93%)	490 (97%)	15 (3%)	41	15
1	B	506/541 (94%)	492 (97%)	14 (3%)	43	18
1	C	506/541 (94%)	494 (98%)	12 (2%)	49	23
1	D	506/541 (94%)	494 (98%)	12 (2%)	49	23
1	E	506/541 (94%)	496 (98%)	10 (2%)	55	32
1	F	505/541 (93%)	491 (97%)	14 (3%)	43	18
1	G	507/541 (94%)	497 (98%)	10 (2%)	55	32
1	H	507/541 (94%)	493 (97%)	14 (3%)	43	18
All	All	4048/4328 (94%)	3947 (98%)	101 (2%)	47	22

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ILE
1	A	112	MET
1	A	168	TRP
1	A	185	LYS
1	A	206	PHE
1	A	312	LYS
1	A	341	ASN

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Mol	Chain	Res	Type
1	A	392	SER
1	A	400	SER
1	A	401	THR
1	A	408	TRP
1	A	450	HIS
1	A	496	ASN
1	A	593	ASN
1	A	619	THR
1	B	45	ILE
1	B	112	MET
1	B	168	TRP
1	B	185	LYS
1	B	206	PHE
1	B	312	LYS
1	B	385	THR
1	B	389	LEU
1	B	403	LYS
1	B	408	TRP
1	B	450	HIS
1	B	490	LYS
1	B	496	ASN
1	B	593	ASN
1	D	100	ILE
1	D	110	GLN
1	D	132[A]	GLN
1	D	132[B]	GLN
1	D	168	TRP
1	D	206	PHE
1	D	231	LYS
1	D	385	THR
1	D	390	THR
1	D	450	HIS
1	D	593	ASN
1	D	618	PHE
1	C	100	ILE
1	C	168	TRP
1	C	341	ASN
1	C	385	THR
1	C	389	LEU
1	C	408	TRP
1	C	418	GLN
1	C	450	HIS

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Mol	Chain	Res	Type
1	C	455	SER
1	C	490	LYS
1	C	496	ASN
1	C	593	ASN
1	E	100	ILE
1	E	168	TRP
1	E	185	LYS
1	E	206	PHE
1	E	231	LYS
1	E	341	ASN
1	E	403	LYS
1	E	450	HIS
1	E	593	ASN
1	E	618	PHE
1	F	112	MET
1	F	168	TRP
1	F	178	GLU
1	F	206	PHE
1	F	272	GLU
1	F	285	ARG
1	F	328	LEU
1	F	385	THR
1	F	408	TRP
1	F	450	HIS
1	F	496	ASN
1	F	576	LYS
1	F	593	ASN
1	F	618	PHE
1	H	100	ILE
1	H	132[A]	GLN
1	H	132[B]	GLN
1	H	168	TRP
1	H	185	LYS
1	H	206	PHE
1	H	231	LYS
1	H	272	GLU
1	H	341	ASN
1	H	385	THR
1	H	450	HIS
1	H	452	ASP
1	H	593	ASN
1	H	618	PHE

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Mol	Chain	Res	Type
1	G	84	LEU
1	G	168	TRP
1	G	385	THR
1	G	390	THR
1	G	408	TRP
1	G	450	HIS
1	G	490	LYS
1	G	496	ASN
1	G	593	ASN
1	G	618	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	299	HIS
1	A	341	ASN
1	A	460	GLN
1	A	563	ASN
1	B	341	ASN
1	B	460	GLN
1	D	105	ASN
1	D	263	GLN
1	D	341	ASN
1	D	460	GLN
1	C	99	ASN
1	C	105	ASN
1	C	108	GLN
1	C	263	GLN
1	C	341	ASN
1	C	344	ASN
1	C	418	GLN
1	E	99	ASN
1	E	105	ASN
1	E	341	ASN
1	E	418	GLN
1	E	460	GLN
1	F	105	ASN
1	F	108	GLN
1	F	132	GLN
1	F	263	GLN
1	F	341	ASN
1	F	460	GLN

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Mol	Chain	Res	Type
1	H	105	ASN
1	H	108	GLN
1	H	263	GLN
1	H	341	ASN
1	H	418	GLN
1	H	460	GLN
1	H	563	ASN
1	G	105	ASN
1	G	108	GLN
1	G	263	GLN
1	G	418	GLN
1	G	460	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FAD	C	7004	-	51,58,58	1.64	12 (23%)	60,89,89	2.60	20 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	FAD	B	7002	-	51,58,58	1.36	6 (11%)	60,89,89	3.22	21 (35%)
2	FAD	E	7005	-	51,58,58	1.51	8 (15%)	60,89,89	2.55	18 (30%)
2	FAD	A	7001	-	51,58,58	1.71	11 (21%)	60,89,89	2.83	17 (28%)
2	FAD	F	7006	-	51,58,58	1.60	13 (25%)	60,89,89	2.98	18 (30%)
2	FAD	G	7008	-	51,58,58	1.44	10 (19%)	60,89,89	2.75	16 (26%)
3	MES	E	8007	-	12,12,12	1.90	1 (8%)	14,16,16	6.45	11 (78%)
3	MES	A	8002	-	12,12,12	1.67	1 (8%)	14,16,16	4.38	7 (50%)
2	FAD	H	7007	-	51,58,58	1.55	8 (15%)	60,89,89	2.27	16 (26%)
3	MES	D	8005	-	12,12,12	1.69	1 (8%)	14,16,16	6.80	7 (50%)
3	MES	C	8008	-	12,12,12	1.68	1 (8%)	14,16,16	5.48	8 (57%)
3	MES	H	8004	-	12,12,12	2.23	1 (8%)	14,16,16	3.80	7 (50%)
3	MES	F	8001	-	12,12,12	1.64	1 (8%)	14,16,16	4.11	8 (57%)
2	FAD	D	7003	-	51,58,58	1.51	8 (15%)	60,89,89	2.21	15 (25%)
3	MES	G	8006	-	12,12,12	1.84	1 (8%)	14,16,16	5.89	8 (57%)
3	MES	B	8003	-	12,12,12	1.98	1 (8%)	14,16,16	4.87	6 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	C	7004	-	-	3/30/50/50	0/6/6/6
2	FAD	B	7002	-	-	1/30/50/50	0/6/6/6
2	FAD	E	7005	-	-	3/30/50/50	0/6/6/6
2	FAD	A	7001	-	-	2/30/50/50	0/6/6/6
2	FAD	F	7006	-	-	3/30/50/50	0/6/6/6
2	FAD	G	7008	-	-	2/30/50/50	0/6/6/6
3	MES	E	8007	-	-	5/6/14/14	0/1/1/1
3	MES	A	8002	-	-	2/6/14/14	0/1/1/1
2	FAD	H	7007	-	-	2/30/50/50	0/6/6/6
3	MES	D	8005	-	-	2/6/14/14	0/1/1/1
3	MES	C	8008	-	-	2/6/14/14	0/1/1/1
3	MES	H	8004	-	-	5/6/14/14	0/1/1/1
3	MES	F	8001	-	-	2/6/14/14	0/1/1/1
2	FAD	D	7003	-	-	3/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MES	G	8006	-	-	2/6/14/14	0/1/1/1
3	MES	B	8003	-	-	2/6/14/14	0/1/1/1

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	8004	MES	C8-S	-7.64	1.66	1.77
3	B	8003	MES	C8-S	-6.51	1.68	1.77
3	G	8006	MES	C8-S	-6.05	1.68	1.77
3	E	8007	MES	C8-S	-6.04	1.68	1.77
3	C	8008	MES	C8-S	-5.43	1.69	1.77
3	A	8002	MES	C8-S	-5.42	1.69	1.77
3	D	8005	MES	C8-S	-5.29	1.70	1.77
3	F	8001	MES	C8-S	-5.10	1.70	1.77
2	A	7001	FAD	C10-N1	4.88	1.39	1.33
2	C	7004	FAD	C10-N1	4.31	1.38	1.33
2	H	7007	FAD	C2B-C1B	-4.12	1.47	1.53
2	D	7003	FAD	C10-N1	3.96	1.38	1.33
2	H	7007	FAD	C10-N1	3.81	1.38	1.33
2	F	7006	FAD	C10-N1	3.74	1.38	1.33
2	D	7003	FAD	O4B-C4B	-3.74	1.36	1.45
2	A	7001	FAD	C2B-C1B	-3.69	1.48	1.53
2	E	7005	FAD	C4-N3	3.62	1.39	1.33
2	F	7006	FAD	C4-N3	3.53	1.39	1.33
2	C	7004	FAD	O4B-C4B	-3.40	1.37	1.45
2	E	7005	FAD	C4-C4X	3.37	1.47	1.41
2	C	7004	FAD	C2A-N3A	3.34	1.37	1.32
2	A	7001	FAD	C9A-N10	3.33	1.43	1.38
2	G	7008	FAD	C2A-N3A	3.32	1.37	1.32
2	D	7003	FAD	C4-N3	3.24	1.38	1.33
2	A	7001	FAD	C4-N3	3.23	1.38	1.33
2	H	7007	FAD	C2A-N3A	3.14	1.37	1.32
2	E	7005	FAD	C10-N1	3.12	1.37	1.33
2	H	7007	FAD	C4-N3	3.11	1.38	1.33
2	D	7003	FAD	C1'-N10	-3.08	1.45	1.48
2	C	7004	FAD	C4-N3	3.06	1.38	1.33
2	E	7005	FAD	O3B-C3B	-3.05	1.35	1.43
2	A	7001	FAD	C2B-C3B	-3.04	1.45	1.53
2	H	7007	FAD	C2-N1	-3.03	1.32	1.38
2	E	7005	FAD	C2A-N3A	3.03	1.37	1.32
2	F	7006	FAD	C2-N3	-2.99	1.32	1.38
2	C	7004	FAD	O3B-C3B	-2.99	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	7006	FAD	C4-C4X	2.98	1.46	1.41
2	B	7002	FAD	C4X-C10	2.97	1.41	1.38
2	A	7001	FAD	C4-C4X	2.94	1.46	1.41
2	B	7002	FAD	C10-N1	2.89	1.37	1.33
2	E	7005	FAD	O4B-C4B	-2.88	1.38	1.45
2	D	7003	FAD	C2B-C1B	-2.86	1.49	1.53
2	F	7006	FAD	O4B-C4B	-2.84	1.38	1.45
2	B	7002	FAD	C2-N1	-2.81	1.32	1.38
2	H	7007	FAD	O3B-C3B	-2.80	1.36	1.43
2	F	7006	FAD	C4X-N5	2.77	1.37	1.33
2	D	7003	FAD	C4-C4X	2.73	1.46	1.41
2	C	7004	FAD	C4-C4X	2.71	1.46	1.41
2	C	7004	FAD	C2B-C3B	-2.67	1.46	1.53
2	F	7006	FAD	C2B-C1B	-2.63	1.49	1.53
2	A	7001	FAD	C2A-N3A	2.63	1.36	1.32
2	B	7002	FAD	C2B-C1B	-2.59	1.49	1.53
2	A	7001	FAD	C4X-N5	2.56	1.37	1.33
2	F	7006	FAD	C1'-N10	-2.54	1.45	1.48
2	C	7004	FAD	C2-N1	-2.54	1.33	1.38
2	G	7008	FAD	C5'-C4'	2.48	1.55	1.51
2	E	7005	FAD	C2B-C3B	-2.46	1.46	1.53
2	C	7004	FAD	C4X-N5	2.45	1.36	1.33
2	F	7006	FAD	O3B-C3B	-2.44	1.37	1.43
2	G	7008	FAD	C4-C4X	2.44	1.45	1.41
2	C	7004	FAD	C9A-N10	2.42	1.41	1.38
2	F	7006	FAD	C8A-N7A	-2.37	1.30	1.34
2	E	7005	FAD	C4X-C10	2.36	1.41	1.38
2	B	7002	FAD	C4-C4X	2.32	1.45	1.41
2	F	7006	FAD	C9A-N10	2.30	1.41	1.38
2	F	7006	FAD	C2B-C3B	-2.29	1.47	1.53
2	C	7004	FAD	C2A-N1A	2.28	1.38	1.33
2	G	7008	FAD	C9A-N10	2.27	1.41	1.38
2	D	7003	FAD	C2B-C3B	-2.25	1.47	1.53
2	D	7003	FAD	O3B-C3B	-2.25	1.37	1.43
2	G	7008	FAD	C4A-N3A	-2.24	1.32	1.35
2	G	7008	FAD	P-O1P	-2.22	1.43	1.50
2	A	7001	FAD	C4A-N3A	-2.21	1.32	1.35
2	H	7007	FAD	C4-C4X	2.18	1.45	1.41
2	G	7008	FAD	C2B-C1B	-2.17	1.50	1.53
2	A	7001	FAD	C9A-C5X	-2.16	1.38	1.42
2	G	7008	FAD	O4B-C4B	-2.12	1.40	1.45
2	G	7008	FAD	C4X-C10	2.12	1.40	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	7004	FAD	C2-N3	-2.10	1.34	1.38
2	H	7007	FAD	C2B-C3B	-2.08	1.47	1.53
2	F	7006	FAD	C2-N1	-2.07	1.34	1.38
2	A	7001	FAD	C2-N1	-2.04	1.34	1.38
2	B	7002	FAD	O3B-C3B	-2.01	1.38	1.43
2	G	7008	FAD	C2'-C3'	2.00	1.57	1.53

All (203) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	8005	MES	O2S-S-C8	-22.09	80.31	106.92
3	G	8006	MES	O2S-S-C8	-18.46	84.68	106.92
2	F	7006	FAD	C4-N3-C2	16.00	128.65	115.14
2	A	7001	FAD	C4-N3-C2	15.07	127.87	115.14
2	G	7008	FAD	C4-N3-C2	13.83	126.81	115.14
3	C	8008	MES	O3S-S-C8	-13.59	83.79	105.77
3	B	8003	MES	O1S-S-C8	-13.26	90.95	106.92
3	E	8007	MES	O1S-S-C8	-12.89	91.40	106.92
3	A	8002	MES	O1S-S-C8	-12.00	92.47	106.92
2	B	7002	FAD	C4-N3-C2	11.91	125.19	115.14
2	E	7005	FAD	C4-N3-C2	11.86	125.16	115.14
3	E	8007	MES	O3S-S-C8	-11.59	87.02	105.77
3	E	8007	MES	C6-C5-N4	-10.23	94.59	110.10
2	C	7004	FAD	C4-N3-C2	10.23	123.78	115.14
2	B	7002	FAD	C1'-N10-C9A	9.34	125.64	118.29
3	H	8004	MES	O2S-S-C8	-9.33	95.68	106.92
2	F	7006	FAD	C4X-C4-N3	-9.09	111.00	123.43
3	C	8008	MES	O1S-S-C8	-9.07	96.00	106.92
2	C	7004	FAD	C4-C4X-C10	-9.02	113.98	119.95
3	F	8001	MES	O3S-S-C8	-9.00	91.22	105.77
2	A	7001	FAD	C4X-C4-N3	-8.70	111.53	123.43
2	D	7003	FAD	C4-C4X-C10	-8.69	114.20	119.95
2	B	7002	FAD	C4-C4X-C10	-8.28	114.47	119.95
3	E	8007	MES	C7-N4-C3	8.27	132.38	111.23
3	B	8003	MES	O2S-S-C8	-7.99	97.30	106.92
3	F	8001	MES	O1S-S-C8	-7.87	97.44	106.92
2	H	7007	FAD	N3A-C2A-N1A	-7.67	116.69	128.68
2	B	7002	FAD	C4-C4X-N5	7.29	126.93	118.60
2	A	7001	FAD	N3A-C2A-N1A	-6.87	117.95	128.68
3	C	8008	MES	C5-N4-C3	6.86	124.28	108.83
3	G	8006	MES	C5-N4-C3	6.55	123.57	108.83
2	E	7005	FAD	C4X-C4-N3	-6.51	114.53	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	7008	FAD	N3A-C2A-N1A	-6.32	118.80	128.68
2	H	7007	FAD	C4-N3-C2	6.16	120.34	115.14
3	H	8004	MES	O1S-S-C8	-6.13	99.53	106.92
3	D	8005	MES	C5-N4-C3	6.08	122.52	108.83
3	B	8003	MES	C5-N4-C3	6.00	122.34	108.83
2	E	7005	FAD	N3A-C2A-N1A	-5.95	119.38	128.68
3	A	8002	MES	C5-N4-C3	5.82	121.94	108.83
3	H	8004	MES	C5-N4-C3	5.80	121.89	108.83
2	B	7002	FAD	C1'-N10-C10	-5.77	113.24	118.41
3	D	8005	MES	O3S-S-C8	-5.66	96.61	105.77
2	G	7008	FAD	C4X-C4-N3	-5.60	115.77	123.43
2	B	7002	FAD	C4X-N5-C5X	5.59	122.36	116.77
2	B	7002	FAD	N3A-C2A-N1A	-5.59	119.95	128.68
3	G	8006	MES	O3S-S-C8	-5.56	96.78	105.77
3	A	8002	MES	O2S-S-C8	-5.46	100.34	106.92
3	F	8001	MES	C5-N4-C3	5.46	121.11	108.83
3	D	8005	MES	O3S-S-O2S	5.36	124.37	111.27
3	C	8008	MES	O2S-S-C8	-5.22	100.63	106.92
2	G	7008	FAD	C1'-N10-C9A	5.21	122.40	118.29
2	C	7004	FAD	C4X-C4-N3	-5.16	116.38	123.43
3	E	8007	MES	O2S-S-C8	-5.12	100.75	106.92
3	F	8001	MES	C7-N4-C3	5.08	124.24	111.23
3	E	8007	MES	O1-C6-C5	-4.97	100.85	111.80
2	F	7006	FAD	C1'-N10-C9A	4.84	122.11	118.29
3	C	8008	MES	O1-C2-C3	-4.82	101.18	111.80
2	H	7007	FAD	C2A-N1A-C6A	4.79	126.95	118.75
2	E	7005	FAD	C1'-N10-C9A	4.77	122.05	118.29
2	G	7008	FAD	O3B-C3B-C4B	4.74	124.75	111.05
2	G	7008	FAD	C4-C4X-C10	-4.67	116.86	119.95
3	A	8002	MES	C7-N4-C5	4.67	123.17	111.23
3	G	8006	MES	O3S-S-O2S	4.67	122.68	111.27
2	D	7003	FAD	O3B-C3B-C4B	4.60	124.36	111.05
2	D	7003	FAD	C1'-N10-C9A	4.59	121.91	118.29
2	H	7007	FAD	C4X-C4-N3	-4.59	117.16	123.43
3	E	8007	MES	O3S-S-O1S	4.58	122.46	111.27
3	D	8005	MES	C7-N4-C3	4.58	122.94	111.23
3	B	8003	MES	C7-N4-C3	4.57	122.93	111.23
2	B	7002	FAD	C10-C4X-N5	-4.41	118.21	121.26
2	H	7007	FAD	C4X-N5-C5X	4.33	121.10	116.77
2	D	7003	FAD	C4-N3-C2	4.33	118.80	115.14
3	D	8005	MES	O1S-S-C8	-4.32	101.71	106.92
3	E	8007	MES	C2-C3-N4	-4.25	103.66	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	7003	FAD	C4-C4X-N5	4.24	123.45	118.60
2	B	7002	FAD	C2A-N1A-C6A	4.16	125.87	118.75
3	G	8006	MES	C7-N4-C3	4.15	121.85	111.23
2	H	7007	FAD	O2B-C2B-C3B	4.15	125.25	111.82
3	C	8008	MES	C7-N4-C5	4.09	121.69	111.23
2	D	7003	FAD	N3A-C2A-N1A	-4.08	122.30	128.68
3	C	8008	MES	O3S-S-O1S	4.02	121.09	111.27
2	D	7003	FAD	O4B-C1B-C2B	3.97	112.73	106.93
2	B	7002	FAD	O3B-C3B-C4B	3.95	122.46	111.05
2	C	7004	FAD	O2B-C2B-C3B	3.91	124.47	111.82
2	A	7001	FAD	C2A-N1A-C6A	3.81	125.27	118.75
2	F	7006	FAD	N3A-C2A-N1A	-3.77	122.78	128.68
2	B	7002	FAD	C4X-C4-N3	-3.77	118.28	123.43
2	H	7007	FAD	O4B-C1B-C2B	3.76	112.42	106.93
3	B	8003	MES	O1-C6-C5	-3.76	103.52	111.80
3	H	8004	MES	O3S-S-O1S	3.73	120.39	111.27
3	A	8002	MES	O3S-S-C8	-3.63	99.90	105.77
3	B	8003	MES	O3S-S-O2S	3.62	120.12	111.27
2	F	7006	FAD	O2B-C2B-C1B	3.62	124.22	110.85
3	D	8005	MES	O1-C6-C5	-3.60	103.86	111.80
2	F	7006	FAD	O3B-C3B-C4B	3.60	121.45	111.05
2	H	7007	FAD	O3B-C3B-C4B	3.58	121.41	111.05
2	G	7008	FAD	O4'-C4'-C3'	3.57	117.79	109.10
2	C	7004	FAD	C4-C4X-N5	3.57	122.68	118.60
2	C	7004	FAD	N3A-C2A-N1A	-3.55	123.13	128.68
3	C	8008	MES	O3S-S-O2S	3.55	119.95	111.27
2	E	7005	FAD	C4X-N5-C5X	3.55	120.32	116.77
2	E	7005	FAD	C2A-N1A-C6A	3.52	124.77	118.75
2	C	7004	FAD	C10-C4X-N5	-3.41	118.90	121.26
2	D	7003	FAD	O2B-C2B-C1B	3.40	123.40	110.85
2	D	7003	FAD	O2B-C2B-C3B	3.38	122.77	111.82
2	C	7004	FAD	O2A-PA-O1A	3.35	128.81	112.24
3	H	8004	MES	C7-N4-C5	3.35	119.80	111.23
2	C	7004	FAD	O4B-C1B-C2B	3.33	111.80	106.93
2	F	7006	FAD	O4B-C1B-C2B	3.33	111.79	106.93
2	E	7005	FAD	O4B-C4B-C5B	3.32	120.31	109.37
2	A	7001	FAD	C1'-N10-C9A	3.31	120.89	118.29
2	G	7008	FAD	C5'-C4'-C3'	-3.30	105.82	112.20
2	C	7004	FAD	O2B-C2B-C1B	3.28	122.98	110.85
2	E	7005	FAD	O3B-C3B-C4B	3.28	120.53	111.05
2	G	7008	FAD	C2A-N1A-C6A	3.28	124.36	118.75
2	F	7006	FAD	O2B-C2B-C3B	3.26	122.37	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	8002	MES	O3S-S-O2S	3.25	119.22	111.27
2	A	7001	FAD	O3B-C3B-C4B	3.24	120.42	111.05
2	E	7005	FAD	O2B-C2B-C3B	3.22	122.24	111.82
2	A	7001	FAD	O2B-C2B-C3B	3.22	122.23	111.82
2	E	7005	FAD	O4B-C1B-C2B	3.20	111.61	106.93
2	D	7003	FAD	O4B-C4B-C3B	3.20	111.44	105.11
3	G	8006	MES	O1S-S-C8	-3.19	103.08	106.92
3	G	8006	MES	O1-C6-C5	-3.11	104.94	111.80
3	F	8001	MES	O3S-S-O2S	3.11	118.86	111.27
2	H	7007	FAD	O2'-C2'-C3'	3.08	116.59	109.10
3	F	8001	MES	O3S-S-O1S	3.08	118.80	111.27
2	G	7008	FAD	C4-C4X-N5	3.08	122.12	118.60
2	G	7008	FAD	O2B-C2B-C3B	3.07	121.76	111.82
2	H	7007	FAD	N6A-C6A-N1A	3.07	124.95	118.57
2	C	7004	FAD	O5'-P-O1P	-3.01	97.32	109.07
2	H	7007	FAD	C5B-C4B-C3B	2.97	126.31	115.18
2	B	7002	FAD	O4B-C4B-C3B	2.97	110.98	105.11
3	F	8001	MES	C2-C3-N4	2.94	114.56	110.10
2	H	7007	FAD	C1'-N10-C9A	2.93	120.60	118.29
2	A	7001	FAD	C3B-C2B-C1B	2.92	105.37	100.98
2	C	7004	FAD	C4X-N5-C5X	2.89	119.66	116.77
2	B	7002	FAD	O2B-C2B-C1B	2.84	121.36	110.85
2	F	7006	FAD	O3B-C3B-C2B	2.84	121.01	111.82
3	A	8002	MES	O3S-S-O1S	2.82	118.17	111.27
2	B	7002	FAD	O2B-C2B-C3B	2.82	120.94	111.82
2	C	7004	FAD	O3B-C3B-C4B	2.80	119.15	111.05
2	C	7004	FAD	C7-C6-C5X	-2.79	117.27	121.22
2	F	7006	FAD	C2A-N1A-C6A	2.79	123.52	118.75
3	H	8004	MES	C7-N4-C3	2.76	118.28	111.23
2	F	7006	FAD	C5A-C6A-N6A	2.75	124.53	120.35
2	C	7004	FAD	O4B-C4B-C5B	2.63	118.02	109.37
2	B	7002	FAD	C5'-C4'-C3'	-2.61	107.17	112.20
2	H	7007	FAD	O2B-C2B-C1B	2.58	120.39	110.85
2	F	7006	FAD	O2A-PA-O1A	2.58	125.00	112.24
2	H	7007	FAD	C5A-C6A-N1A	-2.57	114.53	120.35
2	H	7007	FAD	O4B-C4B-C3B	2.56	110.18	105.11
2	B	7002	FAD	C5A-C6A-N1A	-2.56	114.56	120.35
2	F	7006	FAD	C5A-C6A-N1A	-2.54	114.60	120.35
2	G	7008	FAD	C5B-C4B-C3B	2.53	124.67	115.18
2	E	7005	FAD	O4B-C4B-C3B	2.53	110.11	105.11
2	D	7003	FAD	O5'-P-O1P	-2.52	99.22	109.07
2	F	7006	FAD	C5B-C4B-C3B	2.51	124.59	115.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	7002	FAD	O4B-C4B-C5B	2.50	117.58	109.37
2	H	7007	FAD	C4X-C10-N10	-2.47	117.76	120.30
2	B	7002	FAD	C3B-C2B-C1B	2.46	104.69	100.98
3	G	8006	MES	O3S-S-O1S	2.44	117.24	111.27
2	G	7008	FAD	O2P-P-O1P	2.43	124.25	112.24
2	F	7006	FAD	O2'-C2'-C3'	2.43	115.00	109.10
2	D	7003	FAD	O4B-C4B-C5B	2.42	117.34	109.37
2	A	7001	FAD	C5A-C6A-N1A	-2.42	114.88	120.35
2	A	7001	FAD	O4B-C4B-C3B	2.41	109.89	105.11
3	E	8007	MES	O2S-S-O1S	2.40	122.26	113.95
2	A	7001	FAD	C4A-C5A-N7A	-2.37	106.93	109.40
2	E	7005	FAD	C4-C4X-C10	-2.32	118.42	119.95
2	G	7008	FAD	C4X-N5-C5X	2.32	119.09	116.77
3	E	8007	MES	C5-N4-C3	2.29	113.98	108.83
2	G	7008	FAD	O4B-C1B-C2B	2.29	110.27	106.93
2	E	7005	FAD	C5B-C4B-C3B	2.28	123.74	115.18
3	H	8004	MES	O2S-S-O1S	2.28	121.84	113.95
2	A	7001	FAD	O4'-C4'-C3'	2.25	114.58	109.10
2	B	7002	FAD	C4X-C10-N10	-2.25	117.99	120.30
2	D	7003	FAD	O2A-PA-O1A	2.24	123.34	112.24
2	F	7006	FAD	C9A-N10-C10	-2.24	118.97	121.91
3	E	8007	MES	C6-O1-C2	2.24	117.36	109.89
2	C	7004	FAD	C2B-C3B-C4B	2.24	106.99	102.64
2	D	7003	FAD	C5B-C4B-C3B	2.23	123.55	115.18
2	F	7006	FAD	C4X-N5-C5X	2.23	119.00	116.77
2	C	7004	FAD	C7M-C7-C6	-2.22	115.03	120.34
2	B	7002	FAD	N6A-C6A-N1A	2.21	123.16	118.57
2	E	7005	FAD	O2B-C2B-C1B	2.20	118.99	110.85
2	A	7001	FAD	C5A-C6A-N6A	2.20	123.70	120.35
2	E	7005	FAD	C5A-C6A-N1A	-2.19	115.38	120.35
2	B	7002	FAD	C1B-N9A-C4A	-2.17	122.82	126.64
2	F	7006	FAD	C4'-C3'-C2'	-2.13	108.93	113.36
2	C	7004	FAD	C1'-N10-C9A	2.13	119.97	118.29
2	A	7001	FAD	C5'-C4'-C3'	-2.12	108.10	112.20
2	C	7004	FAD	C1'-N10-C10	2.12	120.31	118.41
2	E	7005	FAD	O2A-PA-O1A	2.11	122.67	112.24
2	E	7005	FAD	C5'-C4'-C3'	-2.10	108.14	112.20
2	C	7004	FAD	C5B-C4B-C3B	2.05	122.87	115.18
2	D	7003	FAD	C4X-C4-N3	-2.05	120.63	123.43
2	E	7005	FAD	O2P-P-O1P	2.03	122.28	112.24
2	A	7001	FAD	O4B-C1B-C2B	2.03	109.89	106.93
3	F	8001	MES	O1-C2-C3	-2.02	107.35	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	7001	FAD	C4X-N5-C5X	2.02	118.79	116.77
2	A	7001	FAD	O2'-C2'-C3'	2.02	114.00	109.10
2	G	7008	FAD	O4B-C4B-C5B	2.02	116.00	109.37

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	7003	FAD	PA-O3P-P-O5'
2	F	7006	FAD	PA-O3P-P-O5'
3	A	8002	MES	C8-C7-N4-C5
3	A	8002	MES	N4-C7-C8-S
3	B	8003	MES	C8-C7-N4-C3
3	B	8003	MES	N4-C7-C8-S
3	D	8005	MES	C8-C7-N4-C3
3	D	8005	MES	N4-C7-C8-S
3	C	8008	MES	C8-C7-N4-C5
3	C	8008	MES	N4-C7-C8-S
3	E	8007	MES	C8-C7-N4-C5
3	E	8007	MES	N4-C7-C8-S
3	E	8007	MES	C7-C8-S-O1S
3	E	8007	MES	C7-C8-S-O2S
3	E	8007	MES	C7-C8-S-O3S
3	F	8001	MES	C8-C7-N4-C3
3	F	8001	MES	N4-C7-C8-S
3	H	8004	MES	C8-C7-N4-C5
3	H	8004	MES	C7-C8-S-O1S
3	H	8004	MES	C7-C8-S-O2S
3	H	8004	MES	C7-C8-S-O3S
3	G	8006	MES	C8-C7-N4-C3
3	G	8006	MES	N4-C7-C8-S
2	C	7004	FAD	O4B-C4B-C5B-O5B
2	A	7001	FAD	PA-O3P-P-O5'
2	C	7004	FAD	PA-O3P-P-O5'
2	E	7005	FAD	PA-O3P-P-O5'
2	G	7008	FAD	PA-O3P-P-O5'
2	F	7006	FAD	O4B-C4B-C5B-O5B
2	E	7005	FAD	O4B-C4B-C5B-O5B
3	H	8004	MES	N4-C7-C8-S
2	B	7002	FAD	O4B-C4B-C5B-O5B
2	C	7004	FAD	P-O3P-PA-O2A
2	E	7005	FAD	P-O3P-PA-O2A

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Mol	Chain	Res	Type	Atoms
2	F	7006	FAD	P-O3P-PA-O2A
2	H	7007	FAD	O4B-C4B-C5B-O5B
2	H	7007	FAD	PA-O3P-P-O5'
2	G	7008	FAD	O4B-C4B-C5B-O5B
2	D	7003	FAD	P-O3P-PA-O2A
2	A	7001	FAD	O4B-C4B-C5B-O5B
2	D	7003	FAD	O4B-C4B-C5B-O5B

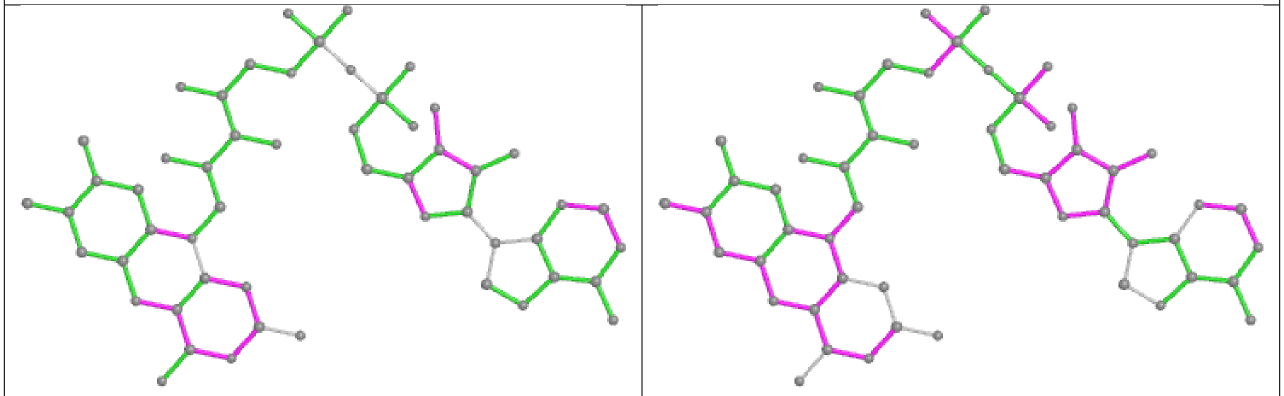
There are no ring outliers.

13 monomers are involved in 84 short contacts:

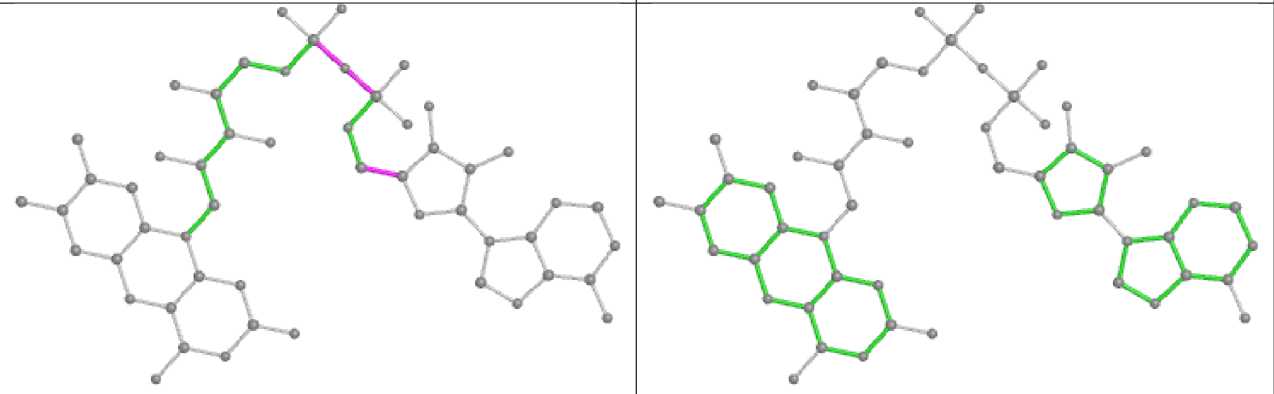
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	7004	FAD	1	0
2	B	7002	FAD	2	0
2	F	7006	FAD	1	0
2	G	7008	FAD	1	0
3	E	8007	MES	11	0
3	A	8002	MES	4	0
3	D	8005	MES	14	0
3	C	8008	MES	10	0
3	H	8004	MES	17	0
3	F	8001	MES	4	0
2	D	7003	FAD	1	0
3	G	8006	MES	9	0
3	B	8003	MES	9	0

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 then 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.

Ligand FAD C 7004

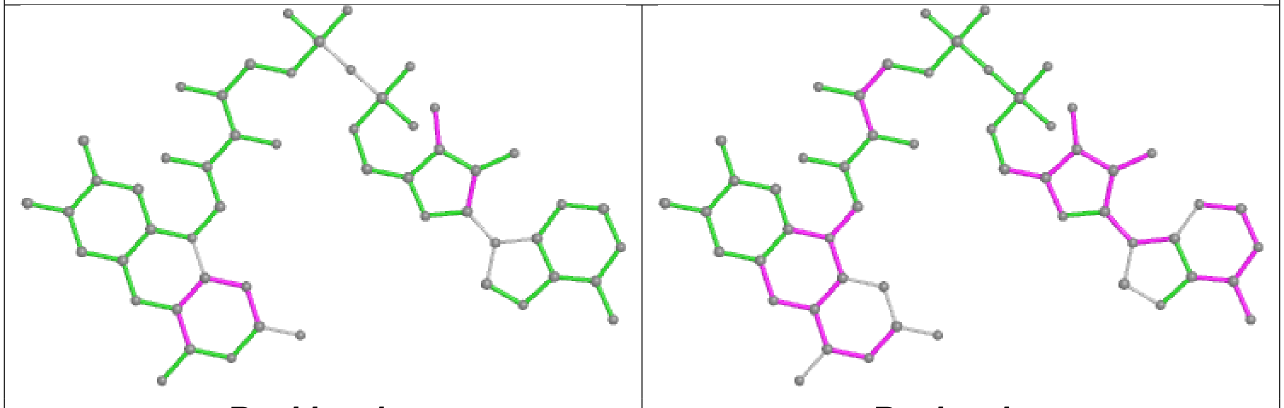


Bond lengths **Bond angles**



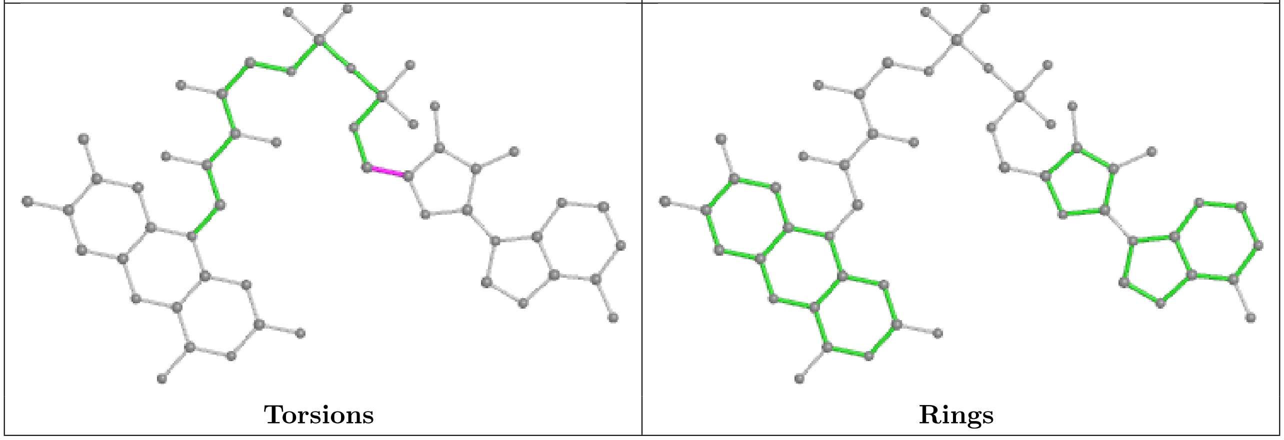
Torsions **Rings**

Ligand FAD B 7002



Bond lengths

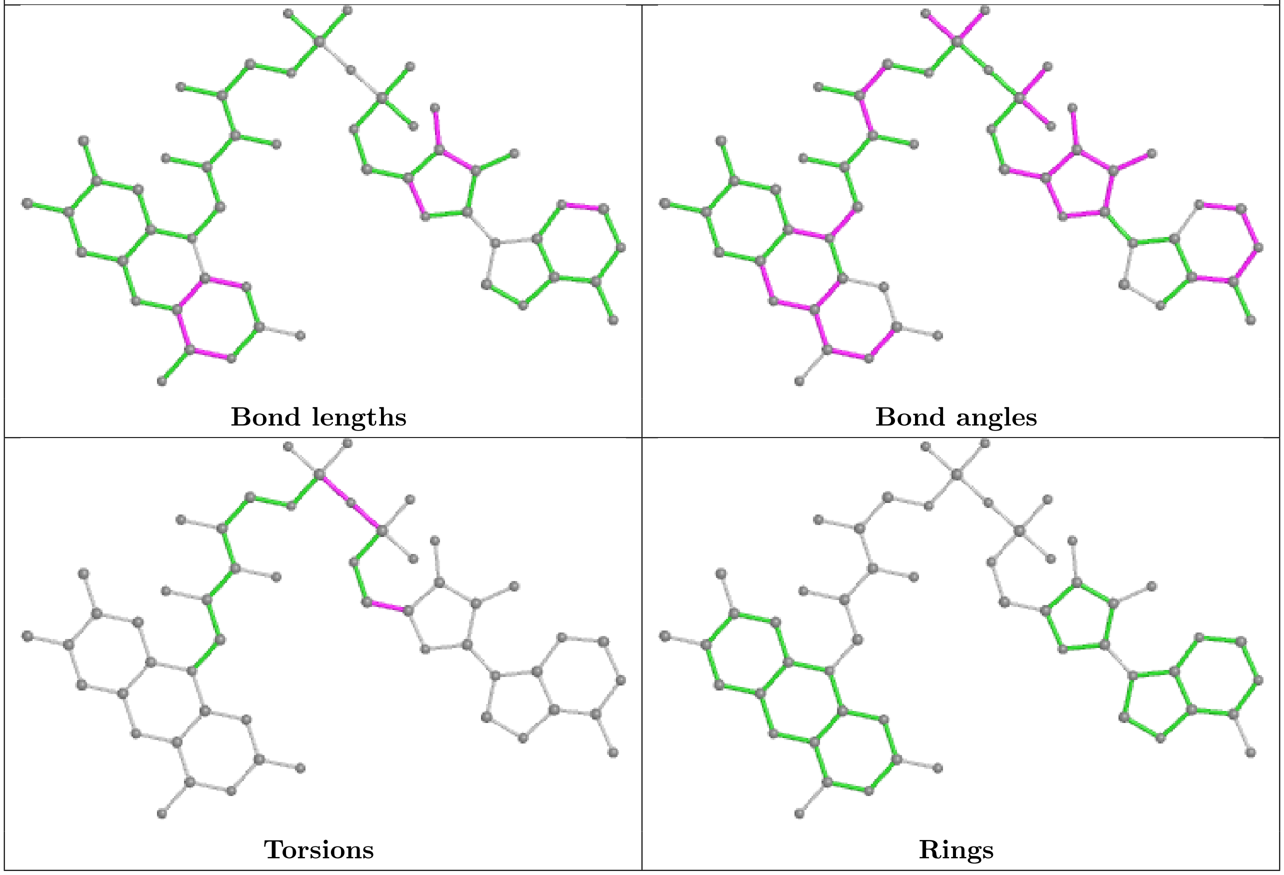
Bond angles



Torsions

Rings

Ligand FAD E 7005



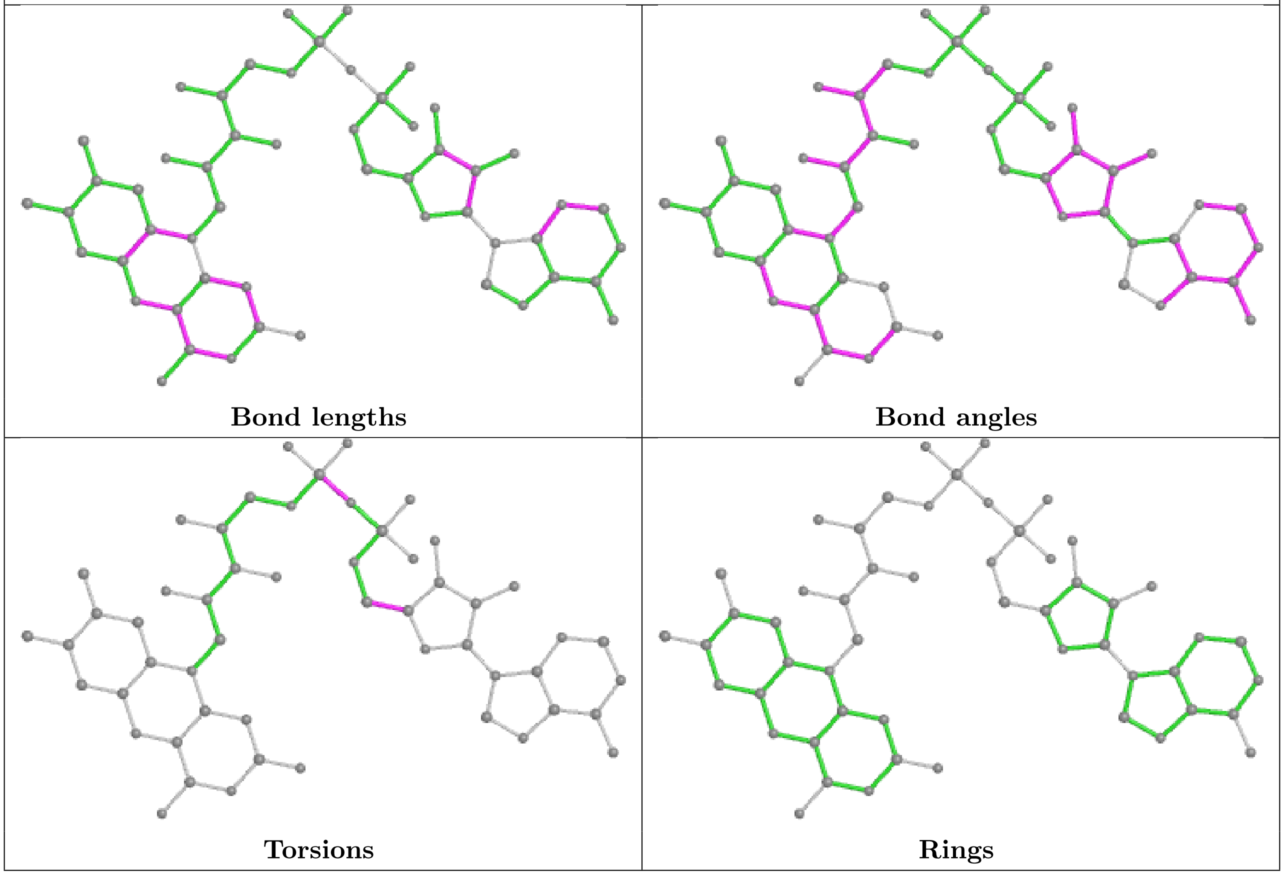
Bond lengths

Bond angles

Torsions

Rings

Ligand FAD A 7001



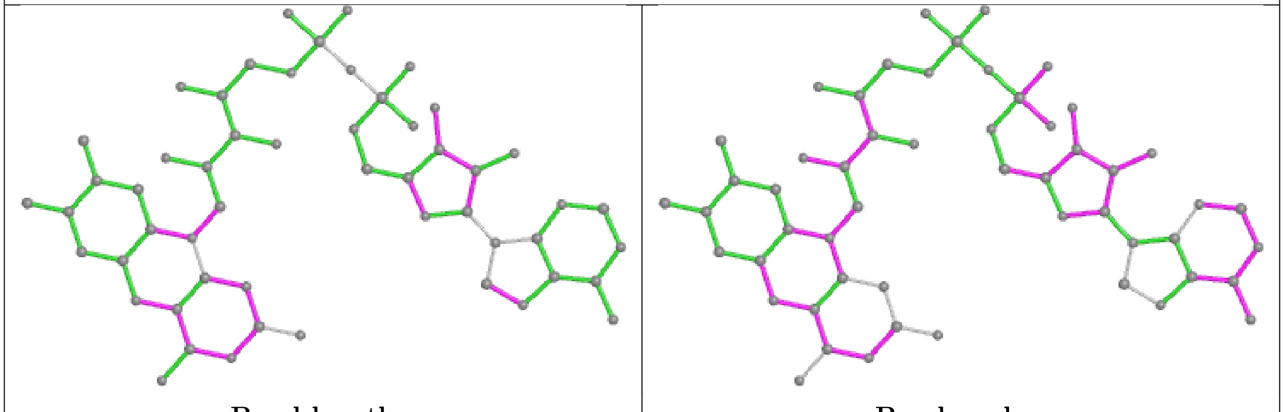
Bond lengths

Bond angles

Torsions

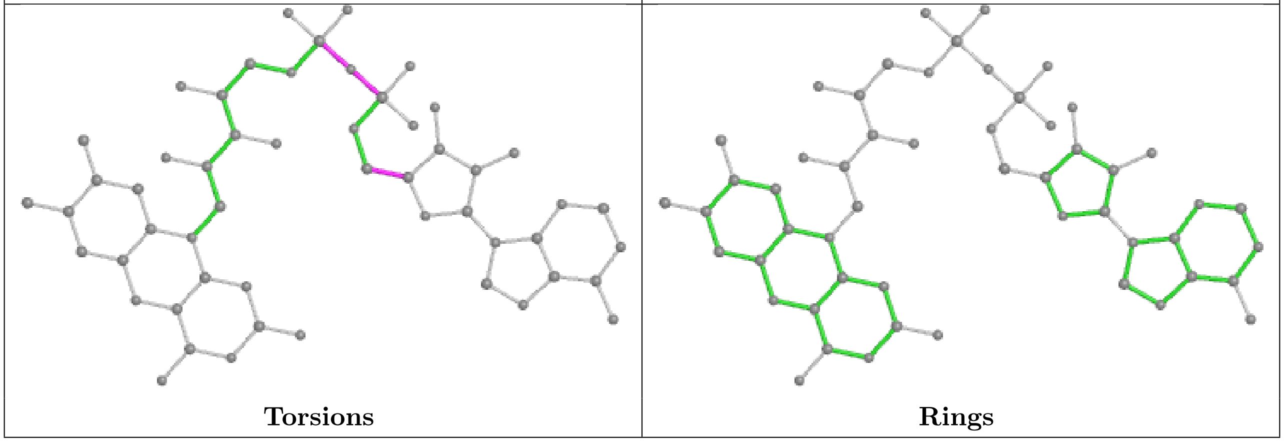
Rings

Ligand FAD F 7006



Bond lengths

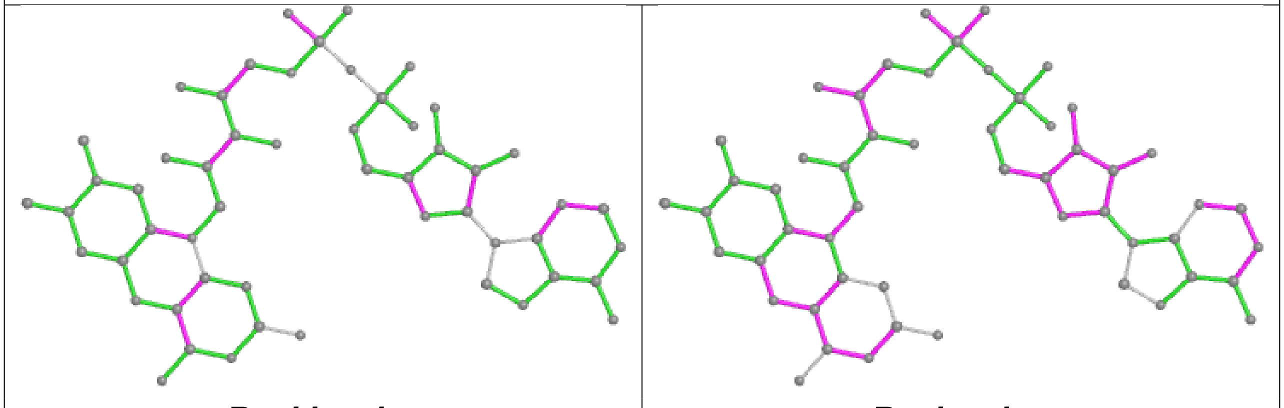
Bond angles



Torsions

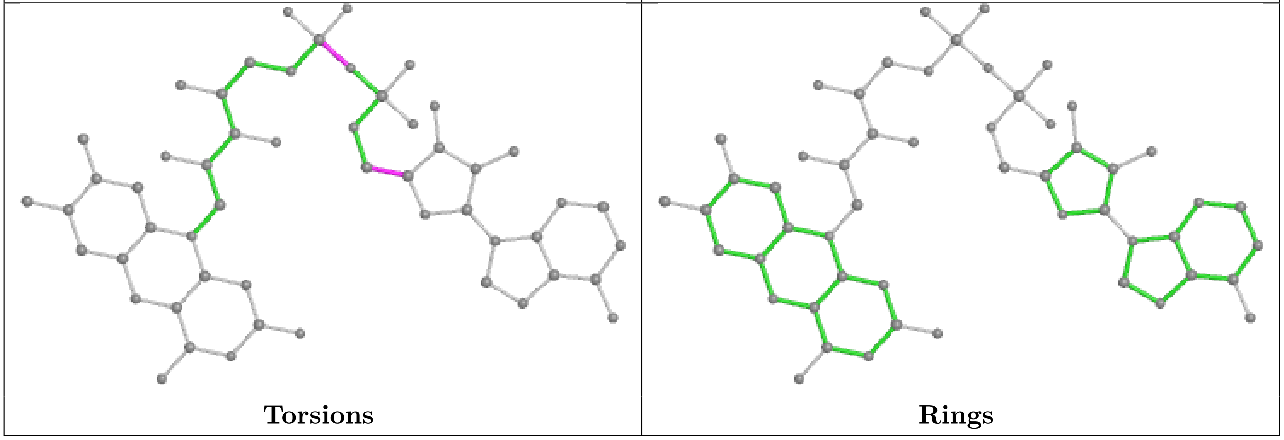
Rings

Ligand FAD G 7008



Bond lengths

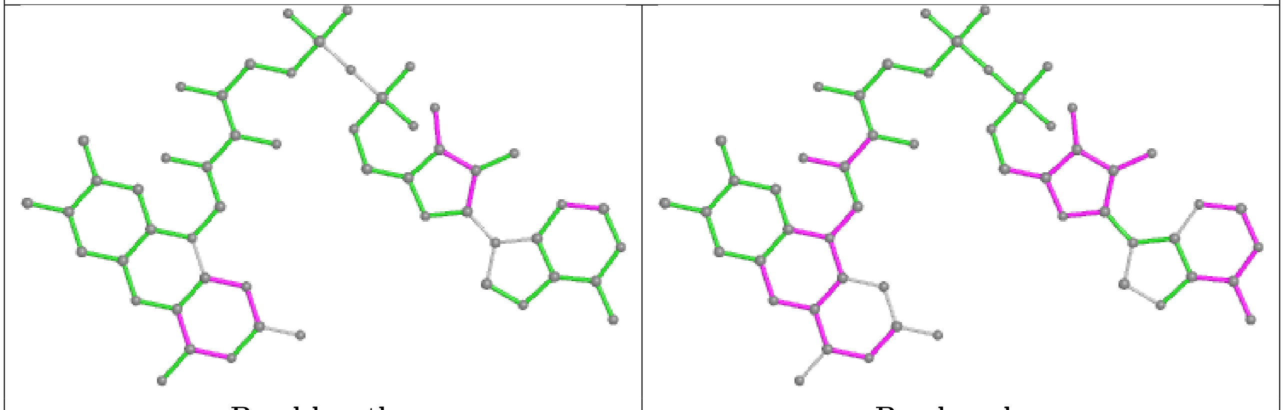
Bond angles



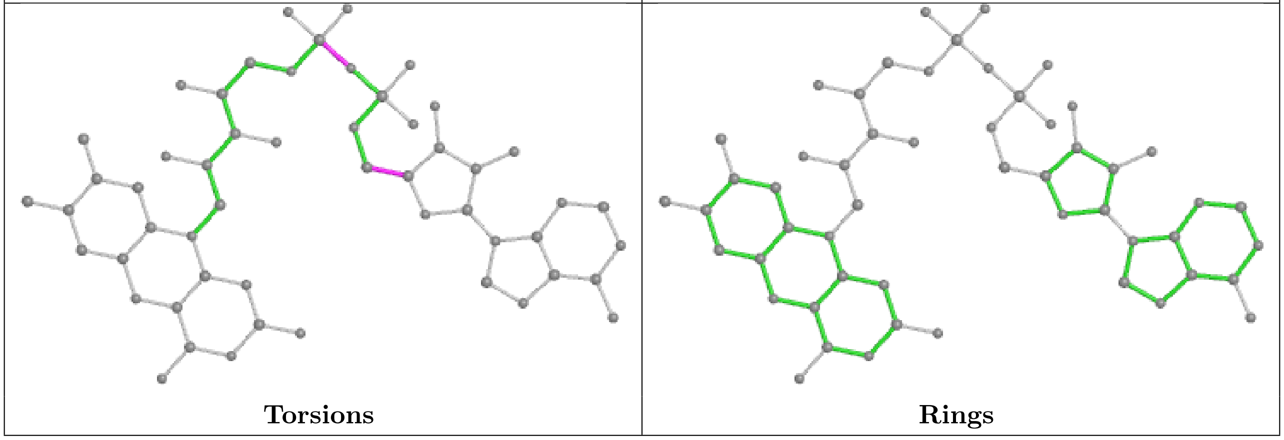
Torsions

Rings

Ligand FAD H 7007

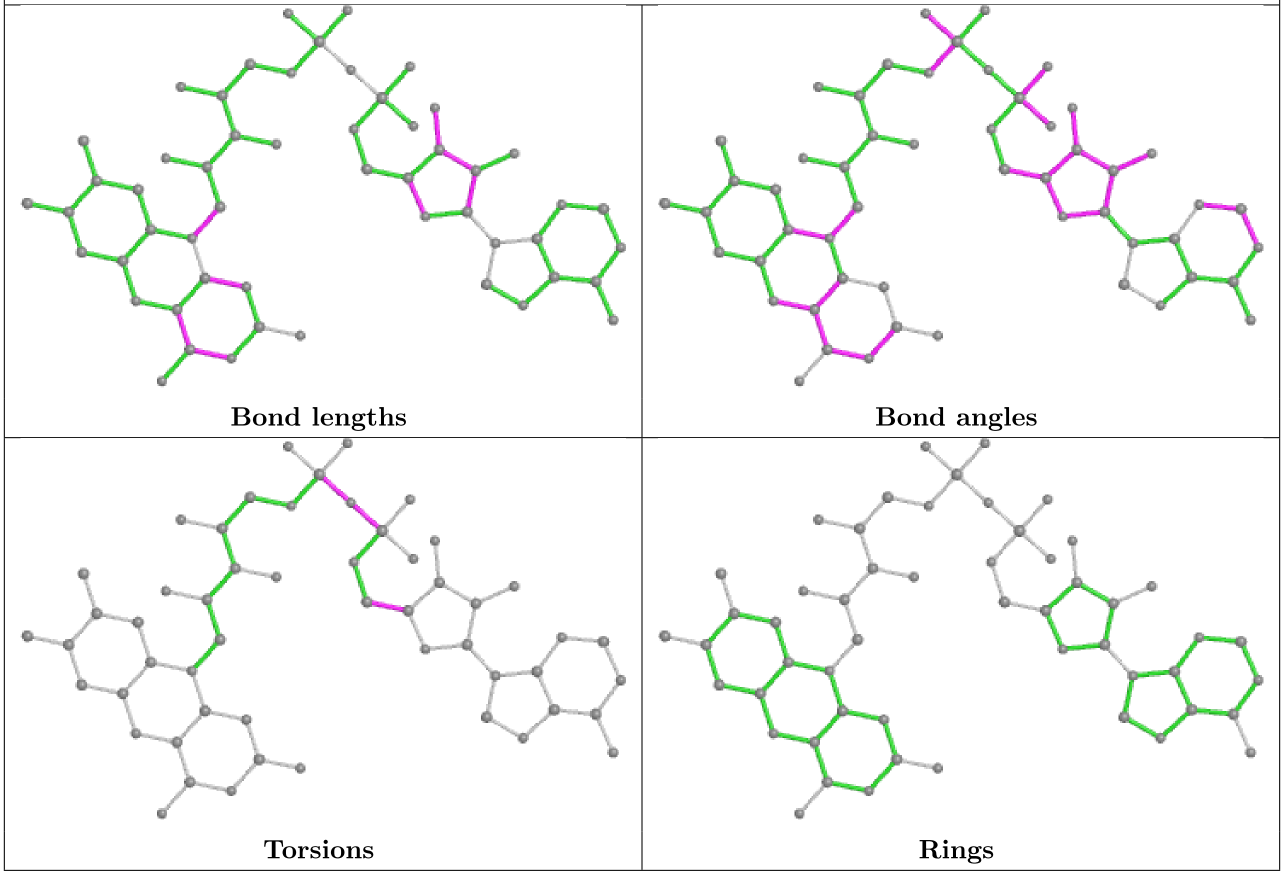


Bond lengths **Bond angles**



Torsions **Rings**

Ligand FAD D 7003



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.11	23 (3%)	38	38	11, 16, 37, 60	0
1	B	577/623 (92%)	-0.13	20 (3%)	44	45	11, 17, 36, 54	0
1	C	577/623 (92%)	0.13	30 (5%)	27	26	13, 23, 43, 64	0
1	D	577/623 (92%)	-0.02	25 (4%)	35	34	13, 21, 40, 59	0
1	E	577/623 (92%)	0.01	32 (5%)	25	24	14, 21, 41, 58	0
1	F	577/623 (92%)	0.04	29 (5%)	28	27	13, 23, 41, 61	0
1	G	577/623 (92%)	-0.08	25 (4%)	35	34	13, 18, 38, 57	0
1	H	577/623 (92%)	-0.19	20 (3%)	44	45	12, 18, 35, 55	0
All	All	4616/4984 (92%)	-0.04	204 (4%)	34	34	11, 20, 40, 64	0

All (204) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	619	THR	13.1
1	C	619	THR	12.7
1	H	619	THR	12.1
1	A	619	THR	11.7
1	E	619	THR	11.4
1	G	619	THR	10.2
1	F	343	ALA	9.3
1	F	619	THR	9.3
1	B	619	THR	9.2
1	C	389	LEU	8.6
1	C	618	PHE	8.3
1	G	45	ILE	7.7
1	B	618	PHE	7.7
1	C	45	ILE	7.6
1	G	343	ALA	7.4
1	H	343	ALA	7.3

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Mol	Chain	Res	Type	RSRZ
1	A	389	LEU	7.3
1	F	44	ASP	7.3
1	C	43	MET	7.1
1	B	343	ALA	7.1
1	A	343	ALA	7.0
1	G	43	MET	7.0
1	E	618	PHE	6.9
1	E	43	MET	6.8
1	G	389	LEU	6.8
1	E	385	THR	6.8
1	D	389	LEU	6.7
1	C	343	ALA	6.7
1	C	384	GLY	6.7
1	G	44	ASP	6.7
1	F	389	LEU	6.6
1	D	618	PHE	6.5
1	A	390	THR	6.5
1	C	44	ASP	6.5
1	E	384	GLY	6.5
1	F	43	MET	6.4
1	H	618	PHE	6.2
1	G	618	PHE	6.2
1	H	459	VAL	6.1
1	E	45	ILE	6.0
1	H	44	ASP	6.0
1	B	45	ILE	5.9
1	E	343	ALA	5.9
1	C	385	THR	5.8
1	B	43	MET	5.7
1	D	343	ALA	5.6
1	D	45	ILE	5.6
1	H	344	ASN	5.6
1	C	383	ARG	5.5
1	F	45	ILE	5.5
1	A	385	THR	5.4
1	D	44	ASP	5.4
1	H	43	MET	5.3
1	E	44	ASP	5.3
1	F	385	THR	5.3
1	D	43	MET	5.3
1	B	389	LEU	5.1
1	B	344	ASN	5.1

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Mol	Chain	Res	Type	RSRZ
1	E	344	ASN	5.0
1	F	344	ASN	4.9
1	F	618	PHE	4.9
1	A	43	MET	4.9
1	D	345	PRO	4.8
1	A	459	VAL	4.8
1	B	44	ASP	4.8
1	G	342	PRO	4.8
1	E	342	PRO	4.7
1	E	389	LEU	4.6
1	F	342	PRO	4.6
1	C	344	ASN	4.5
1	A	383	ARG	4.5
1	A	384	GLY	4.5
1	H	342	PRO	4.5
1	A	344	ASN	4.4
1	C	345	PRO	4.4
1	G	385	THR	4.4
1	C	617	PRO	4.3
1	D	388	GLU	4.3
1	E	388	GLU	4.3
1	G	344	ASN	4.3
1	C	388	GLU	4.3
1	E	345	PRO	4.2
1	A	618	PHE	4.2
1	D	385	THR	4.2
1	C	390	THR	4.0
1	F	383	ARG	4.0
1	E	459	VAL	4.0
1	H	345	PRO	4.0
1	H	341	ASN	3.9
1	B	342	PRO	3.9
1	G	458	ALA	3.9
1	A	388	GLU	3.8
1	A	342	PRO	3.8
1	D	390	THR	3.8
1	G	390	THR	3.8
1	G	459	VAL	3.8
1	F	341	ASN	3.8
1	F	309	PHE	3.7
1	F	390	THR	3.7
1	F	384	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	G	341	ASN	3.7
1	F	388	GLU	3.6
1	G	401	THR	3.6
1	F	345	PRO	3.6
1	E	390	THR	3.5
1	A	400	SER	3.5
1	G	388	GLU	3.5
1	E	386	PRO	3.5
1	B	341	ASN	3.5
1	D	344	ASN	3.5
1	A	345	PRO	3.4
1	A	382	ILE	3.4
1	B	383	ARG	3.4
1	D	342	PRO	3.4
1	C	272	GLU	3.4
1	G	345	PRO	3.4
1	D	272	GLU	3.3
1	B	345	PRO	3.3
1	D	617	PRO	3.3
1	H	458	ALA	3.3
1	H	45	ILE	3.2
1	F	347	GLU	3.2
1	C	342	PRO	3.2
1	E	617	PRO	3.2
1	D	384	GLY	3.2
1	A	341	ASN	3.2
1	A	44	ASP	3.1
1	B	309	PHE	3.1
1	C	341	ASN	3.1
1	C	459	VAL	3.1
1	F	458	ALA	3.0
1	B	385	THR	3.0
1	E	186	ASP	3.0
1	E	341	ASN	2.9
1	H	617	PRO	2.9
1	F	381	THR	2.9
1	D	383	ARG	2.9
1	H	186	ASP	2.8
1	E	458	ALA	2.8
1	C	392	SER	2.8
1	B	186	ASP	2.8
1	D	268	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	271	PRO	2.8
1	D	459	VAL	2.8
1	B	388	GLU	2.7
1	E	232	GLY	2.7
1	D	186	ASP	2.7
1	C	382	ILE	2.7
1	G	399	ALA	2.7
1	G	82	SER	2.7
1	E	268	THR	2.7
1	F	459	VAL	2.7
1	E	272	GLU	2.6
1	C	391	TYR	2.6
1	H	133	ALA	2.6
1	G	617	PRO	2.6
1	E	269	ASP	2.6
1	D	458	ALA	2.6
1	H	269	ASP	2.6
1	E	561	GLU	2.6
1	G	269	ASP	2.6
1	D	309	PHE	2.5
1	G	186	ASP	2.5
1	C	268	THR	2.5
1	B	459	VAL	2.5
1	C	400	SER	2.5
1	F	391	TYR	2.5
1	D	341	ASN	2.5
1	E	383	ARG	2.4
1	C	396	THR	2.4
1	D	382	ILE	2.4
1	E	309	PHE	2.4
1	E	490	LYS	2.4
1	B	133	ALA	2.4
1	F	272	GLU	2.4
1	H	271	PRO	2.4
1	C	458	ALA	2.4
1	C	309	PHE	2.4
1	G	400	SER	2.3
1	A	398	GLY	2.3
1	E	400	SER	2.3
1	E	299	HIS	2.3
1	A	45	ILE	2.3
1	F	271	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	387	GLY	2.3
1	C	387	GLY	2.3
1	E	392	SER	2.3
1	F	269	ASP	2.2
1	A	272	GLU	2.2
1	C	490	LYS	2.2
1	A	391	TYR	2.2
1	E	347	GLU	2.2
1	F	299	HIS	2.1
1	G	384	GLY	2.1
1	D	269	ASP	2.1
1	H	309	PHE	2.1
1	F	186	ASP	2.1
1	B	617	PRO	2.1
1	H	272	GLU	2.1
1	G	383	ARG	2.1
1	B	393	VAL	2.1
1	H	347	GLU	2.1
1	F	268	THR	2.1
1	F	561	GLU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
3	MES	E	8007	12/12	0.91	0.19	29,33,38,39	0
3	MES	G	8006	12/12	0.91	0.19	24,30,33,33	0
3	MES	B	8003	12/12	0.92	0.18	28,32,34,35	0

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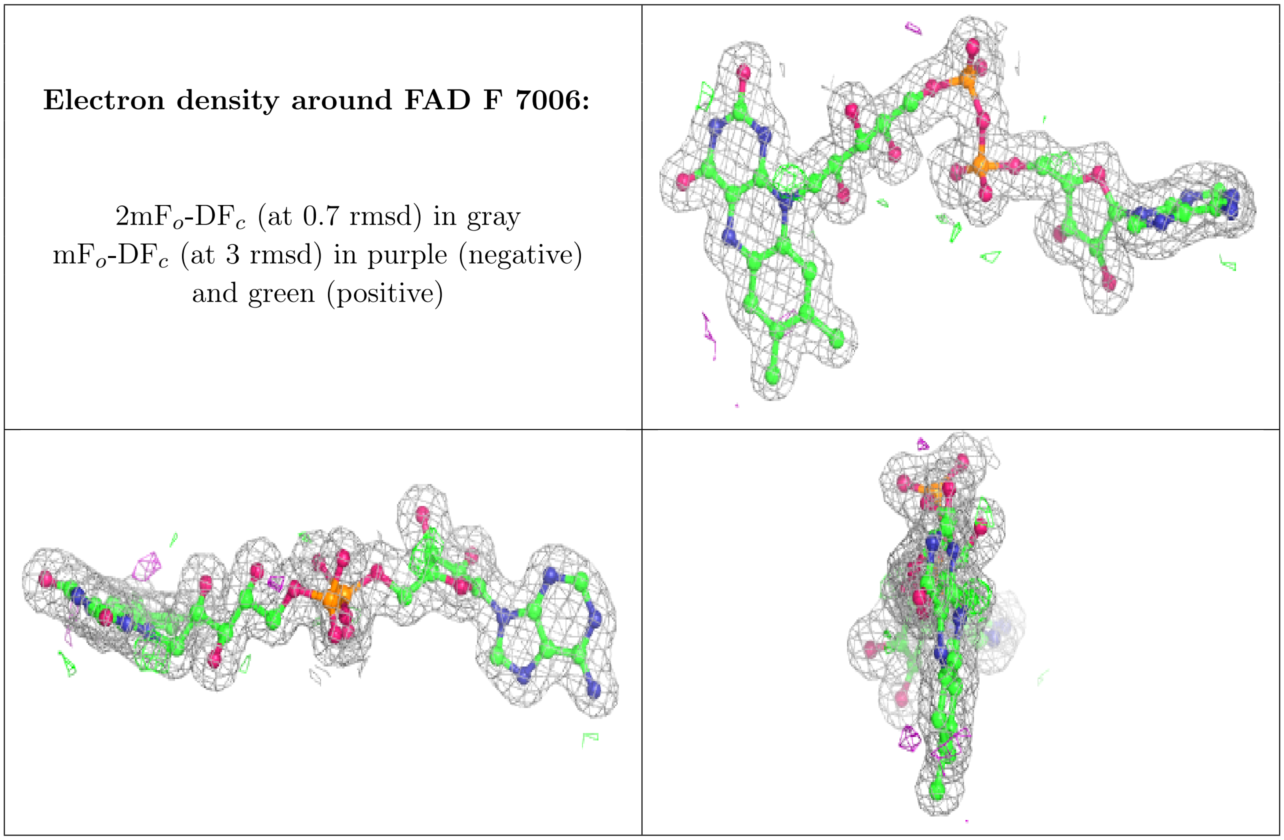
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MES	D	8005	12/12	0.93	0.17	30,32,34,36	0
3	MES	H	8004	12/12	0.93	0.17	27,33,34,35	0
3	MES	C	8008	12/12	0.93	0.19	27,32,38,39	0
3	MES	A	8002	12/12	0.97	0.14	22,26,28,28	0
3	MES	F	8001	12/12	0.97	0.10	20,22,24,25	0
2	FAD	F	7006	53/53	0.98	0.10	14,17,20,22	0
2	FAD	G	7008	53/53	0.98	0.09	11,14,15,17	0
2	FAD	D	7003	53/53	0.98	0.10	14,17,19,22	0
2	FAD	C	7004	53/53	0.98	0.09	15,18,22,22	0
2	FAD	E	7005	53/53	0.98	0.09	15,17,20,21	0
2	FAD	A	7001	53/53	0.99	0.09	10,12,14,16	0
2	FAD	B	7002	53/53	0.99	0.09	10,13,16,20	0
2	FAD	H	7007	53/53	0.99	0.09	10,14,17,19	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.

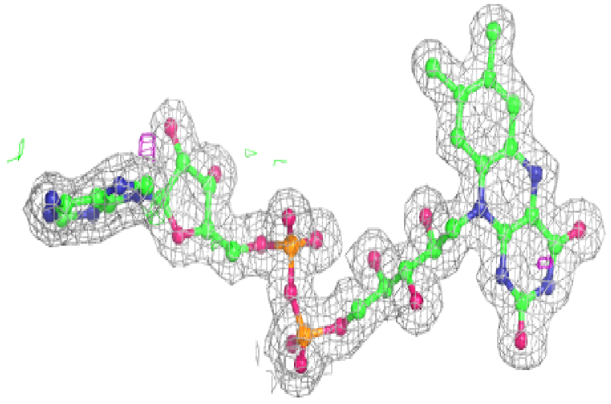


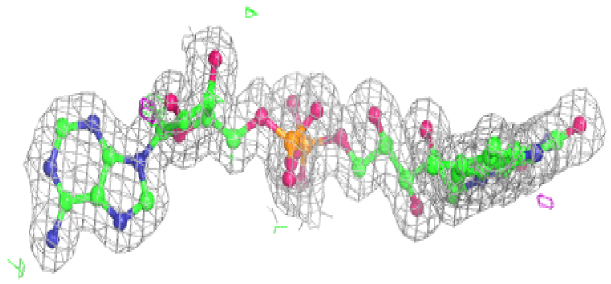
Electron density around FAD F 7006:

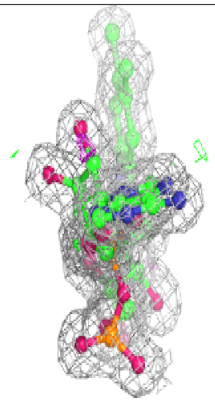
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around FAD G 7008:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

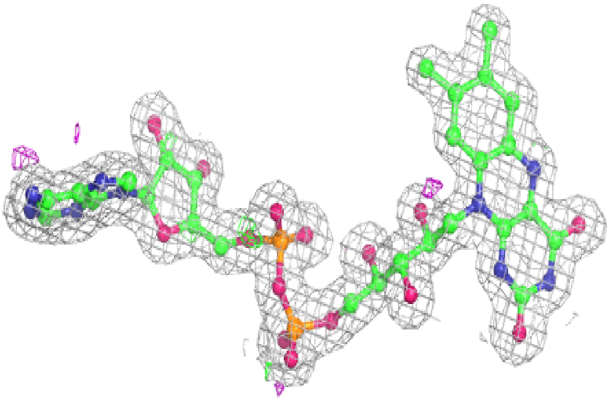


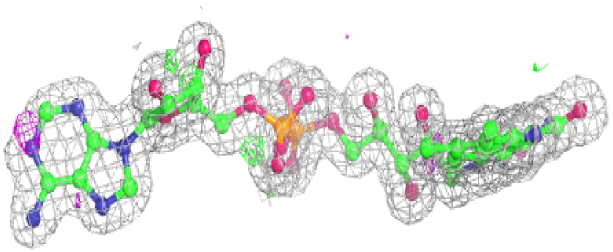


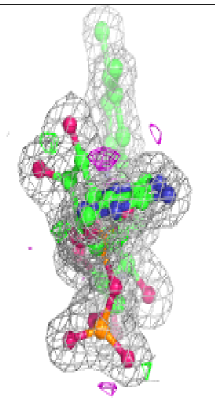


Electron density around FAD D 7003:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

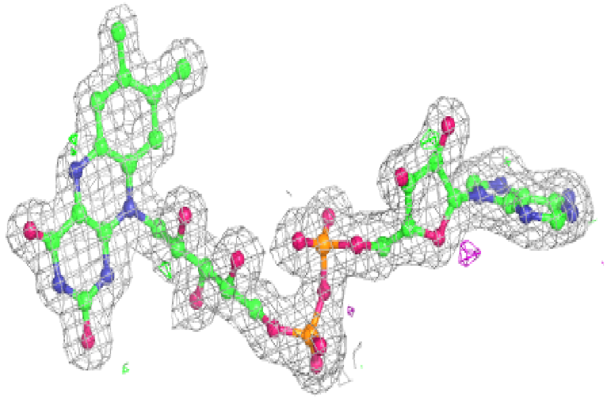


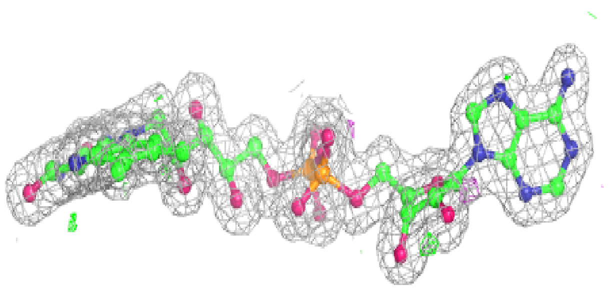


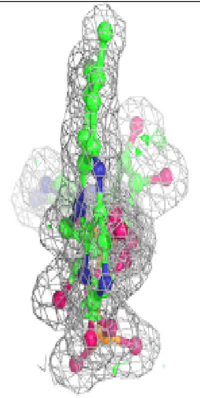


Electron density around FAD C 7004:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

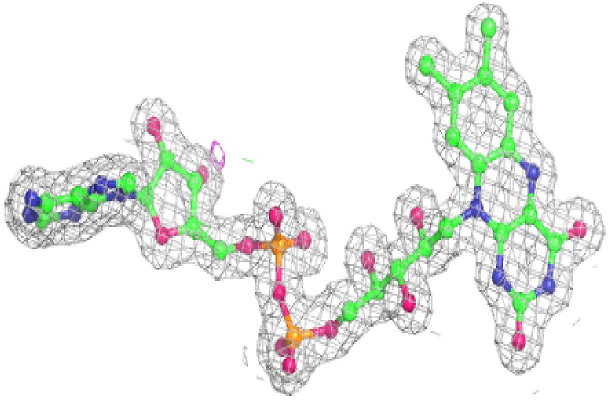


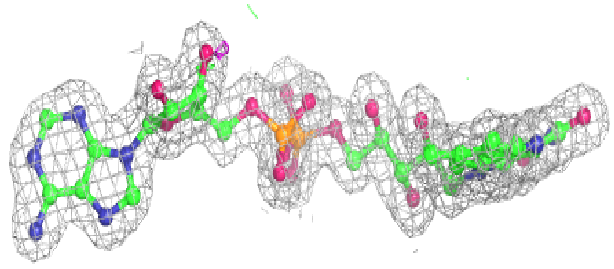


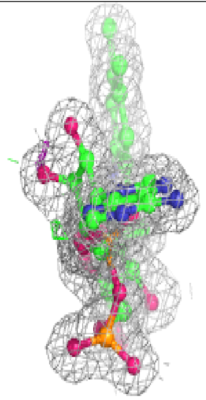


Electron density around FAD E 7005:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

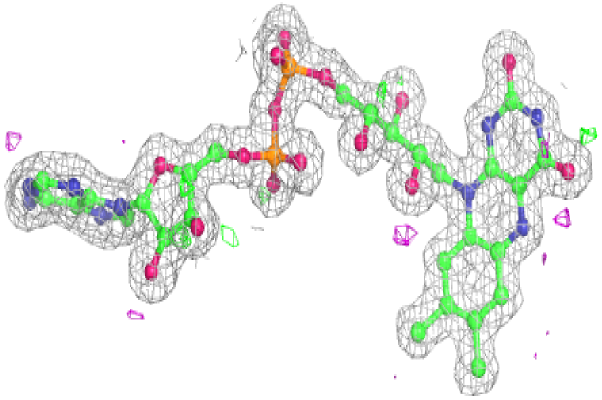


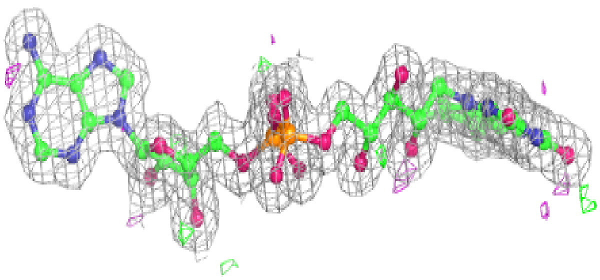


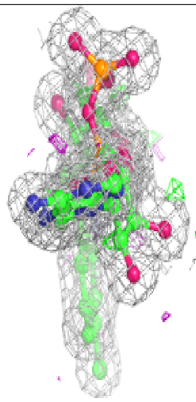


Electron density around FAD A 7001:

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

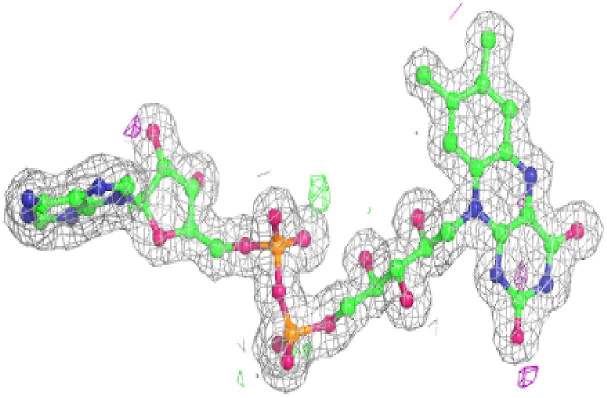


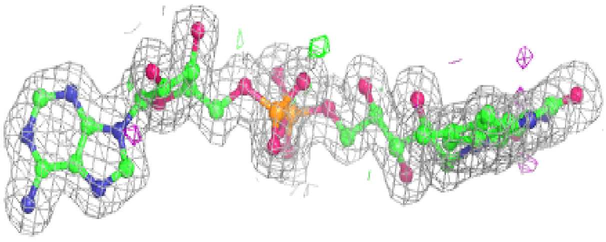


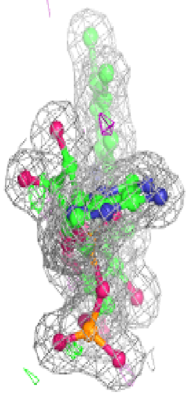


Electron density around FAD B 7002:

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

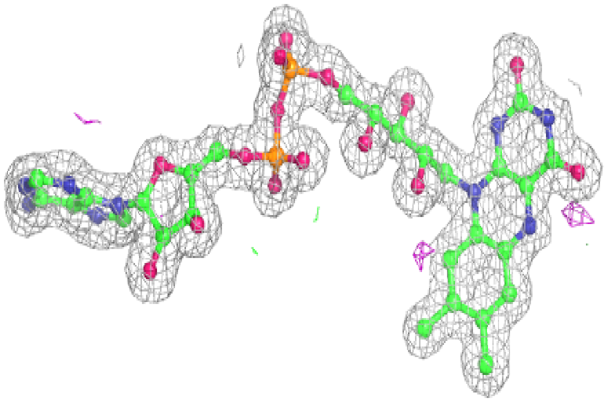


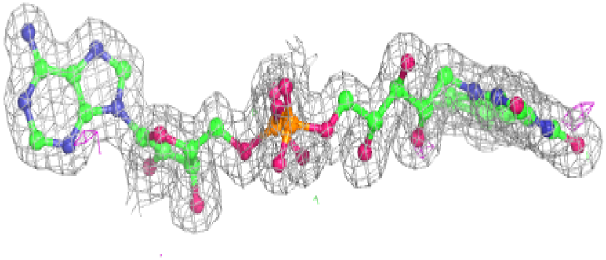


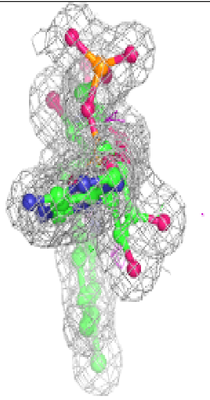


Electron density around FAD H 7007:

$2mF_o$-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

There are no such residues in this entry.