



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:49 AM UTC

PDB ID : 1TZL / pdb_00001tzt
Title : Crystal Structure of Pyranose 2-Oxidase from the White-Rot Fungus *Peniophora* sp.
Authors : Bannwarth, M.; Bastian, S.; Heckmann-Pohl, D.; Giffhorn, F.; Schulz, G.E.
Deposited on : 2004-07-10
Resolution : 2.35 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

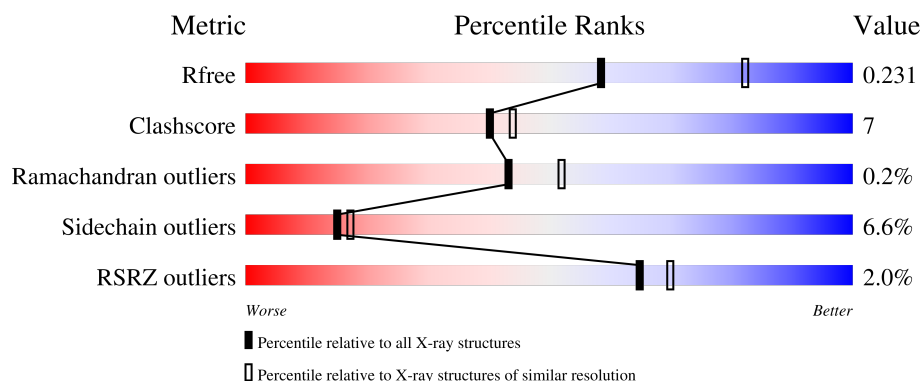
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	622	78% 13% • 7%
1	B	622	66% 22% • • 7%
1	C	622	81% 11% • 7%
1	D	622	78% 14% • 7%
1	E	622	77% 14% • 7%

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Mol	Chain	Length	Quality of chain
1	F	622	% 77% 14% • 7%
1	G	622	2% 78% 13% • 7%
1	H	622	2% 79% 12% • 7%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 38970 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	C	N	O	S	Se	0	0	0
			4549	2872	778	874	9	16			
1	B	577	Total	C	N	O	S	Se	0	0	0
			4549	2872	778	874	9	16			
1	C	577	Total	C	N	O	S	Se	0	0	0
			4549	2872	778	874	9	16			
1	D	577	Total	C	N	O	S	Se	0	0	0
			4549	2872	778	874	9	16			
1	E	577	Total	C	N	O	S	Se	0	0	0
			4549	2872	778	874	9	16			
1	F	577	Total	C	N	O	S	Se	0	0	0
			4549	2872	778	874	9	16			
1	G	577	Total	C	N	O	S	Se	0	0	0
			4549	2872	778	874	9	16			
1	H	577	Total	C	N	O	S	Se	0	0	0
			4549	2872	778	874	9	16			

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	MSE	MET	modified residue	UNP Q8J136
A	74	MSE	MET	modified residue	UNP Q8J136
A	112	MSE	MET	modified residue	UNP Q8J136
A	164	MSE	MET	modified residue	UNP Q8J136
A	368	MSE	MET	modified residue	UNP Q8J136
A	380	MSE	MET	modified residue	UNP Q8J136
A	416	MSE	MET	modified residue	UNP Q8J136
A	417	MSE	MET	modified residue	UNP Q8J136
A	497	MSE	MET	modified residue	UNP Q8J136
A	518	MSE	MET	modified residue	UNP Q8J136
A	519	MSE	MET	modified residue	UNP Q8J136
A	522	MSE	MET	modified residue	UNP Q8J136
A	525	MSE	MET	modified residue	UNP Q8J136

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Chain	Residue	Modelled	Actual	Comment	Reference
A	541	MSE	MET	modified residue	UNP Q8J136
A	555	MSE	MET	modified residue	UNP Q8J136
A	599	MSE	MET	modified residue	UNP Q8J136
B	43	MSE	MET	modified residue	UNP Q8J136
B	74	MSE	MET	modified residue	UNP Q8J136
B	112	MSE	MET	modified residue	UNP Q8J136
B	164	MSE	MET	modified residue	UNP Q8J136
B	368	MSE	MET	modified residue	UNP Q8J136
B	380	MSE	MET	modified residue	UNP Q8J136
B	416	MSE	MET	modified residue	UNP Q8J136
B	417	MSE	MET	modified residue	UNP Q8J136
B	497	MSE	MET	modified residue	UNP Q8J136
B	518	MSE	MET	modified residue	UNP Q8J136
B	519	MSE	MET	modified residue	UNP Q8J136
B	522	MSE	MET	modified residue	UNP Q8J136
B	525	MSE	MET	modified residue	UNP Q8J136
B	541	MSE	MET	modified residue	UNP Q8J136
B	555	MSE	MET	modified residue	UNP Q8J136
B	599	MSE	MET	modified residue	UNP Q8J136
C	43	MSE	MET	modified residue	UNP Q8J136
C	74	MSE	MET	modified residue	UNP Q8J136
C	112	MSE	MET	modified residue	UNP Q8J136
C	164	MSE	MET	modified residue	UNP Q8J136
C	368	MSE	MET	modified residue	UNP Q8J136
C	380	MSE	MET	modified residue	UNP Q8J136
C	416	MSE	MET	modified residue	UNP Q8J136
C	417	MSE	MET	modified residue	UNP Q8J136
C	497	MSE	MET	modified residue	UNP Q8J136
C	518	MSE	MET	modified residue	UNP Q8J136
C	519	MSE	MET	modified residue	UNP Q8J136
C	522	MSE	MET	modified residue	UNP Q8J136
C	525	MSE	MET	modified residue	UNP Q8J136
C	541	MSE	MET	modified residue	UNP Q8J136
C	555	MSE	MET	modified residue	UNP Q8J136
C	599	MSE	MET	modified residue	UNP Q8J136
D	43	MSE	MET	modified residue	UNP Q8J136
D	74	MSE	MET	modified residue	UNP Q8J136
D	112	MSE	MET	modified residue	UNP Q8J136
D	164	MSE	MET	modified residue	UNP Q8J136
D	368	MSE	MET	modified residue	UNP Q8J136
D	380	MSE	MET	modified residue	UNP Q8J136
D	416	MSE	MET	modified residue	UNP Q8J136

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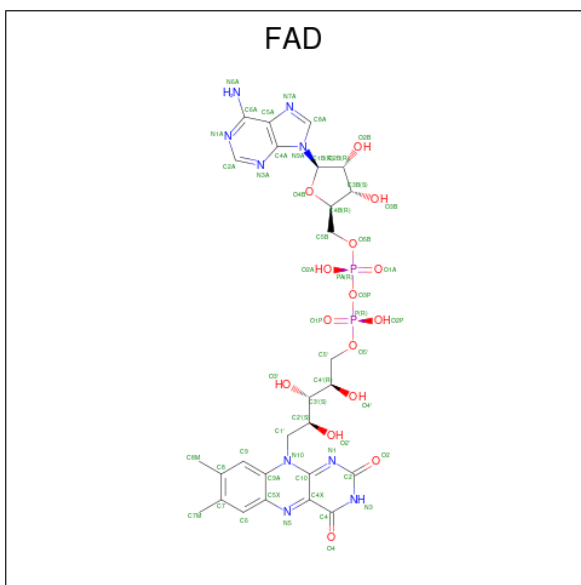
Chain	Residue	Modelled	Actual	Comment	Reference
D	417	MSE	MET	modified residue	UNP Q8J136
D	497	MSE	MET	modified residue	UNP Q8J136
D	518	MSE	MET	modified residue	UNP Q8J136
D	519	MSE	MET	modified residue	UNP Q8J136
D	522	MSE	MET	modified residue	UNP Q8J136
D	525	MSE	MET	modified residue	UNP Q8J136
D	541	MSE	MET	modified residue	UNP Q8J136
D	555	MSE	MET	modified residue	UNP Q8J136
D	599	MSE	MET	modified residue	UNP Q8J136
E	43	MSE	MET	modified residue	UNP Q8J136
E	74	MSE	MET	modified residue	UNP Q8J136
E	112	MSE	MET	modified residue	UNP Q8J136
E	164	MSE	MET	modified residue	UNP Q8J136
E	368	MSE	MET	modified residue	UNP Q8J136
E	380	MSE	MET	modified residue	UNP Q8J136
E	416	MSE	MET	modified residue	UNP Q8J136
E	417	MSE	MET	modified residue	UNP Q8J136
E	497	MSE	MET	modified residue	UNP Q8J136
E	518	MSE	MET	modified residue	UNP Q8J136
E	519	MSE	MET	modified residue	UNP Q8J136
E	522	MSE	MET	modified residue	UNP Q8J136
E	525	MSE	MET	modified residue	UNP Q8J136
E	541	MSE	MET	modified residue	UNP Q8J136
E	555	MSE	MET	modified residue	UNP Q8J136
E	599	MSE	MET	modified residue	UNP Q8J136
F	43	MSE	MET	modified residue	UNP Q8J136
F	74	MSE	MET	modified residue	UNP Q8J136
F	112	MSE	MET	modified residue	UNP Q8J136
F	164	MSE	MET	modified residue	UNP Q8J136
F	368	MSE	MET	modified residue	UNP Q8J136
F	380	MSE	MET	modified residue	UNP Q8J136
F	416	MSE	MET	modified residue	UNP Q8J136
F	417	MSE	MET	modified residue	UNP Q8J136
F	497	MSE	MET	modified residue	UNP Q8J136
F	518	MSE	MET	modified residue	UNP Q8J136
F	519	MSE	MET	modified residue	UNP Q8J136
F	522	MSE	MET	modified residue	UNP Q8J136
F	525	MSE	MET	modified residue	UNP Q8J136
F	541	MSE	MET	modified residue	UNP Q8J136
F	555	MSE	MET	modified residue	UNP Q8J136
F	599	MSE	MET	modified residue	UNP Q8J136
G	43	MSE	MET	modified residue	UNP Q8J136

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Chain	Residue	Modelled	Actual	Comment	Reference
G	74	MSE	MET	modified residue	UNP Q8J136
G	112	MSE	MET	modified residue	UNP Q8J136
G	164	MSE	MET	modified residue	UNP Q8J136
G	368	MSE	MET	modified residue	UNP Q8J136
G	380	MSE	MET	modified residue	UNP Q8J136
G	416	MSE	MET	modified residue	UNP Q8J136
G	417	MSE	MET	modified residue	UNP Q8J136
G	497	MSE	MET	modified residue	UNP Q8J136
G	518	MSE	MET	modified residue	UNP Q8J136
G	519	MSE	MET	modified residue	UNP Q8J136
G	522	MSE	MET	modified residue	UNP Q8J136
G	525	MSE	MET	modified residue	UNP Q8J136
G	541	MSE	MET	modified residue	UNP Q8J136
G	555	MSE	MET	modified residue	UNP Q8J136
G	599	MSE	MET	modified residue	UNP Q8J136
H	43	MSE	MET	modified residue	UNP Q8J136
H	74	MSE	MET	modified residue	UNP Q8J136
H	112	MSE	MET	modified residue	UNP Q8J136
H	164	MSE	MET	modified residue	UNP Q8J136
H	368	MSE	MET	modified residue	UNP Q8J136
H	380	MSE	MET	modified residue	UNP Q8J136
H	416	MSE	MET	modified residue	UNP Q8J136
H	417	MSE	MET	modified residue	UNP Q8J136
H	497	MSE	MET	modified residue	UNP Q8J136
H	518	MSE	MET	modified residue	UNP Q8J136
H	519	MSE	MET	modified residue	UNP Q8J136
H	522	MSE	MET	modified residue	UNP Q8J136
H	525	MSE	MET	modified residue	UNP Q8J136
H	541	MSE	MET	modified residue	UNP Q8J136
H	555	MSE	MET	modified residue	UNP Q8J136
H	599	MSE	MET	modified residue	UNP Q8J136

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



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	290	Total O 290 290	0	0
3	B	221	Total O 221 221	0	0
3	C	274	Total O 274 274	0	0
3	D	172	Total O 172 172	0	0

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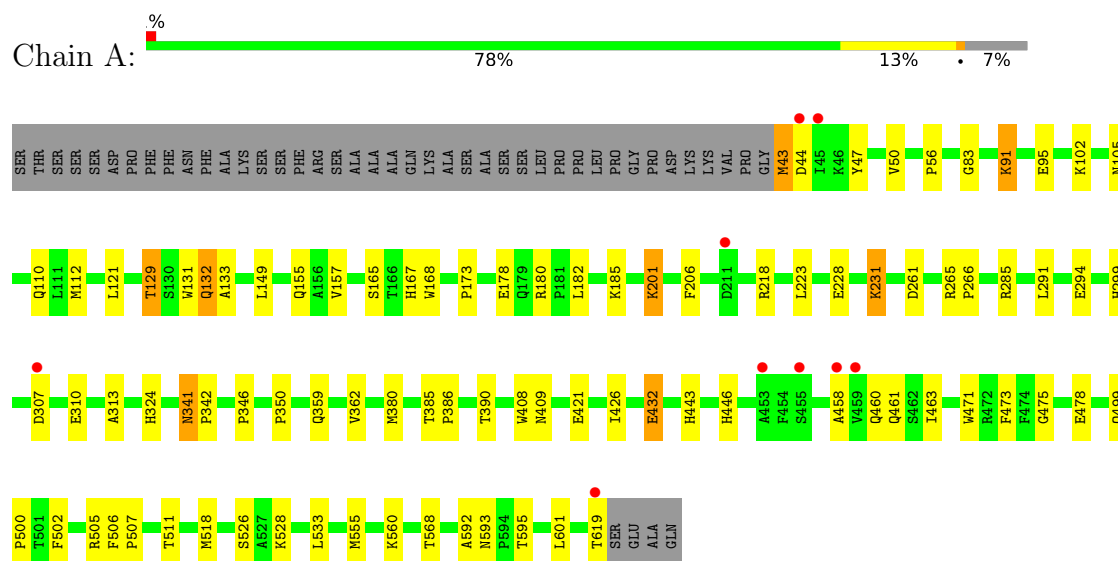
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	303	Total 303	O 303	0	0
3	F	317	Total 317	O 317	0	0
3	G	251	Total 251	O 251	0	0
3	H	326	Total 326	O 326	0	0

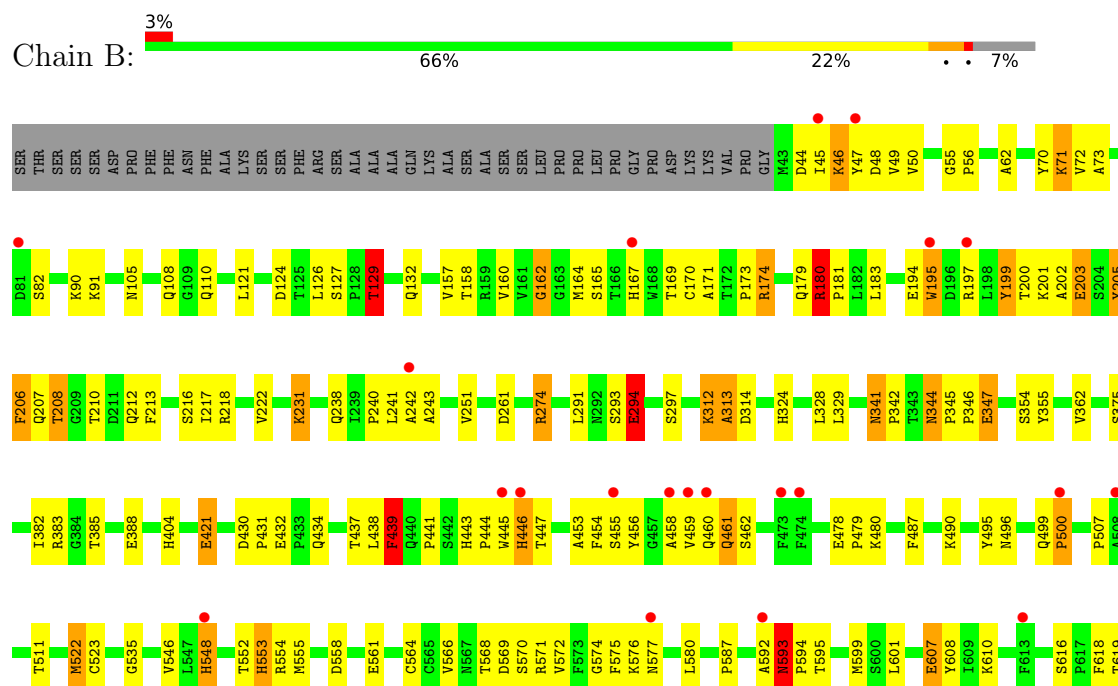
3 Residue-property plots [i](#)

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

• Molecule 1: pyranose oxidase



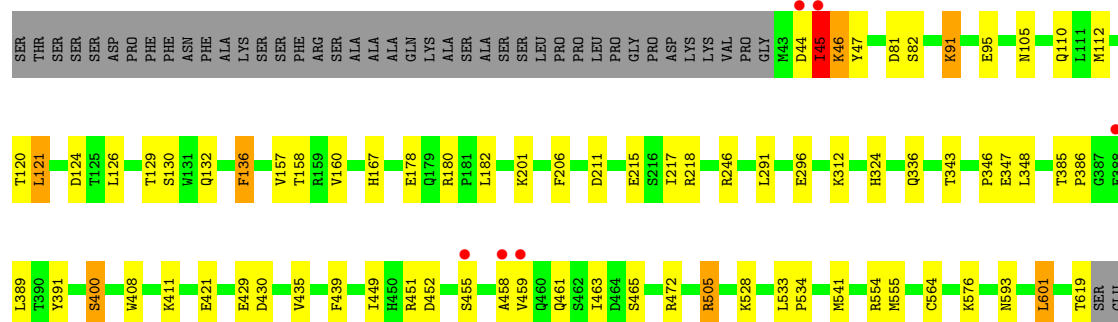
• Molecule 1: pyranose oxidase



SER
GLU
ALA
GLN

- Molecule 1: pyranose oxidase

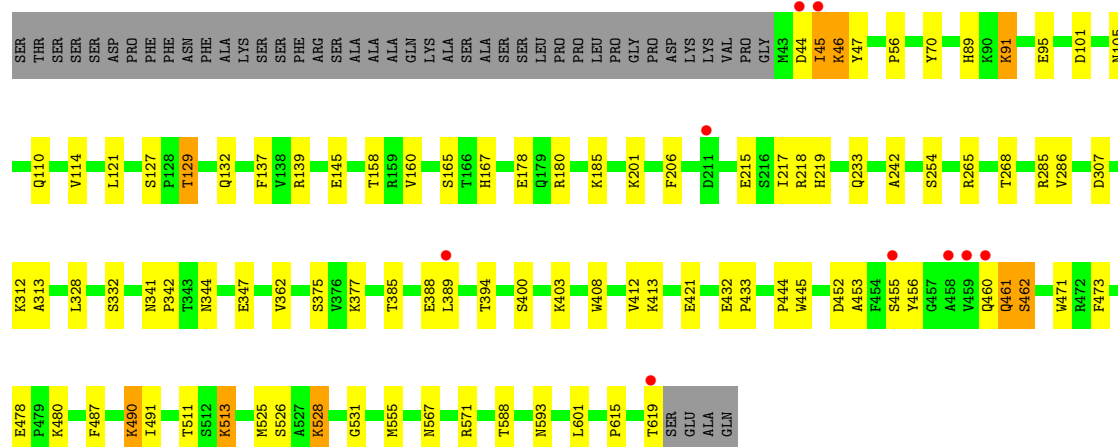
Chain C:  %



ALA
GLN

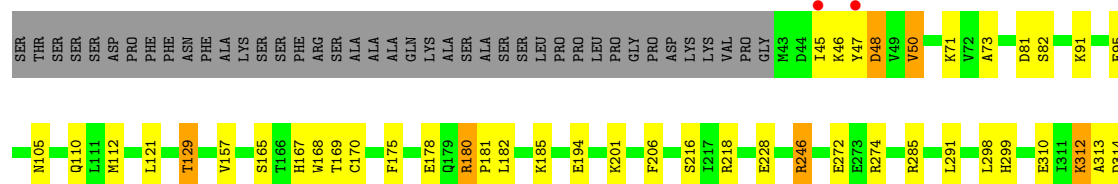
- Molecule 1: pyranose oxidase

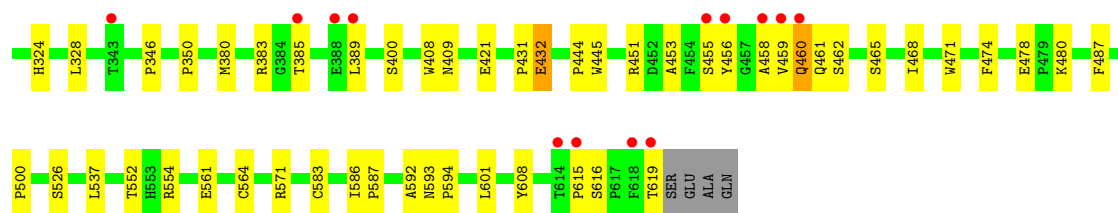
Chain D:  %



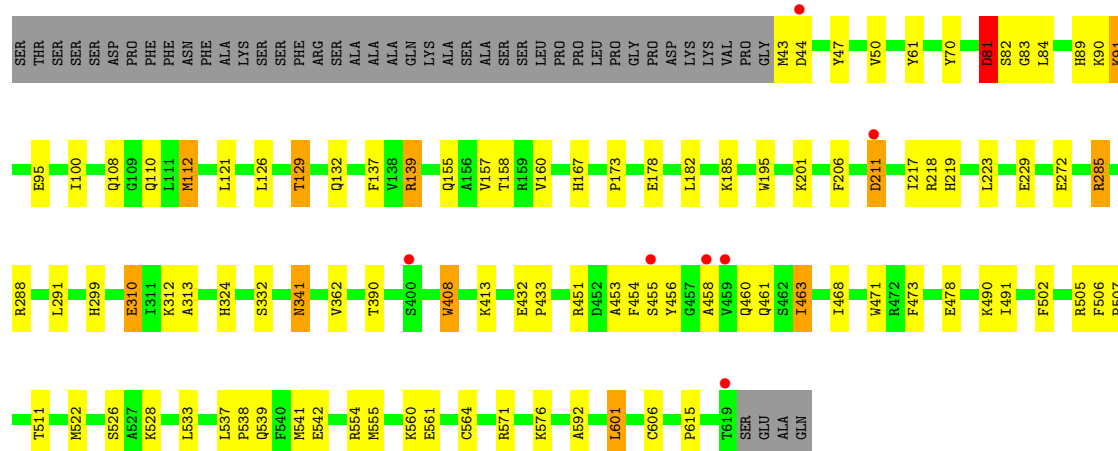
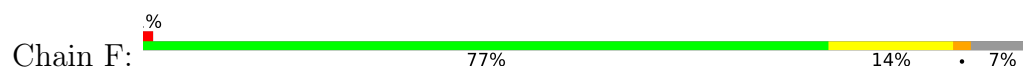
- Molecule 1: pyranose oxidase

Chain E:  %

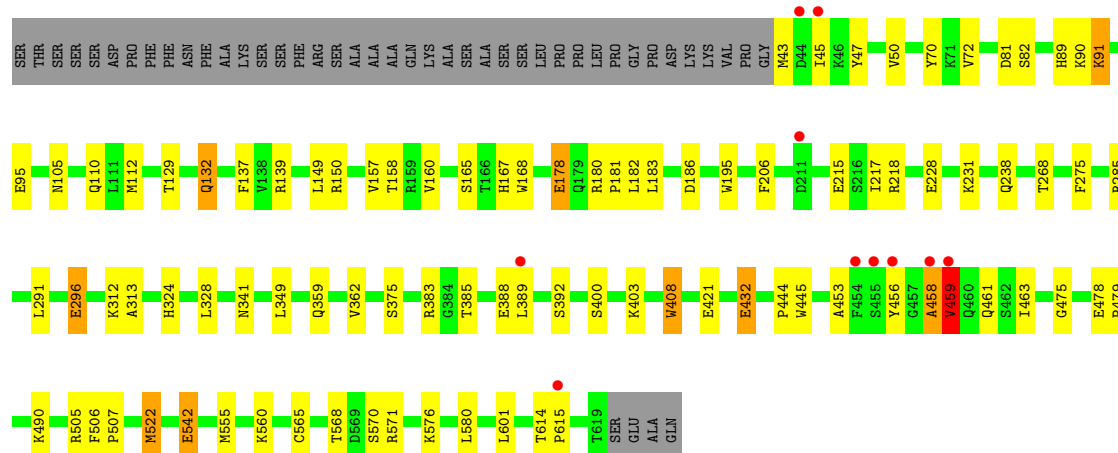
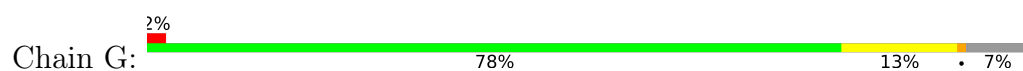




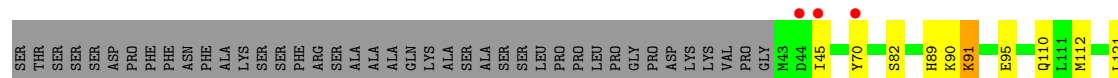
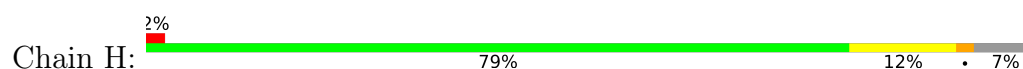
• Molecule 1: pyranose oxidase

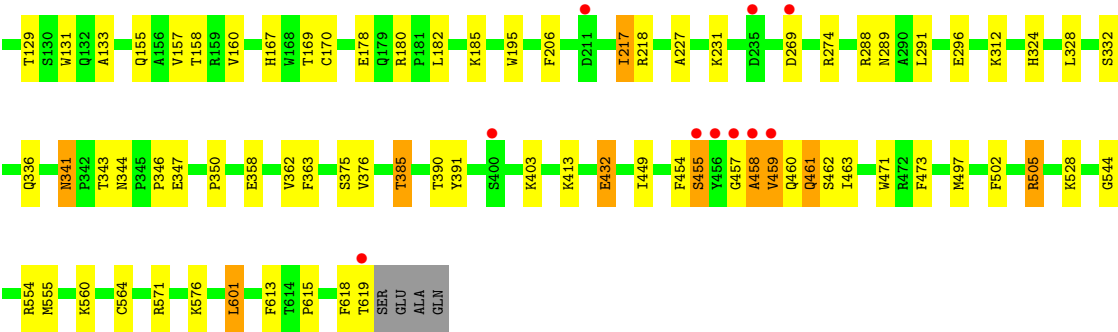


• Molecule 1: pyranose oxidase



• Molecule 1: pyranose oxidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	164.88Å 103.60Å 169.17Å 90.00° 105.25° 90.00°	Depositor
Resolution (Å)	19.70 – 2.35 19.70 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.70-2.35) 99.8 (19.70-2.35)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.96 (at 2.35Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.174 , 0.226 0.196 , 0.231	Depositor DCC
R_{free} test set	9088 reflections (3.98%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.624	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	38970	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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 47.06 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0477e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.84	2/4650 (0.0%)	0.98	3/6298 (0.0%)
1	B	1.40	59/4650 (1.3%)	1.21	17/6298 (0.3%)
1	C	0.82	2/4650 (0.0%)	0.95	0/6298
1	D	0.73	0/4650	0.95	2/6298 (0.0%)
1	E	0.99	6/4650 (0.1%)	1.03	5/6298 (0.1%)
1	F	0.86	1/4650 (0.0%)	0.99	3/6298 (0.0%)
1	G	0.84	1/4650 (0.0%)	0.98	2/6298 (0.0%)
1	H	0.89	1/4650 (0.0%)	1.00	4/6298 (0.1%)
All	All	0.94	72/37200 (0.2%)	1.01	36/50384 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	203	GLU	N-CA	13.22	1.63	1.46
1	B	195	TRP	CD2-CE3	12.57	1.60	1.40
1	B	197	ARG	NE-CZ	12.44	1.46	1.33
1	B	241	LEU	N-CA	11.12	1.59	1.46
1	B	274	ARG	NE-CZ	10.20	1.44	1.33
1	B	194	GLU	CA-C	9.70	1.65	1.52
1	B	313	ALA	N-CA	9.58	1.57	1.46
1	B	608	TYR	CG-CD1	9.56	1.59	1.39
1	B	194	GLU	N-CA	9.08	1.57	1.46
1	B	553	HIS	C-N	9.06	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	48	ASP	N-CA	9.03	1.57	1.46
1	B	242	ALA	CA-C	8.93	1.64	1.52
1	B	197	ARG	CD-NE	8.56	1.58	1.46
1	E	314	ASP	N-CA	7.88	1.56	1.46
1	B	195	TRP	CZ2-CH2	7.84	1.52	1.37
1	B	162	GLY	CA-C	7.77	1.62	1.51
1	B	313	ALA	CA-CB	7.56	1.66	1.53
1	B	180	ARG	CA-C	7.54	1.61	1.52
1	E	608	TYR	CE2-CZ	7.34	1.55	1.38
1	B	199	TYR	CG-CD1	7.29	1.54	1.39
1	B	548	HIS	CA-CB	7.26	1.63	1.53
1	B	195	TRP	CA-C	7.25	1.62	1.52
1	G	522	MSE	SE-CE	-7.22	1.73	1.95
1	B	202	ALA	N-CA	7.22	1.55	1.46
1	B	195	TRP	C-O	6.97	1.33	1.24
1	B	608	TYR	CE2-CZ	6.94	1.54	1.38
1	B	48	ASP	CB-CG	6.88	1.69	1.52
1	E	608	TYR	CG-CD1	6.82	1.53	1.39
1	B	195	TRP	NE1-CE2	6.79	1.45	1.37
1	B	207	GLN	C-O	6.68	1.32	1.23
1	B	568	THR	C-N	6.65	1.43	1.33
1	B	197	ARG	CG-CD	6.65	1.72	1.52
1	B	548	HIS	N-CA	6.63	1.54	1.46
1	B	522	MSE	N-CA	6.37	1.54	1.46
1	B	523	CYS	N-CA	6.26	1.53	1.46
1	B	447	THR	N-CA	6.23	1.53	1.45
1	B	199	TYR	CE2-CZ	6.21	1.53	1.38
1	B	171	ALA	CA-CB	-6.20	1.44	1.53
1	B	179	GLN	N-CA	6.13	1.54	1.45
1	B	71	LYS	CA-C	5.97	1.60	1.52
1	B	552	THR	N-CA	5.94	1.53	1.46
1	B	593	ASN	CA-C	5.90	1.60	1.52
1	A	446	HIS	CG-CD2	5.86	1.42	1.35
1	B	174	ARG	NE-CZ	5.83	1.39	1.33
1	B	62	ALA	C-O	5.82	1.30	1.24
1	B	208	THR	CB-OG1	5.71	1.52	1.43
1	E	194	GLU	CA-C	5.66	1.60	1.52
1	B	576	LYS	CA-C	5.63	1.60	1.52
1	B	439	PHE	CA-C	5.57	1.60	1.52
1	B	438	LEU	CA-CB	5.55	1.62	1.53
1	B	171	ALA	CA-C	5.52	1.60	1.52
1	B	294	GLU	N-CA	5.51	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	112	MSE	SE-CE	5.51	2.12	1.95
1	E	48	ASP	CA-C	-5.46	1.45	1.52
1	B	569	ASP	CG-OD2	5.46	1.35	1.25
1	B	314	ASP	N-CA	5.42	1.53	1.46
1	B	572	VAL	N-CA	5.39	1.52	1.46
1	B	294	GLU	CA-CB	5.39	1.62	1.53
1	B	241	LEU	CA-CB	5.38	1.63	1.53
1	B	205	TYR	N-CA	5.38	1.53	1.46
1	B	500	PRO	CA-C	5.37	1.59	1.52
1	B	48	ASP	N-CA	5.36	1.53	1.46
1	B	572	VAL	CA-C	5.35	1.58	1.52
1	B	48	ASP	CG-OD2	5.34	1.35	1.25
1	B	129	THR	CA-C	5.19	1.59	1.52
1	B	607	GLU	CG-CD	5.18	1.65	1.52
1	C	130	SER	C-O	5.17	1.30	1.23
1	B	593	ASN	CG-ND2	5.14	1.44	1.33
1	B	587	PRO	CA-C	5.12	1.58	1.52
1	A	446	HIS	CA-C	5.12	1.59	1.52
1	C	136	PHE	CG-CD1	5.09	1.49	1.38
1	H	227	ALA	CA-CB	5.03	1.61	1.53

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	314	ASP	N-CA-C	-8.71	101.50	112.90
1	B	552	THR	N-CA-C	7.75	120.71	111.33
1	E	552	THR	N-CA-C	7.55	120.39	111.71
1	E	48	ASP	N-CA-C	-7.35	103.35	111.36
1	H	461	GLN	N-CA-C	-7.16	104.97	113.21
1	B	203	GLU	N-CA-C	-6.98	103.44	112.23
1	B	314	ASP	N-CA-C	-6.92	102.83	112.45
1	B	222	VAL	N-CA-C	6.84	116.99	110.42
1	H	455	SER	N-CA-C	6.61	119.28	111.02
1	G	458	ALA	N-CA-C	6.50	118.24	110.44
1	B	595	THR	N-CA-C	6.27	117.78	111.07
1	A	426	ILE	N-CA-C	6.25	114.00	108.63
1	F	81	ASP	CB-CA-C	-6.23	102.67	111.65
1	B	593	ASN	CA-C-N	6.22	126.34	119.87
1	B	593	ASN	C-N-CA	6.22	126.34	119.87
1	B	194	GLU	N-CA-C	6.12	118.73	111.33
1	E	180	ARG	N-CA-C	6.11	119.45	110.10
1	B	48	ASP	N-CA-C	-6.10	104.19	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	446	HIS	CB-CA-C	6.07	119.76	109.50
1	H	459	VAL	N-CA-C	-6.00	106.57	111.91
1	B	162	GLY	N-CA-C	-5.96	106.86	114.37
1	B	461	GLN	N-CA-C	-5.94	106.38	113.21
1	H	458	ALA	N-CA-C	5.62	118.63	109.24
1	B	242	ALA	N-CA-C	-5.58	98.63	108.23
1	F	82	SER	N-CA-C	5.46	117.53	110.65
1	B	195	TRP	CD2-CE2-CZ2	-5.42	116.98	122.40
1	D	487	PHE	N-CA-C	5.40	117.19	108.34
1	B	297	SER	N-CA-C	5.32	116.36	108.60
1	D	114	VAL	N-CA-C	5.19	115.41	110.42
1	F	285	ARG	N-CA-C	5.19	116.96	108.76
1	B	212	GLN	N-CA-C	5.13	118.80	112.54
1	A	168	TRP	N-CA-C	5.13	116.94	110.33
1	G	614	THR	CB-CA-C	5.06	115.44	109.47
1	E	194	GLU	N-CA-C	5.04	116.78	111.28
1	A	595	THR	N-CA-C	5.04	117.16	111.11
1	B	535	GLY	N-CA-C	-5.03	108.67	115.21

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	240	PRO	Peptide
1	B	553	HIS	Peptide

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	4549	0	4395	57	0
1	B	4549	0	4395	115	0
1	C	4549	0	4395	45	0
1	D	4549	0	4395	48	0
1	E	4549	0	4395	54	0
1	F	4549	0	4395	64	0
1	G	4549	0	4395	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	4549	0	4395	44	0
2	A	53	0	30	0	0
2	B	53	0	30	5	0
2	C	53	0	30	2	0
2	D	53	0	30	2	0
2	E	53	0	30	1	0
2	F	53	0	30	0	0
2	G	53	0	30	0	0
2	H	53	0	30	0	0
3	A	290	0	0	16	0
3	B	221	0	0	8	0
3	C	274	0	0	10	0
3	D	172	0	0	9	0
3	E	303	0	0	7	0
3	F	317	0	0	12	0
3	G	251	0	0	12	0
3	H	326	0	0	9	0
All	All	38970	0	35400	473	0

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

All (473) 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:164:MSE:HB3	1:B:167:HIS:CE1	1.66	1.31
1:B:548:HIS:CE1	1:B:593:ASN:HA	1.87	1.09
1:B:167:HIS:CD2	2:B:625:FAD:C8M	2.41	1.02
1:E:71:LYS:HB2	1:E:274:ARG:NH1	1.74	1.01
1:B:164:MSE:CB	1:B:167:HIS:CE1	2.46	0.98
1:G:110:GLN:HE21	1:G:167:HIS:HD1	1.08	0.98
1:A:112:MSE:HE1	3:A:907:HOH:O	1.64	0.96
1:A:112:MSE:CE	3:A:907:HOH:O	2.14	0.96
1:E:461:GLN:HA	3:E:730:HOH:O	1.66	0.94
1:B:164:MSE:HB3	1:B:167:HIS:NE2	1.84	0.93
1:H:110:GLN:HE21	1:H:167:HIS:HD1	1.16	0.90
1:D:460:GLN:HA	3:D:745:HOH:O	1.71	0.88
1:E:71:LYS:HB2	1:E:274:ARG:CZ	2.04	0.85
1:B:548:HIS:CE1	1:B:593:ASN:CA	2.60	0.85
1:B:458:ALA:HA	1:B:461:GLN:HE21	1.40	0.84
1:G:459:VAL:HA	3:G:840:HOH:O	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:MSE:HE3	1:C:95:GLU:OE1	1.77	0.83
1:B:157:VAL:HG21	1:B:324:HIS:HE1	1.44	0.83
1:A:478:GLU:HB2	3:A:915:HOH:O	1.78	0.82
1:C:110:GLN:HE21	1:C:167:HIS:HD1	1.28	0.81
1:B:548:HIS:CD2	1:B:594:PRO:HD2	2.17	0.80
1:B:446:HIS:CG	1:B:592:ALA:HA	2.18	0.79
1:E:157:VAL:HG21	1:E:324:HIS:HE1	1.49	0.76
1:E:47:TYR:O	1:E:313:ALA:HA	1.84	0.76
1:B:164:MSE:HB3	1:B:167:HIS:HE1	1.49	0.76
1:A:110:GLN:HE21	1:A:167:HIS:HD1	1.33	0.75
1:G:542:GLU:HG2	3:G:734:HOH:O	1.86	0.75
1:E:180:ARG:NH1	3:E:681:HOH:O	2.20	0.74
1:F:110:GLN:HE21	1:F:167:HIS:HD1	1.36	0.73
1:E:180:ARG:HG3	1:E:180:ARG:HH11	1.53	0.73
1:F:458:ALA:CB	1:F:461:GLN:HE21	2.02	0.73
1:F:478:GLU:HG2	1:F:511:THR:OG1	1.88	0.72
1:A:443:HIS:HD2	3:A:641:HOH:O	1.72	0.72
1:B:444:PRO:HD2	1:B:445:TRP:CZ3	2.24	0.72
1:H:505:ARG:HG3	3:H:681:HOH:O	1.88	0.72
1:F:458:ALA:CB	1:F:461:GLN:NE2	2.54	0.71
1:D:145:GLU:HG2	1:D:491:ILE:HD13	1.72	0.71
1:B:47:TYR:O	1:B:313:ALA:HA	1.91	0.70
1:C:44:ASP:HB3	1:C:47:TYR:OH	1.92	0.70
1:C:458:ALA:HB2	3:C:866:HOH:O	1.92	0.69
1:D:453:ALA:O	1:D:456:TYR:HD1	1.75	0.69
1:G:453:ALA:O	1:G:456:TYR:HD1	1.76	0.69
1:A:44:ASP:HB3	1:A:47:TYR:CZ	2.27	0.69
1:B:164:MSE:CA	1:B:167:HIS:CE1	2.75	0.69
1:F:458:ALA:HB1	1:F:461:GLN:NE2	2.08	0.69
1:B:164:MSE:HA	1:B:167:HIS:CE1	2.28	0.68
1:B:169:THR:O	1:B:170:CYS:HB2	1.94	0.68
1:B:385:THR:HB	1:B:388:GLU:HG3	1.75	0.68
1:B:460:GLN:HB2	3:B:790:HOH:O	1.94	0.68
1:E:112:MSE:HE2	1:G:95:GLU:HG3	1.76	0.68
1:B:446:HIS:CD2	1:B:592:ALA:HA	2.28	0.67
1:F:453:ALA:O	1:F:456:TYR:HD1	1.78	0.67
1:G:157:VAL:HG21	1:G:324:HIS:HE1	1.58	0.67
1:F:341:ASN:HB2	3:F:786:HOH:O	1.95	0.67
1:B:46:LYS:HE2	1:B:312:LYS:C	2.20	0.67
1:E:110:GLN:HE21	1:E:167:HIS:HD1	1.41	0.67
1:F:95:GLU:HG3	1:H:112:MSE:HE2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:HIS:ND1	3:B:627:HOH:O	2.27	0.66
1:B:46:LYS:HE2	1:B:312:LYS:O	1.95	0.66
1:B:126:LEU:HD12	1:B:132:GLN:HG3	1.78	0.65
1:F:458:ALA:HB3	3:F:821:HOH:O	1.96	0.65
1:B:362:VAL:O	1:B:522:MSE:HE1	1.98	0.64
1:H:341:ASN:HD21	1:H:344:ASN:HB2	1.63	0.64
1:A:112:MSE:SE	3:A:773:HOH:O	2.65	0.64
1:F:157:VAL:HG21	1:F:324:HIS:HE1	1.62	0.64
1:B:82:SER:HA	3:D:676:HOH:O	1.98	0.64
1:B:458:ALA:HA	1:B:461:GLN:NE2	2.12	0.64
1:B:566:VAL:HA	1:B:571:ARG:O	1.99	0.63
1:F:81:ASP:HB2	3:F:705:HOH:O	1.98	0.63
1:A:299:HIS:CD2	1:A:310:GLU:HG2	2.35	0.62
1:B:495:TYR:OH	1:D:95:GLU:OE2	2.15	0.62
1:D:513:LYS:HE2	3:D:736:HOH:O	1.99	0.62
1:E:571:ARG:NH1	3:E:668:HOH:O	2.32	0.62
1:G:296:GLU:HG3	3:G:780:HOH:O	1.99	0.62
1:E:95:GLU:HG3	1:G:112:MSE:HE2	1.81	0.62
1:G:555:MSE:HE3	1:G:568:THR:HG22	1.82	0.61
1:B:439:PHE:HB2	1:B:445:TRP:C	2.25	0.61
1:C:218:ARG:HG3	1:C:430:ASP:OD2	2.00	0.61
1:H:274:ARG:HD3	1:H:618:PHE:CD1	2.35	0.61
1:G:571:ARG:NH1	3:G:745:HOH:O	2.32	0.61
1:C:461:GLN:HA	3:C:899:HOH:O	1.99	0.61
1:H:455:SER:HB3	3:H:872:HOH:O	2.00	0.61
1:B:167:HIS:CE1	2:B:625:FAD:C8M	2.75	0.60
1:F:458:ALA:HB2	1:F:461:GLN:HE21	1.64	0.60
1:E:218:ARG:HD2	3:E:633:HOH:O	2.00	0.60
1:C:126:LEU:CD1	1:C:132:GLN:HG2	2.32	0.60
1:F:555:MSE:HE1	1:F:601:LEU:HG	1.83	0.60
1:F:129:THR:HG21	3:H:694:HOH:O	2.01	0.60
1:G:110:GLN:NE2	1:G:167:HIS:HD1	1.91	0.60
1:B:375:SER:O	1:B:404:HIS:HE1	1.84	0.60
1:G:408:TRP:CD1	1:G:408:TRP:C	2.80	0.60
1:E:346:PRO:HG2	1:E:350:PRO:HA	1.83	0.60
1:A:132:GLN:HE21	1:A:133:ALA:N	1.99	0.59
1:C:126:LEU:HD13	1:C:132:GLN:HG2	1.83	0.59
1:H:460:GLN:C	1:H:462:SER:H	2.10	0.59
1:B:548:HIS:CG	1:B:594:PRO:CD	2.86	0.59
1:H:218:ARG:HD2	3:H:674:HOH:O	2.03	0.58
1:A:83:GLY:N	3:A:850:HOH:O	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:458:ALA:HA	1:C:461:GLN:HE21	1.68	0.58
1:E:453:ALA:O	1:E:456:TYR:HD1	1.86	0.58
1:B:167:HIS:NE2	2:B:625:FAD:C8	2.61	0.58
1:D:89:HIS:CE1	1:D:91:LYS:HB2	2.38	0.58
1:H:131:TRP:CH2	1:H:133:ALA:HB2	2.39	0.58
1:A:359:GLN:HG2	1:A:475:GLY:O	2.04	0.58
1:B:362:VAL:HG23	1:B:522:MSE:HE3	1.86	0.57
1:B:203:GLU:HB3	1:B:208:THR:HB	1.84	0.57
1:B:362:VAL:HG23	1:B:522:MSE:CE	2.34	0.57
1:A:149:LEU:O	1:A:505:ARG:NH2	2.38	0.57
1:B:558:ASP:OD2	1:B:561:GLU:HG2	2.04	0.57
1:C:400:SER:HB2	3:C:849:HOH:O	2.03	0.57
1:H:158:THR:HG22	1:H:160:VAL:HG22	1.86	0.57
1:B:167:HIS:CD2	2:B:625:FAD:C8	2.87	0.57
1:B:439:PHE:CD1	1:B:445:TRP:N	2.73	0.57
1:B:548:HIS:CE1	1:B:593:ASN:CB	2.88	0.57
1:C:157:VAL:HG21	1:C:324:HIS:HE1	1.69	0.57
1:H:571:ARG:NH1	3:H:729:HOH:O	2.39	0.56
1:D:462:SER:HB2	3:D:745:HOH:O	2.05	0.56
1:G:70:TYR:CE1	1:G:615:PRO:HG3	2.40	0.56
1:F:108:GLN:NE2	1:F:454:PHE:HE2	2.04	0.56
1:D:444:PRO:HD2	1:D:445:TRP:CZ3	2.41	0.56
1:H:274:ARG:HD3	1:H:618:PHE:HD1	1.71	0.56
1:B:180:ARG:HD2	3:B:734:HOH:O	2.06	0.56
1:C:336:GLN:HB2	1:C:346:PRO:HG3	1.87	0.56
1:H:461:GLN:HA	3:H:903:HOH:O	2.06	0.55
1:C:555:MSE:HE1	1:C:601:LEU:HG	1.87	0.55
1:D:56:PRO:HD3	1:D:165:SER:HB3	1.88	0.55
1:E:48:ASP:HB2	1:E:71:LYS:O	2.05	0.55
1:G:362:VAL:O	1:G:522:MSE:HE1	2.07	0.55
1:G:453:ALA:O	1:G:456:TYR:CD1	2.57	0.55
3:B:694:HOH:O	1:D:129:THR:HG21	2.06	0.55
1:D:219:HIS:HB2	1:D:433:PRO:HA	1.87	0.55
1:A:132:GLN:NE2	1:A:133:ALA:N	2.55	0.55
1:A:432:GLU:H	1:A:432:GLU:CD	2.15	0.55
1:H:432:GLU:H	1:H:432:GLU:CD	2.14	0.55
1:A:132:GLN:HE21	1:A:132:GLN:C	2.15	0.55
1:F:108:GLN:NE2	1:F:454:PHE:CE2	2.75	0.55
1:G:132:GLN:HG2	3:G:657:HOH:O	2.06	0.55
1:G:157:VAL:HG21	1:G:324:HIS:CE1	2.40	0.55
1:B:183:LEU:HG	1:B:195:TRP:NE1	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:528:LYS:NZ	3:F:903:HOH:O	2.33	0.54
1:D:158:THR:HG22	1:D:160:VAL:HG22	1.90	0.54
1:H:341:ASN:ND2	1:H:344:ASN:HB2	2.21	0.54
1:B:129:THR:HG21	3:D:678:HOH:O	2.05	0.54
1:D:44:ASP:OD1	1:D:45:ILE:N	2.33	0.54
1:A:131:TRP:CH2	1:A:133:ALA:HB2	2.42	0.54
1:A:443:HIS:HE1	3:A:741:HOH:O	1.90	0.54
1:D:70:TYR:CZ	1:D:615:PRO:HD3	2.42	0.54
1:H:458:ALA:HB1	1:H:460:GLN:H	1.71	0.54
1:C:533:LEU:HD12	1:C:534:PRO:HD2	1.90	0.54
1:E:180:ARG:HH11	1:E:180:ARG:CG	2.17	0.54
1:A:173:PRO:HG2	1:A:592:ALA:HB1	1.89	0.54
1:C:347:GLU:HG2	1:C:348:LEU:HG	1.90	0.54
1:F:458:ALA:HB2	1:F:461:GLN:NE2	2.21	0.54
1:F:362:VAL:CG2	1:F:473:PHE:HB2	2.38	0.54
1:B:110:GLN:HE21	1:B:167:HIS:HD1	1.55	0.53
1:F:473:PHE:CD1	1:F:522:MSE:HE3	2.43	0.53
1:B:218:ARG:HG3	1:B:430:ASP:OD2	2.08	0.53
1:G:70:TYR:CZ	1:G:615:PRO:HD3	2.43	0.53
1:C:505:ARG:HG3	3:C:675:HOH:O	2.09	0.53
1:H:555:MSE:HE1	1:H:601:LEU:HG	1.91	0.53
1:E:47:TYR:CG	1:E:73:ALA:HB2	2.43	0.53
1:B:70:TYR:OH	1:B:610:LYS:HA	2.08	0.53
1:F:89:HIS:CE1	1:F:91:LYS:HB2	2.44	0.53
1:F:112:MSE:HE2	1:H:95:GLU:HG3	1.89	0.53
1:G:505:ARG:NH1	3:G:850:HOH:O	2.42	0.53
1:H:289:ASN:HB3	1:H:296:GLU:HG2	1.91	0.52
1:A:380:MSE:HE1	1:A:409:ASN:HB3	1.91	0.52
1:H:70:TYR:CZ	1:H:615:PRO:HG3	2.44	0.52
1:D:44:ASP:HB3	1:D:47:TYR:OH	2.08	0.52
1:B:439:PHE:HB2	1:B:445:TRP:O	2.09	0.52
1:B:341:ASN:HB2	3:B:678:HOH:O	2.09	0.52
1:B:453:ALA:O	1:B:456:TYR:HD1	1.93	0.51
1:G:362:VAL:HG23	1:G:522:MSE:CE	2.41	0.51
1:H:497:MSE:HA	1:H:497:MSE:HE2	1.91	0.51
1:E:471:TRP:CH2	1:E:526:SER:HA	2.45	0.51
1:B:554:ARG:O	1:B:564:CYS:HB2	2.11	0.51
1:H:157:VAL:HG21	1:H:324:HIS:HE1	1.75	0.51
1:B:441:PRO:HD3	3:B:832:HOH:O	2.10	0.51
1:D:286:VAL:O	1:D:332:SER:HB3	2.11	0.51
1:D:471:TRP:CH2	1:D:526:SER:HA	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:432:GLU:CD	1:F:432:GLU:H	2.18	0.51
1:E:455:SER:HB3	3:E:847:HOH:O	2.10	0.51
1:G:150:ARG:HD2	3:G:874:HOH:O	2.10	0.51
1:A:362:VAL:CG2	1:A:473:PHE:HB2	2.40	0.51
1:B:181:PRO:HB2	1:B:555:MSE:HE2	1.92	0.51
1:A:95:GLU:HG3	1:C:112:MSE:HE2	1.92	0.51
1:E:478:GLU:HG2	1:E:480:LYS:HD3	1.93	0.51
1:G:70:TYR:CD1	1:G:615:PRO:HG3	2.46	0.51
1:B:548:HIS:CE1	1:B:593:ASN:HB3	2.46	0.50
1:B:548:HIS:CG	1:B:594:PRO:HD2	2.44	0.50
1:D:46:LYS:HE3	1:D:312:LYS:HG3	1.92	0.50
1:D:70:TYR:CD2	1:D:615:PRO:HB3	2.46	0.50
1:D:478:GLU:HG2	1:D:511:THR:OG1	2.11	0.50
1:H:110:GLN:NE2	1:H:167:HIS:HD1	1.98	0.50
1:D:47:TYR:O	1:D:313:ALA:HA	2.11	0.50
1:D:480:LYS:HE2	3:D:705:HOH:O	2.12	0.50
1:F:554:ARG:O	1:F:564:CYS:HB2	2.12	0.50
1:H:169:THR:O	1:H:170:CYS:HB2	2.11	0.50
1:B:173:PRO:HG3	1:B:446:HIS:CE1	2.47	0.50
1:B:293:SER:HA	1:B:574:GLY:O	2.12	0.50
1:B:570:SER:HB3	1:B:580:LEU:O	2.12	0.50
1:G:180:ARG:HB2	1:G:181:PRO:HD2	1.93	0.50
1:B:443:HIS:HB2	1:B:445:TRP:NE1	2.27	0.50
1:E:47:TYR:CD1	1:E:73:ALA:HB2	2.46	0.50
1:G:183:LEU:CD2	1:G:555:MSE:HE1	2.41	0.50
1:D:408:TRP:O	1:D:412:VAL:HG23	2.12	0.49
1:F:455:SER:HB3	3:F:801:HOH:O	2.11	0.49
1:B:47:TYR:CD1	1:B:73:ALA:HB2	2.48	0.49
1:B:444:PRO:HD2	1:B:445:TRP:CH2	2.47	0.49
1:F:173:PRO:HG2	1:F:592:ALA:HB1	1.94	0.49
1:A:201:LYS:HE2	3:A:862:HOH:O	2.13	0.49
1:D:110:GLN:HE21	1:D:167:HIS:HD1	1.59	0.49
1:H:554:ARG:O	1:H:564:CYS:HB2	2.12	0.49
1:B:47:TYR:CG	1:B:73:ALA:HB2	2.48	0.49
1:F:505:ARG:HG2	3:F:816:HOH:O	2.13	0.49
1:G:72:VAL:O	1:G:275:PHE:HA	2.12	0.49
1:E:380:MSE:HE1	1:E:409:ASN:HA	1.95	0.49
1:F:453:ALA:O	1:F:456:TYR:CD1	2.62	0.49
1:G:183:LEU:HD23	1:G:555:MSE:HE1	1.95	0.49
1:H:346:PRO:HG2	1:H:350:PRO:HA	1.95	0.49
1:E:165:SER:HA	1:E:168:TRP:CD1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:349:LEU:HD13	1:G:565:CYS:HB3	1.95	0.48
1:B:157:VAL:HG21	1:B:324:HIS:CE1	2.35	0.48
1:E:444:PRO:HD2	1:E:445:TRP:CZ3	2.49	0.48
1:F:528:LYS:HE3	3:F:771:HOH:O	2.12	0.48
1:G:89:HIS:ND1	1:G:91:LYS:HB2	2.28	0.48
1:B:383:ARG:HG3	1:B:383:ARG:HH11	1.78	0.48
1:C:44:ASP:CG	1:C:45:ILE:H	2.22	0.48
1:G:178:GLU:O	1:G:178:GLU:HG3	2.14	0.48
1:A:47:TYR:O	1:A:313:ALA:HA	2.12	0.48
1:E:299:HIS:CD2	1:E:310:GLU:HG2	2.47	0.48
1:G:459:VAL:CA	3:G:840:HOH:O	2.48	0.48
1:H:217:ILE:HD13	1:H:376:VAL:HG13	1.95	0.48
1:G:459:VAL:C	3:G:840:HOH:O	2.57	0.48
1:B:108:GLN:HE21	1:B:454:PHE:HE2	1.60	0.48
1:B:158:THR:HG22	1:B:160:VAL:HG22	1.95	0.48
1:G:47:TYR:O	1:G:313:ALA:HA	2.14	0.48
1:B:173:PRO:HG2	1:B:592:ALA:HB1	1.96	0.48
1:A:475:GLY:N	1:A:518:MSE:SE	2.97	0.48
1:D:408:TRP:CD1	1:D:408:TRP:C	2.92	0.48
1:F:537:LEU:HB3	1:F:538:PRO:HD2	1.94	0.48
1:C:167:HIS:HD2	2:C:625:FAD:HM72	1.79	0.47
1:E:105:ASN:HB3	1:G:105:ASN:O	2.15	0.47
1:G:570:SER:HB3	1:G:580:LEU:O	2.13	0.47
1:E:47:TYR:CD2	1:E:73:ALA:HB2	2.50	0.47
1:A:408:TRP:CD1	1:A:408:TRP:C	2.93	0.47
3:B:777:HOH:O	1:C:121:LEU:HD13	2.15	0.47
1:E:180:ARG:HB2	1:E:181:PRO:HD2	1.96	0.47
1:G:82:SER:HB3	1:G:90:LYS:HG3	1.96	0.47
3:A:850:HOH:O	1:C:81:ASP:C	2.57	0.47
1:B:105:ASN:O	1:D:105:ASN:HB3	2.15	0.47
1:G:444:PRO:HD2	1:G:445:TRP:CZ3	2.49	0.47
1:D:490:LYS:HG3	3:D:756:HOH:O	2.15	0.47
1:F:89:HIS:ND1	1:F:91:LYS:HB2	2.30	0.47
1:F:91:LYS:HE2	3:F:848:HOH:O	2.13	0.47
1:F:463:ILE:HD13	1:F:533:LEU:CD1	2.45	0.47
1:G:70:TYR:CZ	1:G:615:PRO:HG3	2.49	0.47
1:B:294:GLU:HG2	1:B:577:ASN:ND2	2.29	0.47
1:G:218:ARG:HD2	3:G:643:HOH:O	2.15	0.47
1:G:385:THR:O	1:G:388:GLU:HB2	2.15	0.47
1:A:231:LYS:HE3	3:A:883:HOH:O	2.14	0.47
1:B:487:PHE:CD1	1:B:500:PRO:HA	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:LYS:HD2	1:E:312:LYS:O	2.13	0.47
1:A:307:ASP:HB2	3:A:879:HOH:O	2.15	0.47
1:B:507:PRO:HD2	1:B:511:THR:HG21	1.97	0.47
1:F:50:VAL:HG23	1:F:313:ALA:HB2	1.97	0.47
1:H:460:GLN:C	1:H:462:SER:N	2.73	0.47
3:A:784:HOH:O	1:C:129:THR:HG21	2.15	0.46
1:B:201:LYS:HE2	1:B:205:TYR:OH	2.15	0.46
1:E:408:TRP:CD1	1:E:408:TRP:C	2.92	0.46
1:E:71:LYS:CB	1:E:274:ARG:NH1	2.63	0.46
1:G:215:GLU:O	1:G:215:GLU:HG2	2.16	0.46
1:G:362:VAL:HG23	1:G:522:MSE:HE3	1.97	0.46
1:H:288:ARG:HD3	1:H:332:SER:O	2.14	0.46
1:B:56:PRO:HD3	1:B:165:SER:HB3	1.97	0.46
1:B:124:ASP:HA	3:B:706:HOH:O	2.16	0.46
1:F:408:TRP:CD1	1:F:408:TRP:C	2.92	0.46
1:A:265:ARG:HA	1:A:266:PRO:C	2.41	0.46
1:G:158:THR:HG22	1:G:160:VAL:HG22	1.97	0.46
1:A:56:PRO:HD3	1:A:165:SER:HB3	1.98	0.46
1:B:499:GLN:HA	1:B:500:PRO:HD2	1.82	0.46
1:B:495:TYR:O	1:B:496:ASN:HB2	2.16	0.46
1:B:548:HIS:NE2	1:B:594:PRO:HD2	2.31	0.45
1:D:167:HIS:CD2	2:D:625:FAD:HM72	2.51	0.45
1:E:458:ALA:HA	1:E:461:GLN:NE2	2.30	0.45
1:G:458:ALA:HA	1:G:461:GLN:HE21	1.81	0.45
1:B:437:THR:HG23	1:B:437:THR:O	2.16	0.45
1:E:554:ARG:O	1:E:564:CYS:HB2	2.16	0.45
1:B:231:LYS:HZ3	1:B:231:LYS:HB2	1.81	0.45
1:F:84:LEU:HD23	3:H:723:HOH:O	2.15	0.45
1:C:218:ARG:HD2	3:C:657:HOH:O	2.17	0.45
1:F:507:PRO:HD2	1:F:511:THR:HG21	1.99	0.45
1:G:110:GLN:HB2	1:G:158:THR:HG23	1.98	0.45
1:C:45:ILE:HG23	1:C:46:LYS:H	1.82	0.45
1:A:506:PHE:HA	1:A:507:PRO:HD3	1.86	0.45
1:F:211:ASP:HB2	3:F:862:HOH:O	2.16	0.45
1:F:288:ARG:HD3	1:F:332:SER:O	2.15	0.45
1:B:548:HIS:CG	1:B:594:PRO:HD3	2.51	0.44
1:G:89:HIS:CE1	1:G:91:LYS:HB2	2.51	0.44
1:B:446:HIS:CB	1:B:592:ALA:HA	2.46	0.44
1:F:157:VAL:HG21	1:F:324:HIS:CE1	2.48	0.44
1:G:478:GLU:HA	1:G:479:PRO:HD3	1.85	0.44
1:D:455:SER:HB3	3:D:767:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:525:MSE:O	1:D:528:LYS:HG3	2.17	0.44
1:A:362:VAL:HG22	1:A:518:MSE:HE3	1.98	0.44
1:A:362:VAL:HG23	1:A:473:PHE:HB2	1.99	0.44
1:B:329:LEU:HD11	1:B:580:LEU:HD21	2.00	0.44
1:B:341:ASN:OD1	1:B:344:ASN:HB2	2.18	0.44
1:C:400:SER:CB	3:C:849:HOH:O	2.63	0.44
1:E:180:ARG:NH1	1:E:180:ARG:CG	2.78	0.44
1:A:261:ASP:OD1	1:A:261:ASP:C	2.61	0.44
1:B:341:ASN:HA	1:B:342:PRO:HD3	1.79	0.44
1:B:355:TYR:HA	1:B:480:LYS:O	2.17	0.44
1:H:155:GLN:HG2	1:H:502:PHE:CZ	2.52	0.44
1:C:541:MSE:HE2	3:C:716:HOH:O	2.18	0.44
1:F:126:LEU:HD12	1:F:132:GLN:HG3	2.00	0.44
1:G:215:GLU:HB3	3:G:757:HOH:O	2.17	0.44
1:B:213:PHE:CD1	1:B:434:GLN:HG3	2.52	0.44
1:B:294:GLU:N	1:B:575:PHE:CD1	2.86	0.44
1:C:554:ARG:O	1:C:564:CYS:HB2	2.18	0.44
1:D:167:HIS:CD2	1:D:167:HIS:C	2.95	0.44
1:H:358:GLU:HG2	1:H:544:GLY:HA2	2.00	0.44
1:C:44:ASP:CG	1:C:45:ILE:N	2.76	0.44
1:C:215:GLU:O	1:C:411:LYS:NZ	2.51	0.44
1:C:435:VAL:HB	1:C:449:ILE:HB	1.99	0.44
1:C:439:PHE:C	1:C:439:PHE:CD2	2.96	0.44
1:F:218:ARG:HD2	3:F:671:HOH:O	2.18	0.44
1:H:336:GLN:HG3	3:H:745:HOH:O	2.18	0.44
1:B:243:ALA:HB1	1:B:251:VAL:CG1	2.47	0.43
1:B:439:PHE:C	1:B:439:PHE:CD2	2.96	0.43
1:D:178:GLU:HG3	1:D:178:GLU:O	2.18	0.43
1:D:342:PRO:C	1:D:344:ASN:H	2.26	0.43
1:D:567:ASN:HD21	1:D:571:ARG:NH1	2.16	0.43
1:F:155:GLN:HG2	1:F:502:PHE:CZ	2.53	0.43
1:F:219:HIS:HB2	1:F:433:PRO:HA	2.00	0.43
1:G:432:GLU:CD	1:G:432:GLU:H	2.25	0.43
1:A:458:ALA:HB1	1:A:461:GLN:OE1	2.18	0.43
1:B:548:HIS:CD2	1:B:594:PRO:CD	2.95	0.43
1:E:216:SER:HB2	1:E:431:PRO:HB2	2.00	0.43
1:C:120:THR:HA	1:C:136:PHE:CD2	2.53	0.43
1:D:218:ARG:HD2	3:D:683:HOH:O	2.17	0.43
1:E:432:GLU:CD	1:E:432:GLU:H	2.26	0.43
1:F:83:GLY:N	3:F:940:HOH:O	2.09	0.43
1:F:541:MSE:HE2	3:F:745:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:TYR:CD2	1:B:73:ALA:HB2	2.53	0.43
1:E:129:THR:HG21	3:G:684:HOH:O	2.18	0.43
1:E:169:THR:O	1:E:170:CYS:HB2	2.18	0.43
1:F:195:TRP:CH2	1:F:601:LEU:HD13	2.54	0.43
1:A:463:ILE:HD13	1:A:533:LEU:CD1	2.49	0.43
1:A:555:MSE:HE3	1:A:568:THR:HG22	1.99	0.43
1:B:127:SER:HB3	1:D:531:GLY:HA3	2.00	0.43
1:A:132:GLN:NE2	1:A:132:GLN:CA	2.81	0.43
1:B:261:ASP:OD1	1:B:261:ASP:C	2.62	0.43
1:B:421:GLU:CD	1:B:421:GLU:H	2.27	0.43
1:E:95:GLU:CG	1:G:112:MSE:HE2	2.46	0.43
1:B:47:TYR:CE1	1:B:73:ALA:HB2	2.54	0.43
1:D:44:ASP:CB	1:D:47:TYR:OH	2.66	0.43
1:F:44:ASP:HB3	1:F:47:TYR:CZ	2.54	0.43
1:F:473:PHE:CD1	1:F:522:MSE:CE	3.02	0.43
1:A:157:VAL:HG21	1:A:324:HIS:HE1	1.84	0.43
1:G:542:GLU:HG2	1:G:542:GLU:H	1.54	0.43
1:A:499:GLN:HA	1:A:500:PRO:HD2	1.93	0.43
1:B:439:PHE:CD1	1:B:444:PRO:C	2.97	0.43
1:D:461:GLN:H	1:D:461:GLN:HG3	1.57	0.43
1:A:91:LYS:HE2	3:A:808:HOH:O	2.18	0.42
1:E:274:ARG:HH12	1:E:616:SER:HG	1.66	0.42
1:H:362:VAL:CG2	1:H:473:PHE:HB2	2.49	0.42
1:A:167:HIS:CD2	1:A:167:HIS:C	2.97	0.42
1:B:446:HIS:NE2	1:B:593:ASN:OD1	2.52	0.42
1:B:453:ALA:O	1:B:456:TYR:CD1	2.72	0.42
1:F:70:TYR:CZ	1:F:615:PRO:HG3	2.54	0.42
1:G:167:HIS:CD2	1:G:167:HIS:C	2.97	0.42
1:C:124:ASP:OD1	1:C:124:ASP:N	2.52	0.42
1:C:167:HIS:CD2	2:C:625:FAD:HM72	2.54	0.42
1:F:463:ILE:HD13	1:F:533:LEU:HD11	2.00	0.42
1:H:413:LYS:HE3	3:H:864:HOH:O	2.18	0.42
1:C:46:LYS:HE2	1:C:47:TYR:O	2.19	0.42
1:C:211:ASP:HB2	3:C:730:HOH:O	2.19	0.42
1:D:44:ASP:HB3	1:D:47:TYR:CZ	2.54	0.42
1:E:167:HIS:CD2	1:E:167:HIS:C	2.96	0.42
1:H:385:THR:O	1:H:391:TYR:HB2	2.19	0.42
1:B:49:VAL:HB	1:B:72:VAL:HG22	2.01	0.42
1:B:548:HIS:ND1	1:B:593:ASN:HA	2.29	0.42
1:B:174:ARG:HG2	1:B:199:TYR:CG	2.54	0.42
1:B:345:PRO:HA	1:B:346:PRO:HD3	1.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:ARG:HG3	1:B:383:ARG:NH1	2.35	0.42
1:C:408:TRP:CD1	1:C:408:TRP:C	2.98	0.42
1:E:460:GLN:C	1:E:462:SER:H	2.27	0.42
1:A:132:GLN:HE21	1:A:132:GLN:CA	2.33	0.42
1:B:105:ASN:HB3	1:D:105:ASN:O	2.19	0.42
1:C:158:THR:HG22	1:C:160:VAL:HG22	2.01	0.42
1:E:246:ARG:HA	1:E:246:ARG:HD3	1.76	0.42
1:G:149:LEU:O	1:G:505:ARG:NH2	2.53	0.42
1:B:206:PHE:CE1	1:B:599:MSE:CE	3.03	0.42
1:F:61:TYR:HA	1:F:606:CYS:SG	2.60	0.42
1:B:55:GLY:HA2	1:B:162:GLY:O	2.20	0.41
1:D:89:HIS:ND1	1:D:91:LYS:HB2	2.35	0.41
1:G:81:ASP:OD2	1:G:90:LYS:NZ	2.53	0.41
1:C:167:HIS:CD2	1:C:167:HIS:C	2.97	0.41
1:A:341:ASN:HA	1:A:342:PRO:HD3	1.73	0.41
1:F:70:TYR:CE1	1:F:615:PRO:HG3	2.55	0.41
1:A:44:ASP:CB	1:A:47:TYR:OH	2.68	0.41
1:B:274:ARG:HD3	1:B:618:PHE:HD1	1.86	0.41
1:D:362:VAL:HG22	1:D:473:PHE:HB2	2.01	0.41
1:E:586:ILE:HA	1:E:587:PRO:HD3	1.81	0.41
1:F:167:HIS:CD2	1:F:167:HIS:C	2.98	0.41
1:F:506:PHE:HA	1:F:507:PRO:HD3	1.91	0.41
1:H:70:TYR:CE2	1:H:615:PRO:HG3	2.55	0.41
1:B:347:GLU:H	1:B:347:GLU:HG3	1.67	0.41
1:B:460:GLN:C	1:B:462:SER:H	2.27	0.41
1:C:451:ARG:HH22	1:C:465:SER:HB2	1.85	0.41
1:F:95:GLU:CG	1:H:112:MSE:HE2	2.45	0.41
1:H:70:TYR:CE1	1:H:615:PRO:HG3	2.56	0.41
1:A:44:ASP:HB3	1:A:47:TYR:OH	2.20	0.41
1:A:218:ARG:HD2	3:A:640:HOH:O	2.21	0.41
1:A:478:GLU:HG2	1:A:511:THR:OG1	2.21	0.41
1:B:164:MSE:CB	1:B:167:HIS:HE1	2.12	0.41
1:E:46:LYS:HG3	3:E:897:HOH:O	2.21	0.41
1:E:50:VAL:HG11	1:E:298:LEU:HD22	2.02	0.41
1:E:487:PHE:CD1	1:E:500:PRO:HA	2.55	0.41
1:F:229:GLU:HG3	1:F:528:LYS:HG2	2.03	0.41
1:H:89:HIS:CE1	1:H:91:LYS:HB2	2.55	0.41
1:H:363:PHE:HA	1:H:471:TRP:O	2.20	0.41
1:A:471:TRP:CH2	1:A:526:SER:HA	2.56	0.41
1:C:386:PRO:HG3	1:C:391:TYR:CE1	2.56	0.41
1:D:145:GLU:CG	1:D:491:ILE:HD13	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:299:HIS:NE2	1:F:310:GLU:OE2	2.52	0.41
1:G:137:PHE:O	1:G:139:ARG:HD3	2.21	0.41
1:H:70:TYR:OH	1:H:613:PHE:O	2.31	0.41
1:B:210:THR:HA	1:B:238:GLN:NE2	2.36	0.41
1:B:216:SER:HB2	1:B:431:PRO:HB2	2.03	0.41
1:B:478:GLU:HA	1:B:479:PRO:HD3	1.93	0.41
1:C:91:LYS:NZ	3:C:853:HOH:O	2.54	0.41
1:D:127:SER:C	1:D:129:THR:H	2.29	0.41
1:E:328:LEU:HD23	1:E:328:LEU:O	2.20	0.41
1:E:458:ALA:HB2	3:E:841:HOH:O	2.20	0.41
1:E:537:LEU:HD13	1:F:539:GLN:HB3	2.03	0.41
2:E:625:FAD:H2'	2:E:625:FAD:N1	2.35	0.41
1:F:137:PHE:O	1:F:139:ARG:HD3	2.21	0.41
1:F:451:ARG:HD3	1:F:468:ILE:O	2.21	0.41
1:G:181:PRO:HG2	1:G:195:TRP:HZ2	1.86	0.41
1:G:359:GLN:HB3	1:G:475:GLY:O	2.20	0.41
1:H:217:ILE:CD1	1:H:376:VAL:HG13	2.51	0.41
1:A:43:MSE:N	3:A:723:HOH:O	2.54	0.41
1:C:452:ASP:HB2	1:C:472:ARG:NH1	2.36	0.41
1:F:571:ARG:HH11	1:F:571:ARG:HG2	1.86	0.41
1:G:165:SER:HA	1:G:168:TRP:CD1	2.56	0.41
1:A:155:GLN:HG2	1:A:502:PHE:CZ	2.57	0.40
1:A:507:PRO:HD2	1:A:511:THR:HG21	2.03	0.40
1:B:206:PHE:CZ	1:B:599:MSE:HE1	2.56	0.40
1:D:137:PHE:O	1:D:139:ARG:HD3	2.21	0.40
1:E:175:PHE:CE1	1:E:592:ALA:HB3	2.56	0.40
1:E:451:ARG:HD3	1:E:468:ILE:O	2.21	0.40
1:H:449:ILE:HG12	1:H:471:TRP:CE3	2.56	0.40
1:G:181:PRO:HB2	1:G:555:MSE:HE2	2.03	0.40
1:H:180:ARG:HD2	1:H:195:TRP:CD1	2.56	0.40
1:A:105:ASN:O	1:C:105:ASN:HB3	2.21	0.40
1:A:346:PRO:HG2	1:A:350:PRO:HA	2.03	0.40
1:A:458:ALA:HB3	3:A:771:HOH:O	2.21	0.40
1:B:47:TYR:CZ	1:B:73:ALA:HB2	2.56	0.40
1:D:242:ALA:HB1	1:D:254:SER:HB2	2.02	0.40
1:G:506:PHE:HA	1:G:507:PRO:HD3	1.93	0.40
1:A:385:THR:HG22	1:A:386:PRO:O	2.20	0.40
1:C:386:PRO:HG3	1:C:391:TYR:CZ	2.56	0.40
1:D:167:HIS:CD2	2:D:625:FAD:C7M	3.04	0.40
1:F:158:THR:HG22	1:F:160:VAL:HG22	2.03	0.40
1:F:471:TRP:CH2	1:F:526:SER:HA	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:THR:HG21	3:C:710:HOH:O	2.21	0.40
1:B:71:LYS:HB2	1:B:274:ARG:CZ	2.52	0.40
2:B:625:FAD:H9	2:B:625:FAD:H1'1	1.91	0.40
1:D:453:ALA:O	1:D:456:TYR:CD1	2.66	0.40
1:E:451:ARG:HH22	1:E:465:SER:HB2	1.86	0.40
1:E:583:CYS:SG	1:E:594:PRO:HG2	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	575/622 (92%)	554 (96%)	21 (4%)	0	100	100
1	B	575/622 (92%)	549 (96%)	25 (4%)	1 (0%)	43	52
1	C	575/622 (92%)	555 (96%)	18 (3%)	2 (0%)	36	43
1	D	575/622 (92%)	551 (96%)	24 (4%)	0	100	100
1	E	575/622 (92%)	554 (96%)	21 (4%)	0	100	100
1	F	575/622 (92%)	556 (97%)	19 (3%)	0	100	100
1	G	575/622 (92%)	557 (97%)	17 (3%)	1 (0%)	43	52
1	H	575/622 (92%)	551 (96%)	21 (4%)	3 (0%)	24	27
All	All	4600/4976 (92%)	4427 (96%)	166 (4%)	7 (0%)	43	52

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	231	LYS
1	H	454	PHE
1	B	455	SER
1	C	455	SER

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Mol	Chain	Res	Type
1	G	459	VAL
1	H	457	GLY
1	C	45	ILE

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	505/525 (96%)	476 (94%)	29 (6%)	18	23
1	B	505/525 (96%)	472 (94%)	33 (6%)	15	18
1	C	505/525 (96%)	476 (94%)	29 (6%)	18	23
1	D	505/525 (96%)	462 (92%)	43 (8%)	10	11
1	E	505/525 (96%)	473 (94%)	32 (6%)	16	19
1	F	505/525 (96%)	471 (93%)	34 (7%)	15	17
1	G	505/525 (96%)	468 (93%)	37 (7%)	13	14
1	H	505/525 (96%)	474 (94%)	31 (6%)	17	20
All	All	4040/4200 (96%)	3772 (93%)	268 (7%)	15	17

All (268) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	MSE
1	A	50	VAL
1	A	91	LYS
1	A	102	LYS
1	A	121	LEU
1	A	129	THR
1	A	132	GLN
1	A	178	GLU
1	A	180	ARG
1	A	182	LEU
1	A	185	LYS
1	A	201	LYS

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Mol	Chain	Res	Type
1	A	206	PHE
1	A	223	LEU
1	A	228	GLU
1	A	231	LYS
1	A	285	ARG
1	A	291	LEU
1	A	294	GLU
1	A	341	ASN
1	A	390	THR
1	A	421	GLU
1	A	432	GLU
1	A	460	GLN
1	A	528	LYS
1	A	560	LYS
1	A	593	ASN
1	A	601	LEU
1	A	619	THR
1	B	44	ASP
1	B	45	ILE
1	B	46	LYS
1	B	50	VAL
1	B	90	LYS
1	B	91	LYS
1	B	121	LEU
1	B	129	THR
1	B	180	ARG
1	B	200	THR
1	B	206	PHE
1	B	217	ILE
1	B	231	LYS
1	B	291	LEU
1	B	294	GLU
1	B	312	LYS
1	B	328	LEU
1	B	341	ASN
1	B	344	ASN
1	B	347	GLU
1	B	354	SER
1	B	382	ILE
1	B	421	GLU
1	B	432	GLU
1	B	439	PHE

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Mol	Chain	Res	Type
1	B	459	VAL
1	B	490	LYS
1	B	546	VAL
1	B	593	ASN
1	B	601	LEU
1	B	607	GLU
1	B	616	SER
1	B	619	THR
1	C	45	ILE
1	C	46	LYS
1	C	82	SER
1	C	91	LYS
1	C	121	LEU
1	C	178	GLU
1	C	180	ARG
1	C	182	LEU
1	C	201	LYS
1	C	206	PHE
1	C	217	ILE
1	C	246	ARG
1	C	291	LEU
1	C	296	GLU
1	C	312	LYS
1	C	343	THR
1	C	385	THR
1	C	389	LEU
1	C	400	SER
1	C	421	GLU
1	C	429	GLU
1	C	459	VAL
1	C	463	ILE
1	C	505	ARG
1	C	528	LYS
1	C	576	LYS
1	C	593	ASN
1	C	601	LEU
1	C	619	THR
1	D	45	ILE
1	D	46	LYS
1	D	91	LYS
1	D	101	ASP
1	D	121	LEU

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Mol	Chain	Res	Type
1	D	129	THR
1	D	132	GLN
1	D	180	ARG
1	D	185	LYS
1	D	201	LYS
1	D	206	PHE
1	D	215	GLU
1	D	217	ILE
1	D	233	GLN
1	D	265	ARG
1	D	268	THR
1	D	285	ARG
1	D	307	ASP
1	D	328	LEU
1	D	341	ASN
1	D	347	GLU
1	D	375	SER
1	D	377	LYS
1	D	385	THR
1	D	388	GLU
1	D	389	LEU
1	D	394	THR
1	D	400	SER
1	D	403	LYS
1	D	413	LYS
1	D	421	GLU
1	D	432	GLU
1	D	452	ASP
1	D	461	GLN
1	D	462	SER
1	D	490	LYS
1	D	513	LYS
1	D	528	LYS
1	D	555	MSE
1	D	588	THR
1	D	593	ASN
1	D	601	LEU
1	D	619	THR
1	E	45	ILE
1	E	50	VAL
1	E	81	ASP
1	E	82	SER

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Mol	Chain	Res	Type
1	E	91	LYS
1	E	121	LEU
1	E	129	THR
1	E	178	GLU
1	E	182	LEU
1	E	185	LYS
1	E	201	LYS
1	E	206	PHE
1	E	228	GLU
1	E	246	ARG
1	E	272	GLU
1	E	285	ARG
1	E	291	LEU
1	E	312	LYS
1	E	383	ARG
1	E	385	THR
1	E	389	LEU
1	E	400	SER
1	E	421	GLU
1	E	432	GLU
1	E	459	VAL
1	E	460	GLN
1	E	474	PHE
1	E	561	GLU
1	E	593	ASN
1	E	601	LEU
1	E	615	PRO
1	E	619	THR
1	F	43	MSE
1	F	81	ASP
1	F	90	LYS
1	F	91	LYS
1	F	100	ILE
1	F	121	LEU
1	F	129	THR
1	F	139	ARG
1	F	178	GLU
1	F	182	LEU
1	F	185	LYS
1	F	201	LYS
1	F	206	PHE
1	F	211	ASP

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Mol	Chain	Res	Type
1	F	217	ILE
1	F	223	LEU
1	F	272	GLU
1	F	285	ARG
1	F	291	LEU
1	F	310	GLU
1	F	312	LYS
1	F	341	ASN
1	F	390	THR
1	F	408	TRP
1	F	413	LYS
1	F	460	GLN
1	F	463	ILE
1	F	490	LYS
1	F	491	ILE
1	F	542	GLU
1	F	560	LYS
1	F	561	GLU
1	F	576	LYS
1	F	601	LEU
1	G	43	MSE
1	G	45	ILE
1	G	50	VAL
1	G	91	LYS
1	G	129	THR
1	G	132	GLN
1	G	178	GLU
1	G	182	LEU
1	G	186	ASP
1	G	206	PHE
1	G	217	ILE
1	G	228	GLU
1	G	231	LYS
1	G	238	GLN
1	G	268	THR
1	G	285	ARG
1	G	291	LEU
1	G	296	GLU
1	G	312	LYS
1	G	328	LEU
1	G	341	ASN
1	G	375	SER

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Mol	Chain	Res	Type
1	G	383	ARG
1	G	389	LEU
1	G	392	SER
1	G	400	SER
1	G	403	LYS
1	G	408	TRP
1	G	421	GLU
1	G	432	GLU
1	G	459	VAL
1	G	463	ILE
1	G	490	LYS
1	G	542	GLU
1	G	560	LYS
1	G	576	LYS
1	G	601	LEU
1	H	45	ILE
1	H	82	SER
1	H	90	LYS
1	H	91	LYS
1	H	121	LEU
1	H	129	THR
1	H	178	GLU
1	H	182	LEU
1	H	185	LYS
1	H	206	PHE
1	H	217	ILE
1	H	269	ASP
1	H	291	LEU
1	H	312	LYS
1	H	328	LEU
1	H	341	ASN
1	H	343	THR
1	H	347	GLU
1	H	375	SER
1	H	385	THR
1	H	390	THR
1	H	403	LYS
1	H	432	GLU
1	H	459	VAL
1	H	463	ILE
1	H	505	ARG
1	H	528	LYS

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Mol	Chain	Res	Type
1	H	560	LYS
1	H	576	LYS
1	H	601	LEU
1	H	619	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	GLN
1	A	263	GLN
1	A	276	ASN
1	A	299	HIS
1	A	324	HIS
1	A	341	ASN
1	A	418	GLN
1	A	443	HIS
1	B	108	GLN
1	B	155	GLN
1	B	263	GLN
1	B	324	HIS
1	B	404	HIS
1	B	419	HIS
1	B	434	GLN
1	B	461	GLN
1	C	110	GLN
1	C	224	ASN
1	C	324	HIS
1	C	418	GLN
1	C	419	HIS
1	C	440	GLN
1	C	461	GLN
1	C	499	GLN
1	D	110	GLN
1	D	224	ASN
1	D	324	HIS
1	D	331	ASN
1	D	341	ASN
1	D	419	HIS
1	D	434	GLN
1	E	301	HIS
1	E	324	HIS
1	E	434	GLN

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Mol	Chain	Res	Type
1	E	461	GLN
1	F	108	GLN
1	F	324	HIS
1	F	336	GLN
1	F	341	ASN
1	F	365	GLN
1	F	434	GLN
1	F	461	GLN
1	G	257	ASN
1	G	263	GLN
1	G	301	HIS
1	G	324	HIS
1	G	414	ASN
1	G	461	GLN
1	H	224	ASN
1	H	301	HIS
1	H	324	HIS
1	H	341	ASN
1	H	414	ASN
1	H	434	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	F	625	1	58,58,58	1.11	4 (6%)	85,89,89	1.64	19 (22%)
2	FAD	A	625	1	58,58,58	1.22	6 (10%)	85,89,89	1.84	19 (22%)
2	FAD	G	625	1	58,58,58	1.48	6 (10%)	85,89,89	1.62	16 (18%)
2	FAD	C	625	1	58,58,58	1.44	8 (13%)	85,89,89	1.65	16 (18%)
2	FAD	E	625	1	58,58,58	1.48	6 (10%)	85,89,89	1.78	18 (21%)
2	FAD	B	625	1	58,58,58	2.30	10 (17%)	85,89,89	1.77	19 (22%)
2	FAD	H	625	1	58,58,58	1.35	9 (15%)	85,89,89	1.48	16 (18%)
2	FAD	D	625	1	58,58,58	1.24	6 (10%)	85,89,89	1.59	19 (22%)

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	F	625	1	-	4/34/50/50	0/6/6/6
2	FAD	A	625	1	-	4/34/50/50	0/6/6/6
2	FAD	G	625	1	-	1/34/50/50	0/6/6/6
2	FAD	C	625	1	-	2/34/50/50	0/6/6/6
2	FAD	E	625	1	-	7/34/50/50	0/6/6/6
2	FAD	B	625	1	-	4/34/50/50	0/6/6/6
2	FAD	H	625	1	-	2/34/50/50	0/6/6/6
2	FAD	D	625	1	-	2/34/50/50	0/6/6/6

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	625	FAD	P-O3P	12.91	1.73	1.59
2	G	625	FAD	P-O3P	7.57	1.67	1.59
2	E	625	FAD	P-O3P	7.04	1.67	1.59
2	B	625	FAD	PA-O3P	-6.47	1.52	1.59
2	C	625	FAD	P-O3P	5.16	1.65	1.59
2	C	625	FAD	C10-N1	3.96	1.41	1.33
2	H	625	FAD	P-O3P	3.87	1.63	1.59
2	H	625	FAD	C5A-N7A	-3.83	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	625	FAD	C10-N1	3.60	1.40	1.33
2	D	625	FAD	P-O3P	3.46	1.63	1.59
2	D	625	FAD	C10-N1	3.38	1.40	1.33
2	G	625	FAD	C10-N1	3.22	1.39	1.33
2	C	625	FAD	C5X-N5	-3.18	1.33	1.39
2	E	625	FAD	C5X-N5	-3.08	1.33	1.39
2	D	625	FAD	C5A-N7A	-3.07	1.33	1.39
2	B	625	FAD	C5A-N7A	-3.07	1.33	1.39
2	F	625	FAD	C4X-N5	3.07	1.37	1.30
2	F	625	FAD	C10-N1	3.07	1.39	1.33
2	C	625	FAD	C5A-N7A	-3.05	1.33	1.39
2	C	625	FAD	C8M-C8	3.02	1.56	1.51
2	E	625	FAD	C10-N1	2.95	1.39	1.33
2	H	625	FAD	C10-N1	2.87	1.39	1.33
2	H	625	FAD	PA-O3P	2.81	1.62	1.59
2	B	625	FAD	C8M-C8	2.80	1.56	1.51
2	B	625	FAD	C7M-C7	2.79	1.56	1.51
2	G	625	FAD	PA-O3P	2.78	1.62	1.59
2	A	625	FAD	C10-N1	2.76	1.38	1.33
2	H	625	FAD	C7M-C7	2.71	1.56	1.51
2	B	625	FAD	C5X-N5	-2.69	1.34	1.39
2	E	625	FAD	C8M-C8	2.68	1.56	1.51
2	H	625	FAD	C4A-N9A	-2.68	1.32	1.37
2	F	625	FAD	C2-N1	2.66	1.42	1.36
2	B	625	FAD	C8A-N9A	-2.65	1.33	1.37
2	A	625	FAD	C5'-C4'	2.56	1.55	1.51
2	D	625	FAD	C4A-N9A	-2.54	1.32	1.37
2	D	625	FAD	C4X-N5	2.50	1.36	1.30
2	G	625	FAD	C8M-C8	2.48	1.55	1.51
2	A	625	FAD	C4X-N5	2.41	1.36	1.30
2	H	625	FAD	C4X-N5	2.40	1.36	1.30
2	H	625	FAD	C5X-N5	-2.40	1.35	1.39
2	H	625	FAD	C8M-C8	2.40	1.55	1.51
2	E	625	FAD	P-O2P	-2.39	1.44	1.55
2	E	625	FAD	C5A-N7A	-2.37	1.34	1.39
2	D	625	FAD	C5X-N5	-2.35	1.35	1.39
2	G	625	FAD	C4X-N5	2.33	1.35	1.30
2	B	625	FAD	C4X-N5	2.33	1.35	1.30
2	C	625	FAD	PA-O1A	2.32	1.58	1.50
2	A	625	FAD	PA-O5B	2.31	1.68	1.59
2	G	625	FAD	C5X-N5	-2.26	1.35	1.39
2	C	625	FAD	C4X-N5	2.21	1.35	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	625	FAD	C8M-C8	2.19	1.55	1.51
2	F	625	FAD	C5A-N7A	-2.10	1.35	1.39
2	C	625	FAD	C4A-N9A	-2.09	1.33	1.37
2	A	625	FAD	O4B-C4B	-2.08	1.40	1.45
2	B	625	FAD	PA-O1A	2.04	1.57	1.50

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	625	FAD	C5A-C4A-N3A	-6.12	118.29	126.72
2	G	625	FAD	N3A-C2A-N1A	-5.57	120.15	128.58
2	E	625	FAD	C5A-C4A-N3A	-5.38	119.31	126.72
2	A	625	FAD	N3A-C2A-N1A	-5.30	120.56	128.58
2	C	625	FAD	C5A-C4A-N3A	-5.21	119.54	126.72
2	A	625	FAD	C5A-C4A-N3A	-5.14	119.64	126.72
2	F	625	FAD	C5A-C4A-N3A	-4.84	120.06	126.72
2	D	625	FAD	N3A-C2A-N1A	-4.84	121.26	128.58
2	C	625	FAD	N3A-C2A-N1A	-4.81	121.30	128.58
2	H	625	FAD	C5A-C4A-N3A	-4.80	120.10	126.72
2	A	625	FAD	N9A-C8A-N7A	-4.79	107.14	113.94
2	E	625	FAD	N3A-C2A-N1A	-4.77	121.36	128.58
2	D	625	FAD	C5A-C4A-N3A	-4.74	120.19	126.72
2	F	625	FAD	N3A-C2A-N1A	-4.59	121.64	128.58
2	G	625	FAD	C5A-C4A-N3A	-4.46	120.57	126.72
2	A	625	FAD	C4A-N9A-C8A	4.27	110.22	105.74
2	A	625	FAD	N3A-C4A-N9A	4.24	134.38	127.17
2	H	625	FAD	N3A-C2A-N1A	-4.20	122.22	128.58
2	E	625	FAD	N9A-C8A-N7A	-4.16	108.03	113.94
2	A	625	FAD	C2A-N3A-C4A	4.03	121.68	111.83
2	B	625	FAD	O3P-PA-O1A	-3.99	98.70	110.70
2	E	625	FAD	C2A-N3A-C4A	3.97	121.54	111.83
2	F	625	FAD	O2A-PA-O3P	3.96	117.97	107.27
2	G	625	FAD	C2A-N3A-C4A	3.90	121.34	111.83
2	B	625	FAD	C2A-N3A-C4A	3.89	121.34	111.83
2	B	625	FAD	N3A-C4A-N9A	3.86	133.73	127.17
2	G	625	FAD	N9A-C8A-N7A	-3.83	108.50	113.94
2	E	625	FAD	C5A-N7A-C8A	3.82	109.45	103.45
2	B	625	FAD	C4A-C5A-N7A	-3.70	106.35	110.58
2	C	625	FAD	C2A-N3A-C4A	3.70	120.87	111.83
2	E	625	FAD	C4A-C5A-N7A	-3.68	106.38	110.58
2	A	625	FAD	C5A-N7A-C8A	3.66	109.20	103.45
2	E	625	FAD	N3A-C4A-N9A	3.65	133.38	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	625	FAD	N3A-C2A-N1A	-3.65	123.06	128.58
2	F	625	FAD	C2A-N3A-C4A	3.65	120.74	111.83
2	C	625	FAD	O2A-PA-O3P	3.63	117.10	107.27
2	E	625	FAD	C5X-N5-C4X	3.50	123.75	118.09
2	C	625	FAD	N9A-C8A-N7A	-3.48	109.00	113.94
2	C	625	FAD	C4A-C5A-N7A	-3.46	106.63	110.58
2	D	625	FAD	C2A-N3A-C4A	3.38	120.08	111.83
2	B	625	FAD	C5A-N7A-C8A	3.37	108.75	103.45
2	D	625	FAD	N3A-C4A-N9A	3.36	132.88	127.17
2	E	625	FAD	C10-C4X-N5	-3.36	117.96	124.81
2	D	625	FAD	N9A-C8A-N7A	-3.33	109.21	113.94
2	C	625	FAD	C5A-N7A-C8A	3.26	108.58	103.45
2	C	625	FAD	C5X-N5-C4X	3.22	123.30	118.09
2	B	625	FAD	C8M-C8-C9	-3.22	113.91	119.57
2	F	625	FAD	N3A-C4A-N9A	3.21	132.63	127.17
2	A	625	FAD	C4-C4X-N5	3.21	122.64	118.21
2	F	625	FAD	C4-N3-C2	-3.20	119.97	125.64
2	B	625	FAD	N9A-C8A-N7A	-3.17	109.44	113.94
2	H	625	FAD	C2A-N3A-C4A	3.14	119.49	111.83
2	E	625	FAD	C4-N3-C2	-3.13	120.08	125.64
2	B	625	FAD	C5'-C4'-C3'	-3.13	106.32	112.22
2	H	625	FAD	C4-C4X-N5	3.08	122.47	118.21
2	F	625	FAD	N9A-C8A-N7A	-3.01	109.67	113.94
2	H	625	FAD	O2A-PA-O3P	3.00	115.39	107.27
2	D	625	FAD	C4-N3-C2	-2.98	120.35	125.64
2	G	625	FAD	N3A-C4A-N9A	2.98	132.23	127.17
2	A	625	FAD	O2A-PA-O3P	2.97	115.31	107.27
2	E	625	FAD	C4A-N9A-C8A	2.96	108.85	105.74
2	H	625	FAD	N3A-C4A-N9A	2.95	132.19	127.17
2	C	625	FAD	C4-N3-C2	-2.95	120.41	125.64
2	E	625	FAD	C4-C4X-N5	2.94	122.27	118.21
2	H	625	FAD	C10-C4X-N5	-2.94	118.80	124.81
2	F	625	FAD	O3P-PA-O1A	-2.93	101.89	110.70
2	F	625	FAD	C4A-C5A-N7A	-2.91	107.25	110.58
2	D	625	FAD	C4X-C4-N3	2.91	120.65	113.25
2	A	625	FAD	O4B-C1B-N9A	-2.86	102.60	108.09
2	B	625	FAD	C9A-C5X-N5	-2.86	119.42	122.45
2	C	625	FAD	N3A-C4A-N9A	2.84	131.99	127.17
2	F	625	FAD	C4X-C4-N3	2.83	120.46	113.25
2	C	625	FAD	C10-C4X-N5	-2.83	119.04	124.81
2	G	625	FAD	C4A-N9A-C8A	2.82	108.70	105.74
2	F	625	FAD	C5A-N7A-C8A	2.78	107.83	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	625	FAD	C4-C4X-N5	2.78	122.05	118.21
2	F	625	FAD	C10-C4X-N5	-2.78	119.13	124.81
2	A	625	FAD	C4A-C5A-N7A	-2.74	107.44	110.58
2	G	625	FAD	C5A-N7A-C8A	2.73	107.73	103.45
2	C	625	FAD	O3P-PA-O1A	-2.71	102.55	110.70
2	A	625	FAD	C4X-C10-N10	2.71	120.36	116.48
2	B	625	FAD	C4X-C4-N3	2.69	120.11	113.25
2	A	625	FAD	C4X-C4-N3	2.68	120.07	113.25
2	G	625	FAD	O3P-PA-O1A	-2.68	102.66	110.70
2	G	625	FAD	C4-N3-C2	-2.67	120.89	125.64
2	A	625	FAD	C10-N1-C2	2.67	122.63	116.85
2	B	625	FAD	C4-N3-C2	-2.66	120.91	125.64
2	A	625	FAD	C5A-C6A-N6A	-2.65	116.73	123.29
2	A	625	FAD	C10-C4X-N5	-2.63	119.44	124.81
2	C	625	FAD	C4X-C4-N3	2.60	119.88	113.25
2	C	625	FAD	C9A-C5X-N5	-2.60	119.70	122.45
2	A	625	FAD	C4-N3-C2	-2.59	121.05	125.64
2	C	625	FAD	C4-C4X-N5	2.58	121.78	118.21
2	H	625	FAD	O3P-PA-O1A	-2.57	102.97	110.70
2	H	625	FAD	C4-N3-C2	-2.57	121.09	125.64
2	G	625	FAD	C4X-C4-N3	2.54	119.71	113.25
2	H	625	FAD	C4X-C10-N10	2.52	120.09	116.48
2	D	625	FAD	O2A-PA-O3P	2.51	114.06	107.27
2	F	625	FAD	C4-C4X-N5	2.49	121.64	118.21
2	D	625	FAD	C4A-N9A-C8A	2.48	108.34	105.74
2	D	625	FAD	O3P-PA-O1A	-2.48	103.24	110.70
2	H	625	FAD	N9A-C8A-N7A	-2.47	110.43	113.94
2	E	625	FAD	O4B-C1B-N9A	-2.44	103.40	108.09
2	A	625	FAD	N6A-C6A-N1A	2.44	123.81	118.38
2	C	625	FAD	C5A-C4A-N9A	2.43	108.46	105.81
2	H	625	FAD	C5A-N7A-C8A	2.43	107.27	103.45
2	B	625	FAD	O2A-PA-O1A	2.43	123.73	112.44
2	G	625	FAD	C4A-C5A-N7A	-2.42	107.81	110.58
2	A	625	FAD	O3P-PA-O1A	-2.42	103.44	110.70
2	H	625	FAD	C4A-C5A-N7A	-2.40	107.83	110.58
2	E	625	FAD	C4X-C4-N3	2.40	119.35	113.25
2	D	625	FAD	C5A-N7A-C8A	2.39	107.20	103.45
2	D	625	FAD	C4X-C10-N10	2.39	119.90	116.48
2	E	625	FAD	O3B-C3B-C4B	-2.38	104.24	111.08
2	E	625	FAD	O3P-PA-O1A	-2.38	103.54	110.70
2	G	625	FAD	C10-C4X-N5	-2.37	119.97	124.81
2	G	625	FAD	C4X-C10-N10	2.34	119.83	116.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	625	FAD	C8M-C8-C7	2.31	125.48	120.76
2	B	625	FAD	O3B-C3B-C4B	-2.29	104.49	111.08
2	D	625	FAD	O4-C4-C4X	-2.29	120.49	126.53
2	H	625	FAD	C4X-C4-N3	2.26	119.02	113.25
2	B	625	FAD	C4-C4X-N5	2.25	121.32	118.21
2	E	625	FAD	O2A-PA-O3P	2.24	113.34	107.27
2	H	625	FAD	C5'-C4'-C3'	-2.24	107.99	112.22
2	D	625	FAD	C4-C4X-N5	2.22	121.28	118.21
2	G	625	FAD	C5X-N5-C4X	2.21	121.66	118.09
2	E	625	FAD	C4X-C10-N10	2.20	119.63	116.48
2	B	625	FAD	C10-C4X-N5	-2.19	120.33	124.81
2	F	625	FAD	C9A-C5X-N5	-2.16	120.17	122.45
2	D	625	FAD	C5X-N5-C4X	2.13	121.54	118.09
2	G	625	FAD	O3B-C3B-C4B	-2.13	104.96	111.08
2	F	625	FAD	C4A-N9A-C8A	2.13	107.97	105.74
2	F	625	FAD	O3B-C3B-C4B	-2.12	104.98	111.08
2	D	625	FAD	C10-C4X-N5	-2.11	120.49	124.81
2	F	625	FAD	C5X-N5-C4X	2.11	121.51	118.09
2	F	625	FAD	O4B-C1B-N9A	-2.07	104.12	108.09
2	F	625	FAD	O2A-PA-O1A	2.07	122.06	112.44
2	D	625	FAD	O4B-C1B-N9A	-2.06	104.13	108.09
2	D	625	FAD	C5B-C4B-C3B	-2.05	107.85	115.21
2	H	625	FAD	C2A-N1A-C6A	2.02	122.06	118.73
2	B	625	FAD	O4-C4-C4X	-2.02	121.19	126.53
2	D	625	FAD	C5'-C4'-C3'	-2.02	108.41	112.22

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	625	FAD	C5'-O5'-P-O1P
2	B	625	FAD	C5'-O5'-P-O1P
2	C	625	FAD	C5'-O5'-P-O1P
2	C	625	FAD	C5'-O5'-P-O3P
2	E	625	FAD	C5'-O5'-P-O1P
2	G	625	FAD	C5'-O5'-P-O1P
2	H	625	FAD	C5'-O5'-P-O1P
2	H	625	FAD	C5'-O5'-P-O3P
2	F	625	FAD	P-O3P-PA-O1A
2	A	625	FAD	PA-O3P-P-O5'
2	D	625	FAD	PA-O3P-P-O5'
2	E	625	FAD	PA-O3P-P-O5'

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Mol	Chain	Res	Type	Atoms
2	F	625	FAD	PA-O3P-P-O5'
2	B	625	FAD	C5'-O5'-P-O2P
2	B	625	FAD	C5'-O5'-P-O3P
2	D	625	FAD	C5'-O5'-P-O1P
2	E	625	FAD	C5'-O5'-P-O3P
2	F	625	FAD	C5'-O5'-P-O1P
2	A	625	FAD	P-O3P-PA-O1A
2	E	625	FAD	P-O3P-PA-O1A
2	F	625	FAD	P-O3P-PA-O2A
2	E	625	FAD	P-O3P-PA-O2A
2	B	625	FAD	O4B-C4B-C5B-O5B
2	E	625	FAD	O4B-C4B-C5B-O5B
2	E	625	FAD	C2B-C1B-N9A-C8A
2	A	625	FAD	P-O3P-PA-O2A

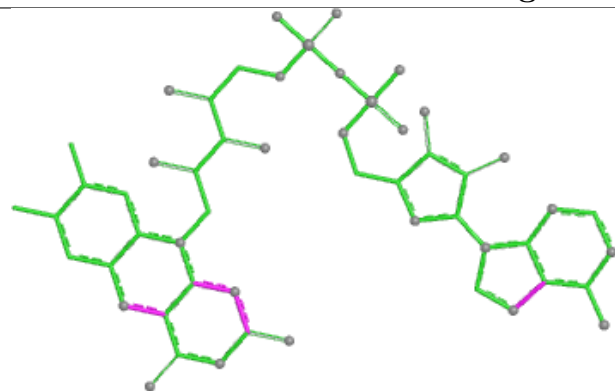
There are no ring outliers.

4 monomers are involved in 10 short contacts:

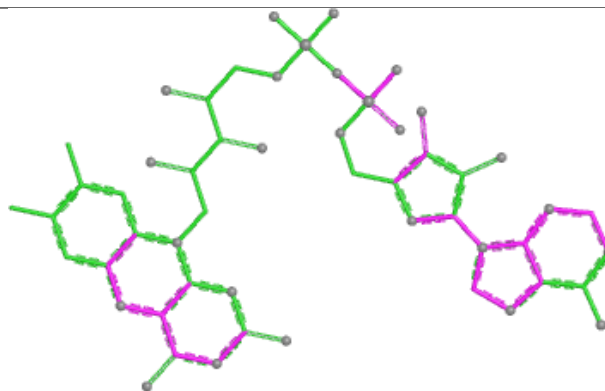
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	625	FAD	2	0
2	E	625	FAD	1	0
2	B	625	FAD	5	0
2	D	625	FAD	2	0

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

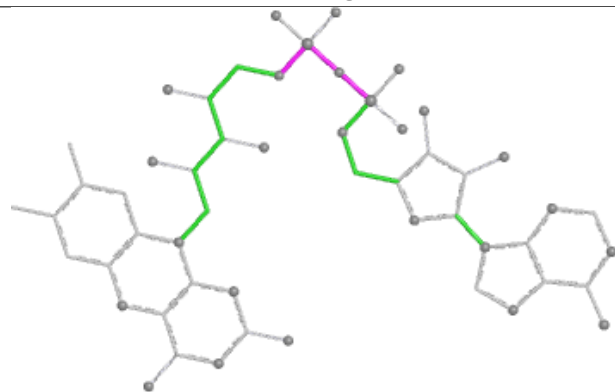
Ligand FAD F 625



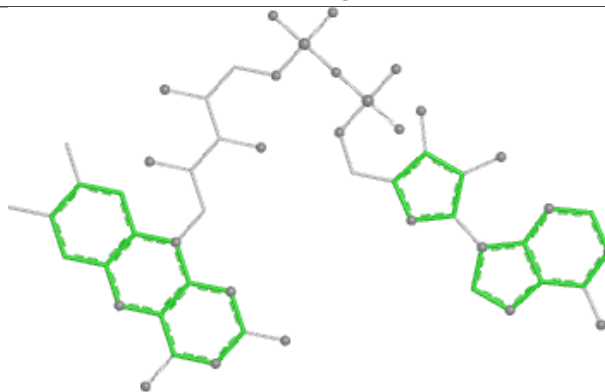
Bond lengths



Bond angles

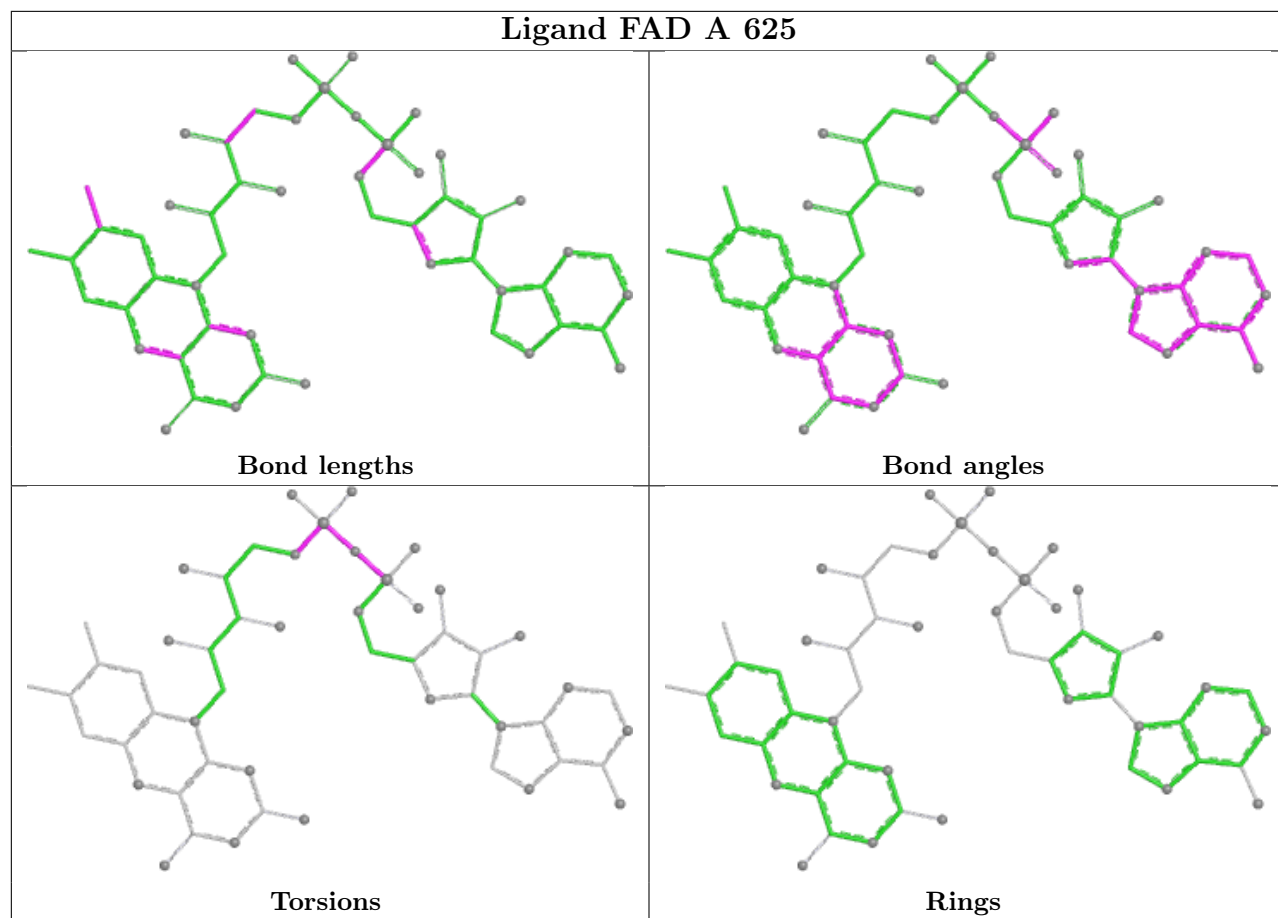


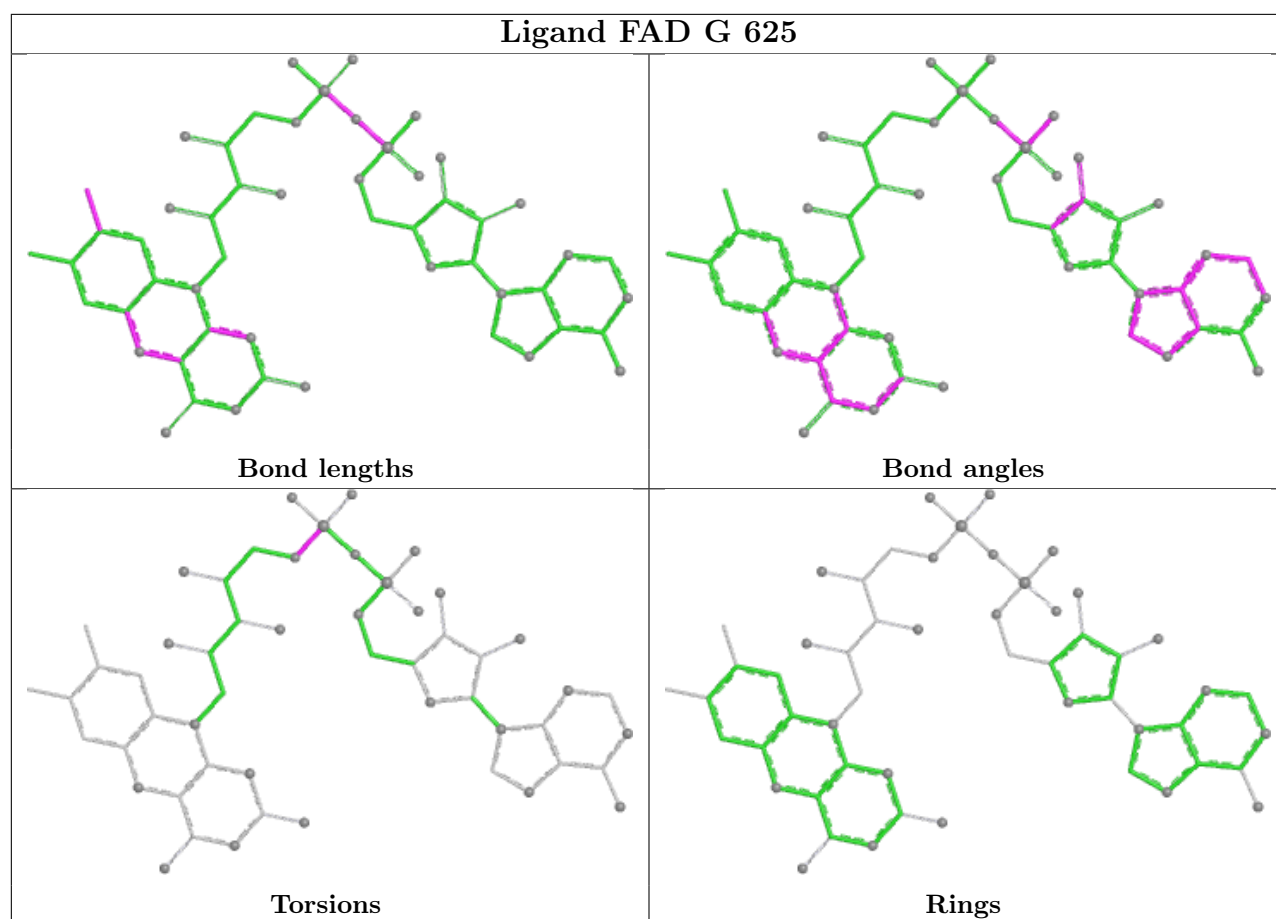
Torsions

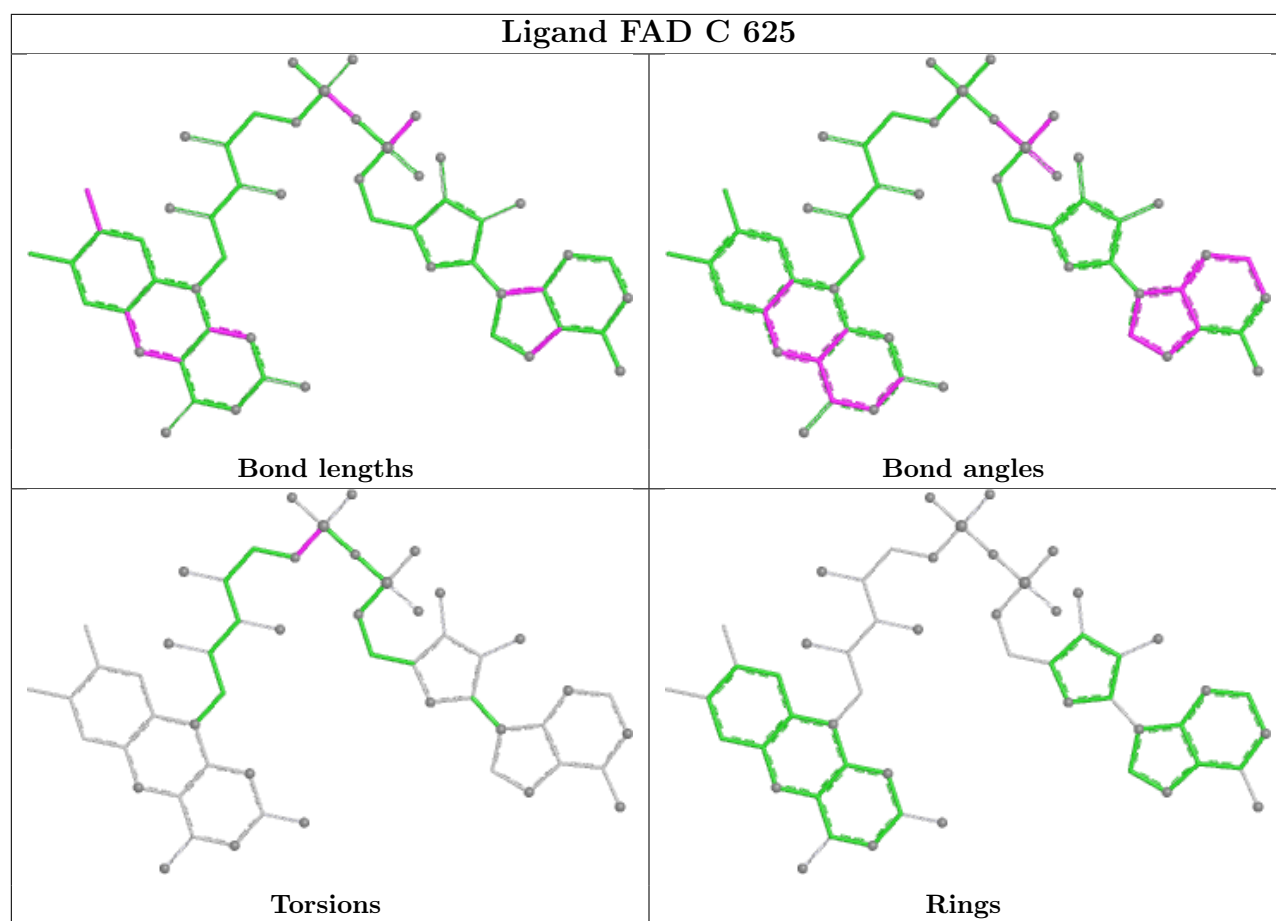


Rings

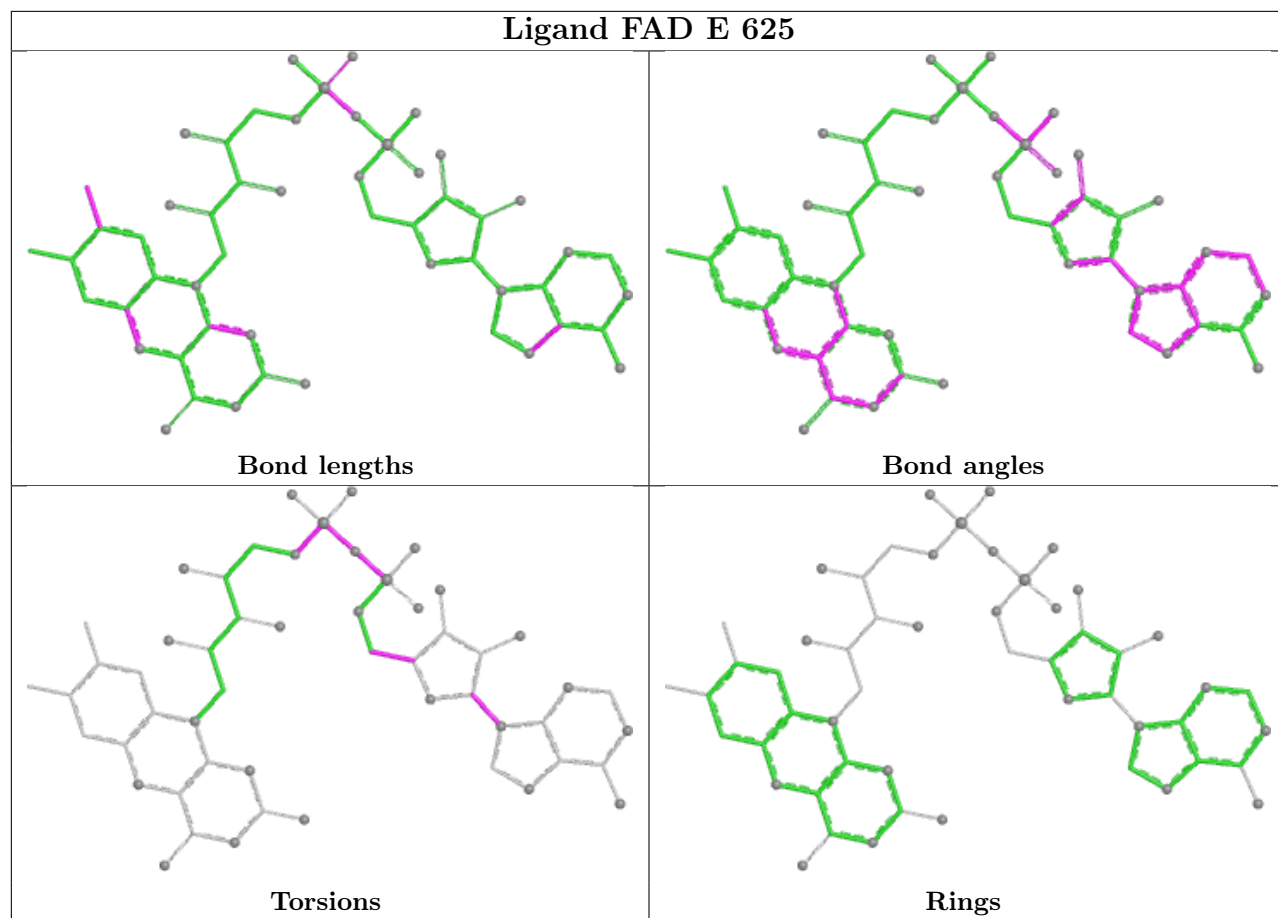
Ligand FAD A 625

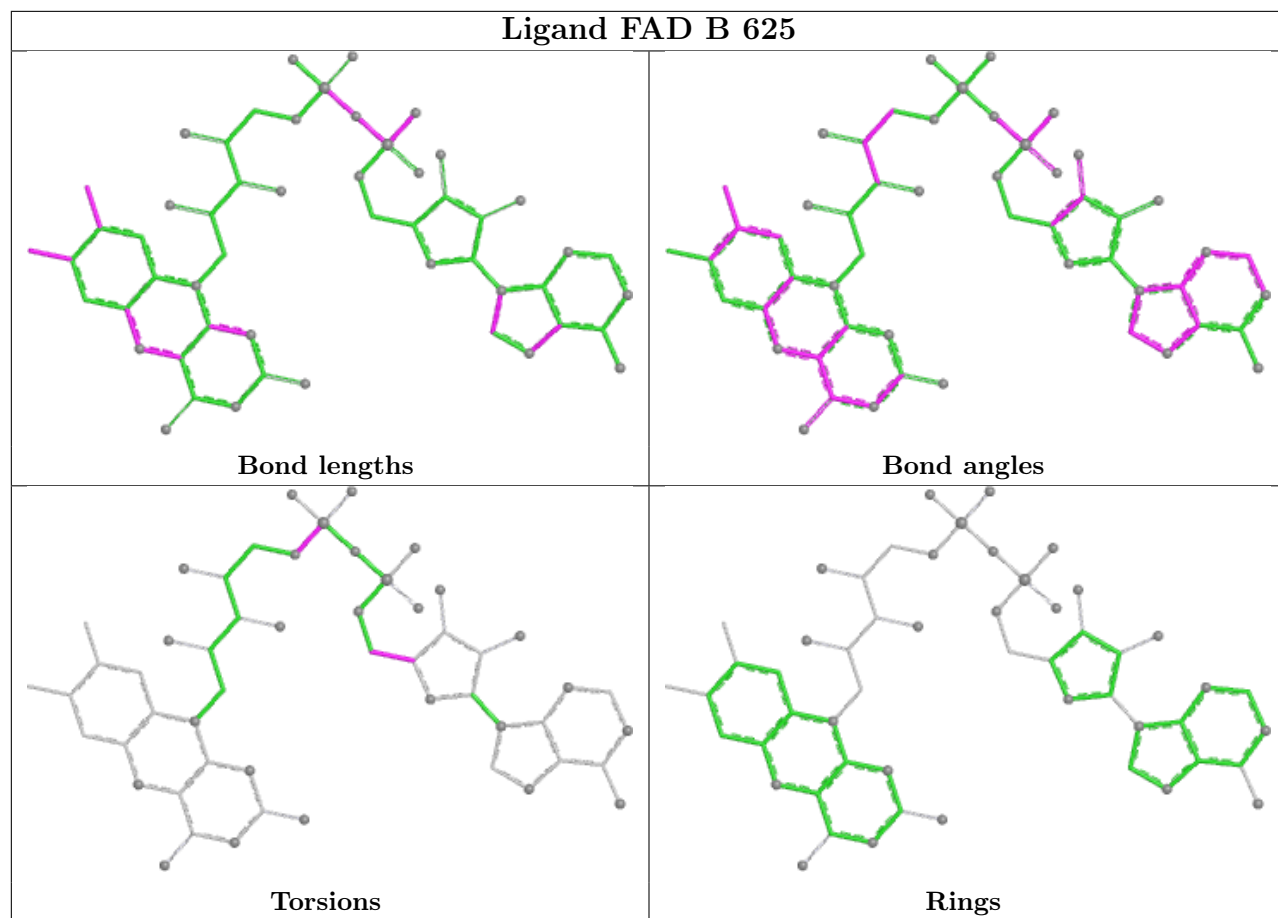


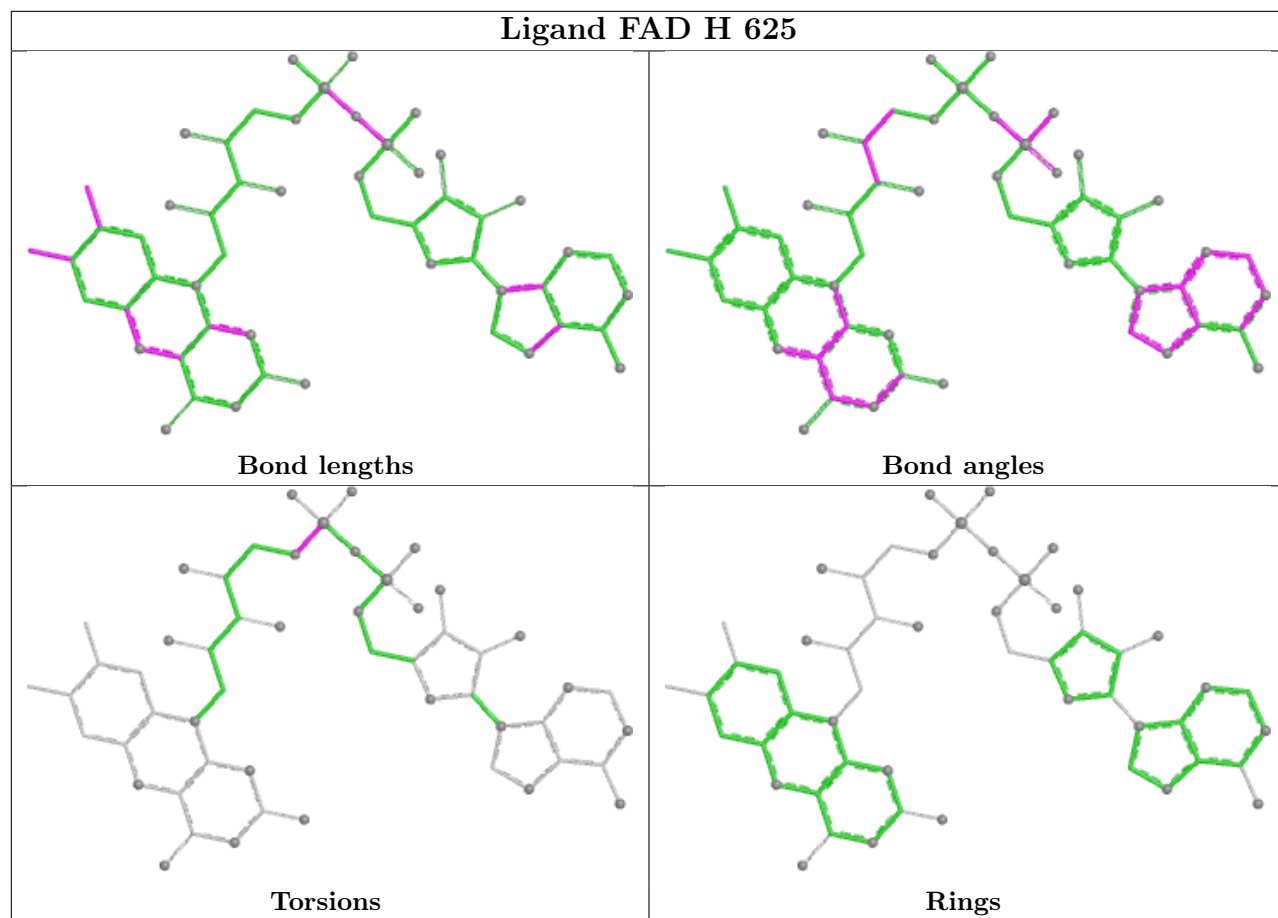


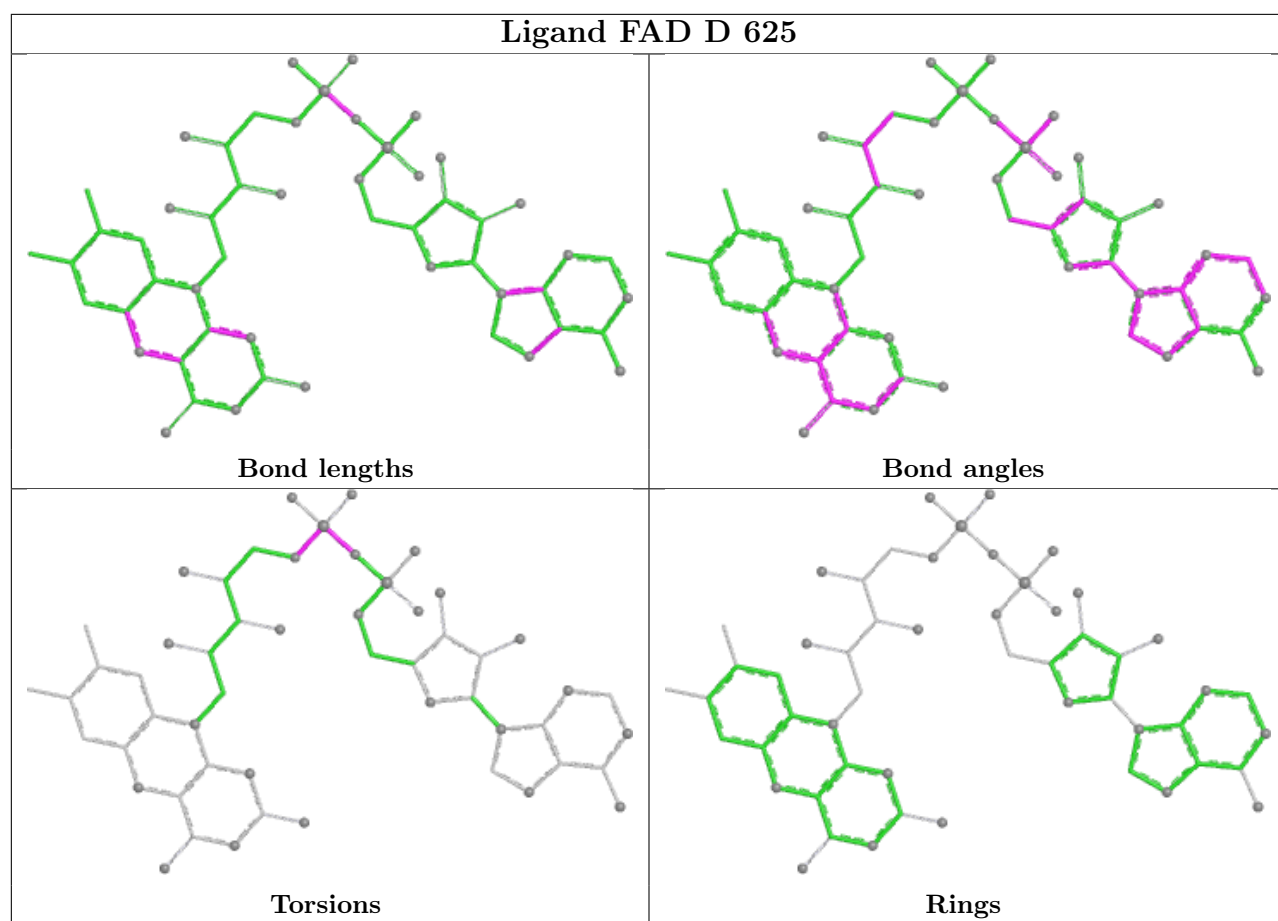


Ligand FAD E 625









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	561/622 (90%)	-0.30	9 (1%) 70 76	8, 16, 31, 51	0
1	B	561/622 (90%)	0.29	21 (3%) 45 51	12, 23, 38, 58	0
1	C	561/622 (90%)	-0.27	6 (1%) 78 82	8, 16, 32, 57	0
1	D	561/622 (90%)	-0.06	9 (1%) 70 76	8, 23, 40, 63	0
1	E	561/622 (90%)	-0.18	15 (2%) 56 63	5, 16, 36, 56	0
1	F	561/622 (90%)	-0.33	7 (1%) 76 81	4, 14, 31, 50	0
1	G	561/622 (90%)	-0.15	10 (1%) 67 72	3, 15, 33, 53	0
1	H	561/622 (90%)	-0.30	13 (2%) 61 66	3, 14, 30, 55	0
All	All	4488/4976 (90%)	-0.16	90 (2%) 65 70	3, 17, 36, 63	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	458	ALA	6.1
1	E	47	TYR	6.1
1	B	445	TRP	5.5
1	D	455	SER	5.4
1	G	44	ASP	5.1
1	H	44	ASP	5.1
1	G	458	ALA	4.7
1	B	47	TYR	4.4
1	E	45	ILE	4.4
1	B	195	TRP	4.3
1	D	458	ALA	4.2
1	B	167	HIS	4.0
1	B	446	HIS	4.0
1	F	458	ALA	3.9
1	F	459	VAL	3.9
1	A	458	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	H	459	VAL	3.8
1	G	455	SER	3.8
1	F	619	THR	3.7
1	F	455	SER	3.7
1	B	473	PHE	3.6
1	B	577	ASN	3.5
1	B	548	HIS	3.5
1	B	197	ARG	3.5
1	E	455	SER	3.4
1	H	45	ILE	3.3
1	A	459	VAL	3.3
1	D	45	ILE	3.3
1	E	458	ALA	3.3
1	B	455	SER	3.3
1	D	619	THR	3.2
1	D	459	VAL	3.2
1	C	455	SER	3.1
1	B	460	GLN	3.1
1	A	455	SER	3.1
1	B	613	PHE	3.1
1	C	459	VAL	3.1
1	E	615	PRO	3.0
1	G	454	PHE	3.0
1	H	457	GLY	3.0
1	E	619	THR	2.9
1	G	456	TYR	2.9
1	A	619	THR	2.8
1	E	385	THR	2.8
1	B	592	ALA	2.8
1	A	211	ASP	2.7
1	B	508	ALA	2.7
1	B	45	ILE	2.7
1	E	618	PHE	2.7
1	B	459	VAL	2.7
1	C	458	ALA	2.6
1	H	70	TYR	2.6
1	A	307	ASP	2.5
1	C	44	ASP	2.5
1	G	459	VAL	2.5
1	G	389	LEU	2.5
1	C	45	ILE	2.4
1	H	458	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	389	LEU	2.4
1	D	44	ASP	2.3
1	G	615	PRO	2.3
1	E	614	THR	2.3
1	H	455	SER	2.3
1	A	453	ALA	2.3
1	H	619	THR	2.3
1	E	389	LEU	2.2
1	A	44	ASP	2.2
1	D	211	ASP	2.2
1	H	211	ASP	2.2
1	H	400	SER	2.2
1	G	45	ILE	2.2
1	H	456	TYR	2.1
1	B	81	ASP	2.1
1	E	388	GLU	2.1
1	H	235	ASP	2.1
1	E	459	VAL	2.1
1	A	45	ILE	2.1
1	G	211	ASP	2.1
1	D	460	GLN	2.1
1	E	460	GLN	2.1
1	B	242	ALA	2.1
1	H	269	ASP	2.1
1	B	474	PHE	2.1
1	F	400	SER	2.0
1	F	44	ASP	2.0
1	E	456	TYR	2.0
1	C	388	GLU	2.0
1	E	343	THR	2.0
1	F	211	ASP	2.0
1	B	500	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

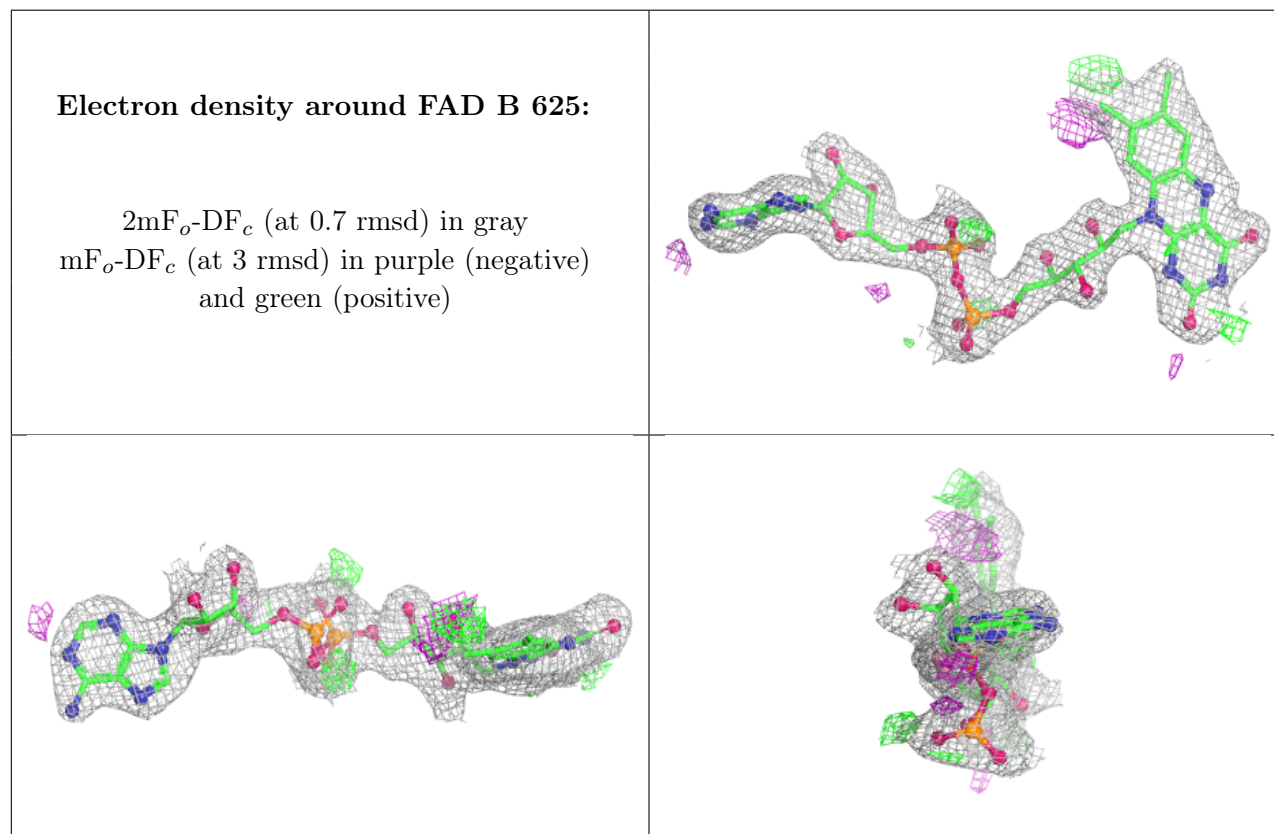
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

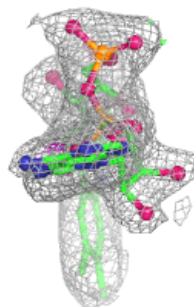
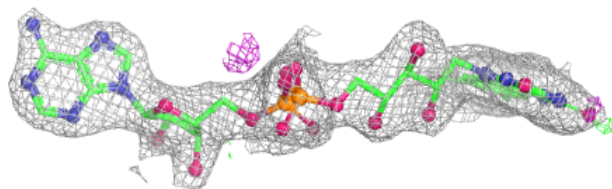
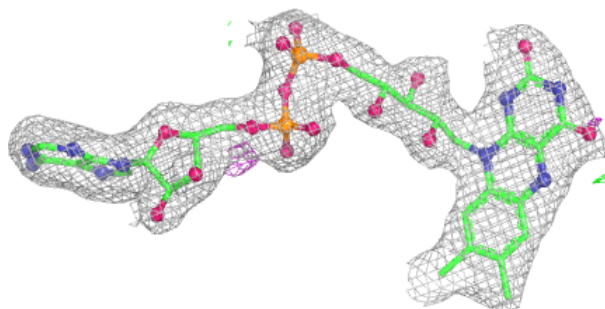
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FAD	B	625	53/53	0.95	0.07	12,23,28,33	0
2	FAD	D	625	53/53	0.95	0.07	17,21,26,27	0
2	FAD	G	625	53/53	0.96	0.06	10,15,20,22	0
2	FAD	A	625	53/53	0.97	0.06	6,14,17,19	0
2	FAD	E	625	53/53	0.97	0.06	10,16,19,23	0
2	FAD	C	625	53/53	0.97	0.06	8,15,18,20	0
2	FAD	H	625	53/53	0.97	0.05	9,13,16,19	0
2	FAD	F	625	53/53	0.98	0.06	10,13,17,20	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.

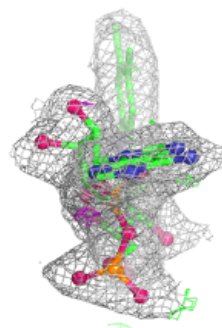
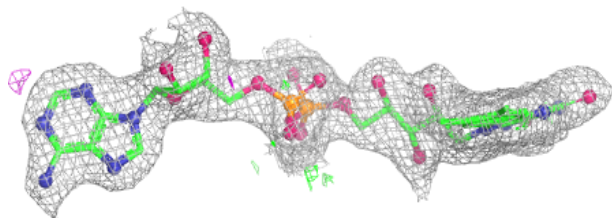
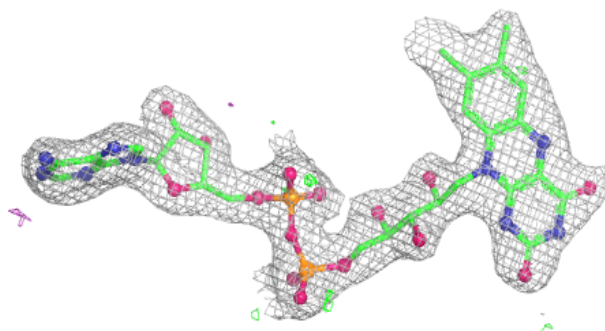


Electron density around FAD D 625:

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

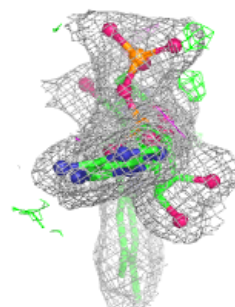
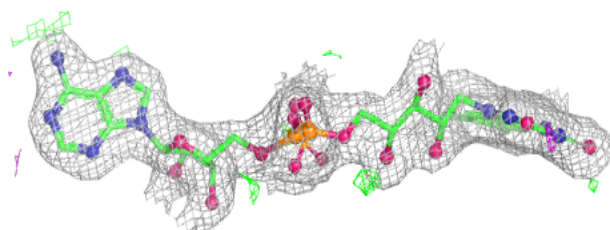
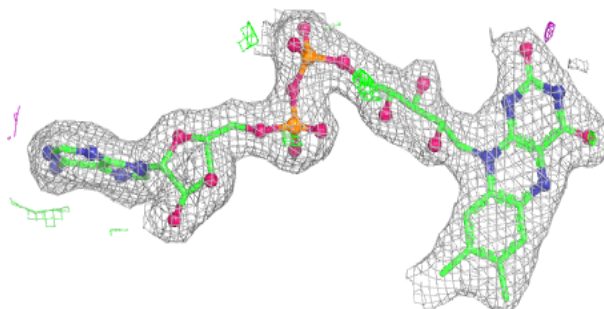
**Electron density around FAD G 625:**

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

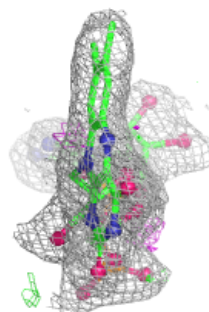
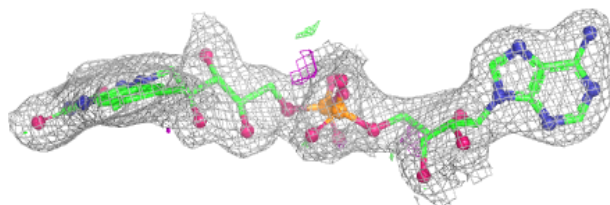
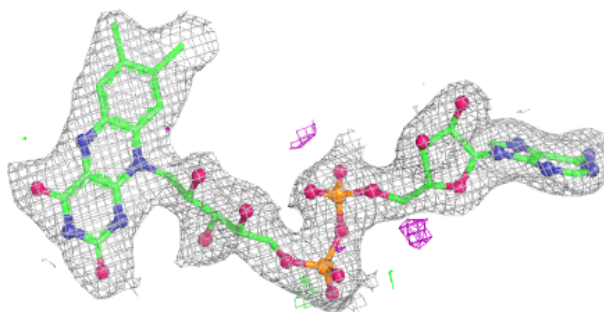


Electron density around FAD A 625:

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

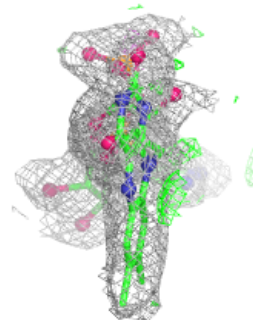
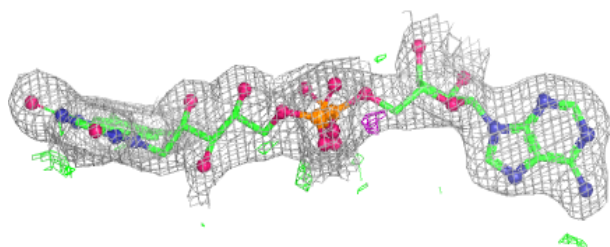
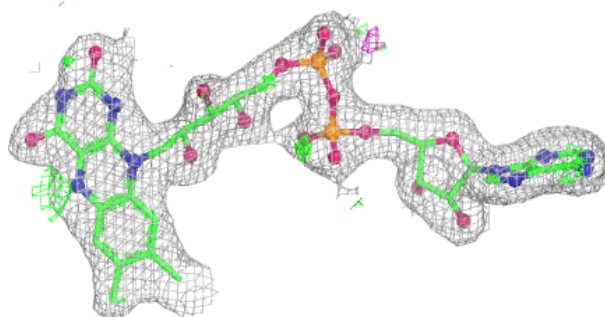
**Electron density around FAD E 625:**

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

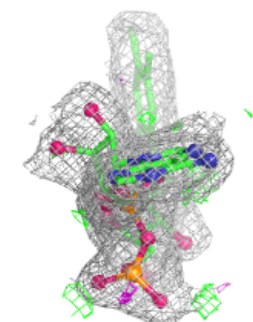
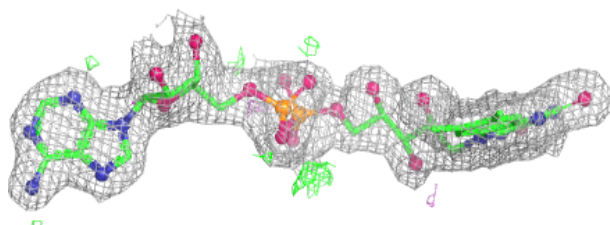
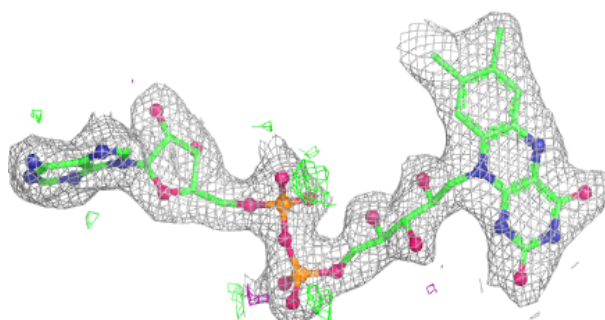


Electron density around FAD C 625:

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

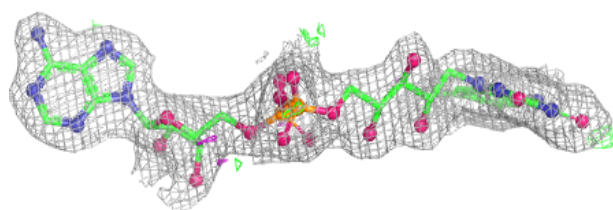
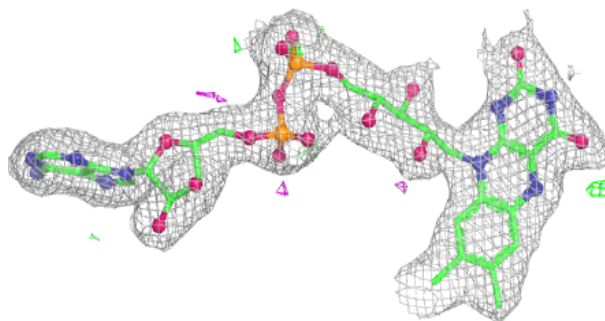
**Electron density around FAD H 625:**

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



Electron density around FAD F 625:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.