



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:09 am BST

PDB ID : 1TZL  
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](mailto: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.

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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 : 2.11  
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) : 2.11

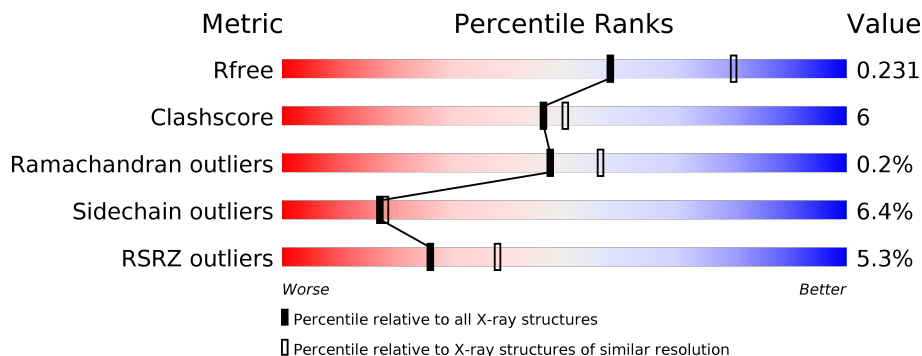
# 1 Overall quality at a glance i

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.



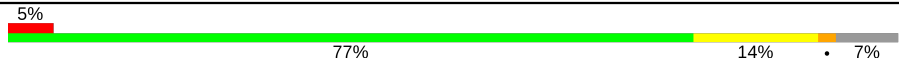

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 78%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">3%      78%      14%      • 7%</p>
1	B	622	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 68%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">8%      68%      20%      • 7%</p>
1	C	622	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 78%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">4%      78%      13%      • 7%</p>
1	D	622	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 76%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">7%      76%      15%      • 7%</p>
1	E	622	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 77%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">5%      77%      14%      • 7%</p>
1	F	622	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 75%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">3%      75%      16%      • 7%</p>

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Mol	Chain	Length	Quality of chain
1	G	622	
1	H	622	

## 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
			Total	C	N	O	S	Se			
1	A	577	4549	2872	778	874	9	16	0	0	0
1	B	577	4549	2872	778	874	9	16	0	0	0
1	C	577	4549	2872	778	874	9	16	0	0	0
1	D	577	4549	2872	778	874	9	16	0	0	0
1	E	577	4549	2872	778	874	9	16	0	0	0
1	F	577	4549	2872	778	874	9	16	0	0	0
1	G	577	4549	2872	778	874	9	16	0	0	0
1	H	577	4549	2872	778	874	9	16	0	0	0

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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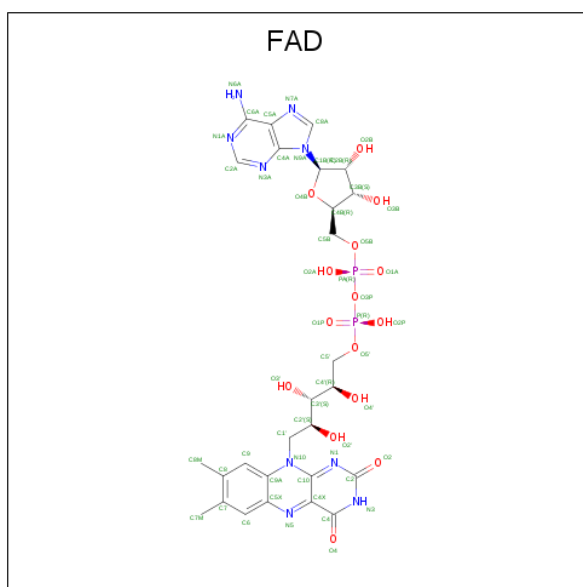
Chain	Residue	Modelled	Actual	Comment	Reference
D	417	MSE	MET	MODIFIED RESIDUE	UNP Q8J136
D	497	MSE	MET	MODIFIED RESIDUE	UNP Q8J136
D	518	MSE	MET	MODIFIED RESIDUE	UNP Q8J136
D	519	MSE	MET	MODIFIED RESIDUE	UNP Q8J136
D	522	MSE	MET	MODIFIED RESIDUE	UNP Q8J136
D	525	MSE	MET	MODIFIED RESIDUE	UNP Q8J136
D	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 (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	C	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	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	G	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		

- Molecule 3 is water.

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

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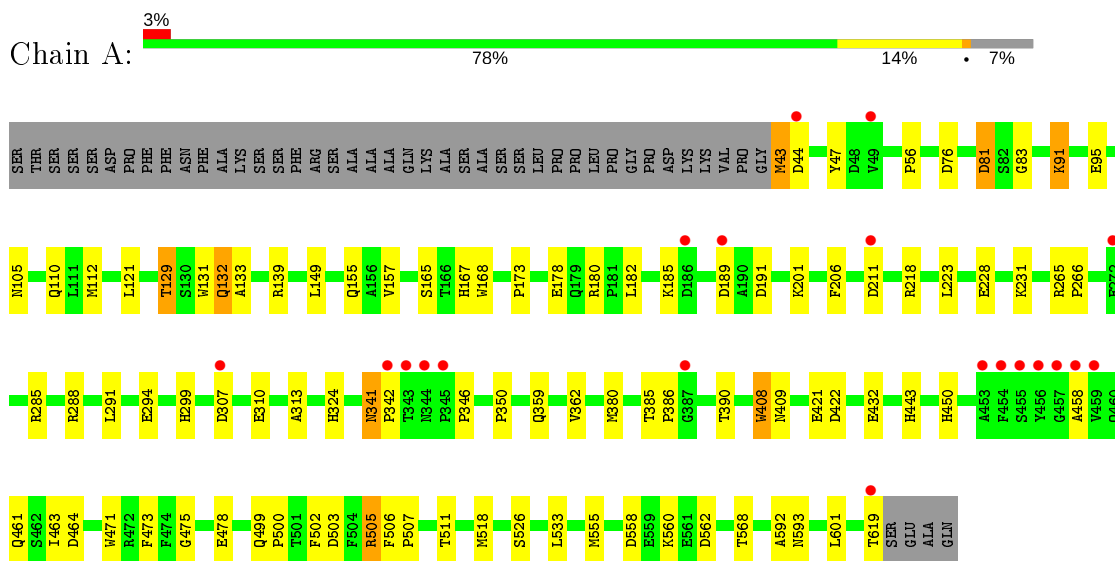
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	E	303	Total 303	O 303	0	0
3	F	317	Total 317	O 317	0	0
3	G	251	Total 251	O 251	0	0
3	H	326	Total 326	O 326	0	0

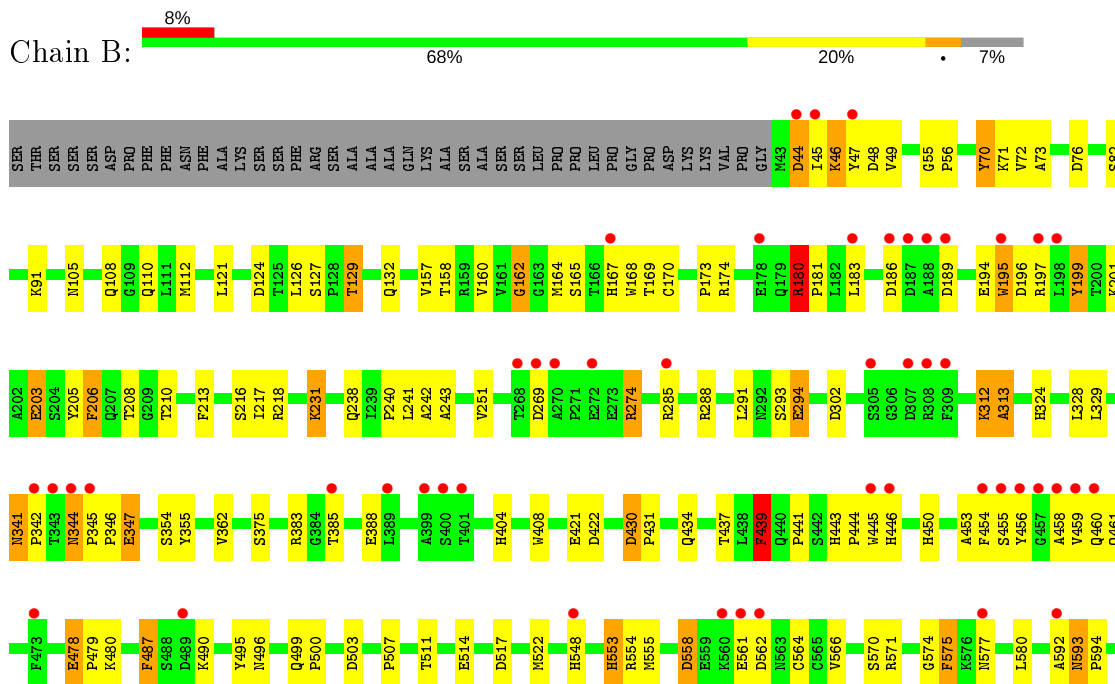
### 3 Residue-property plots [i](#)

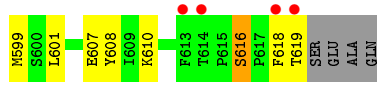
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: pyranose oxidase

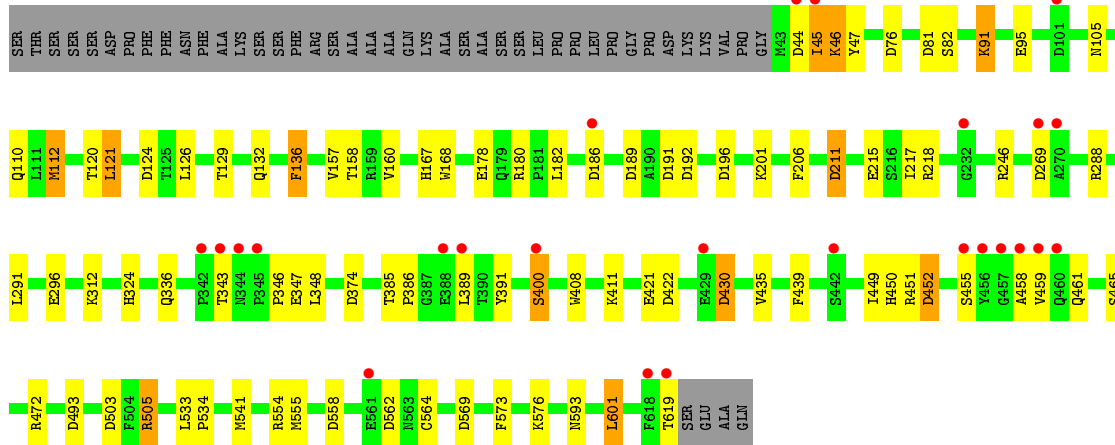
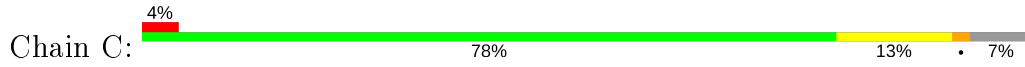


- Molecule 1: pyranose oxidase

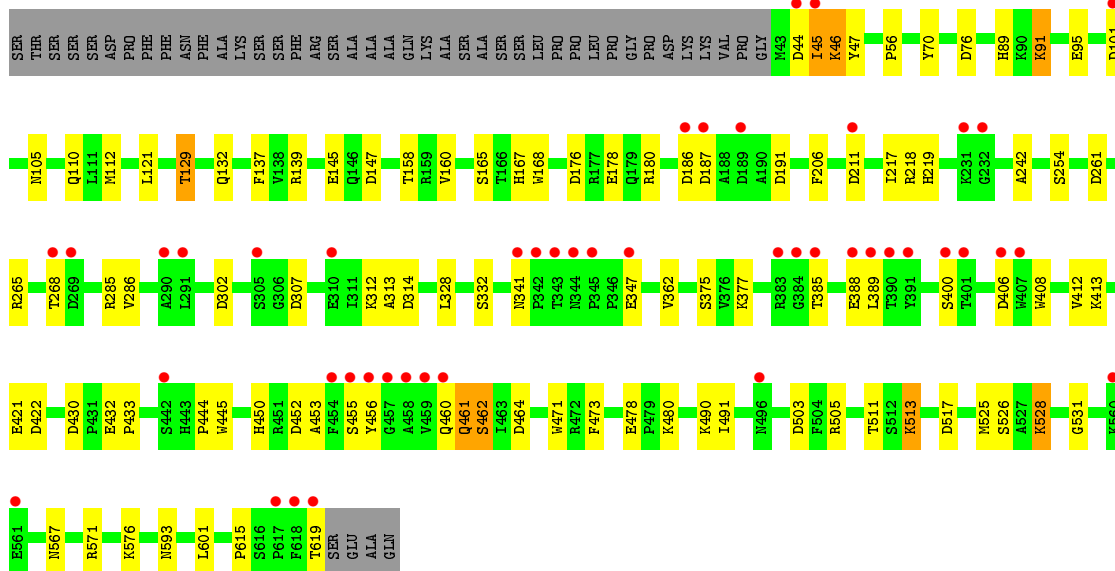
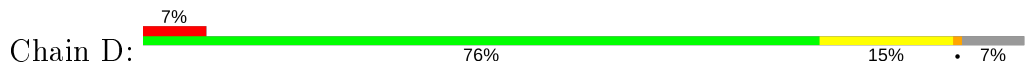




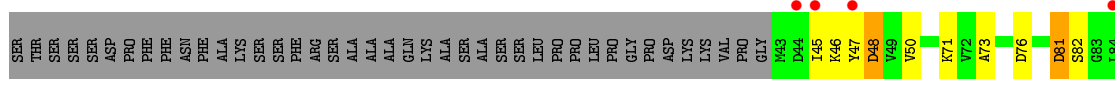
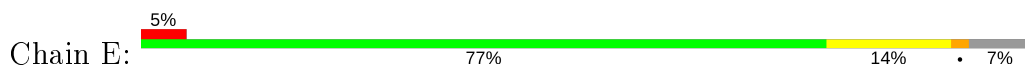
• Molecule 1: pyranose oxidase

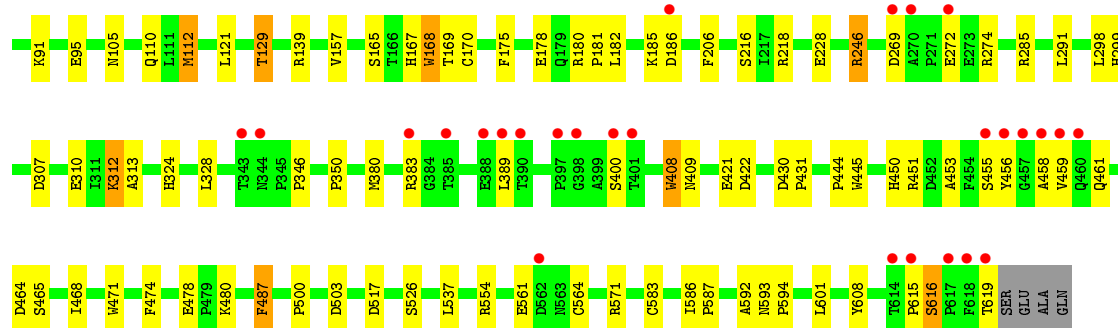


• Molecule 1: pyranose oxidase

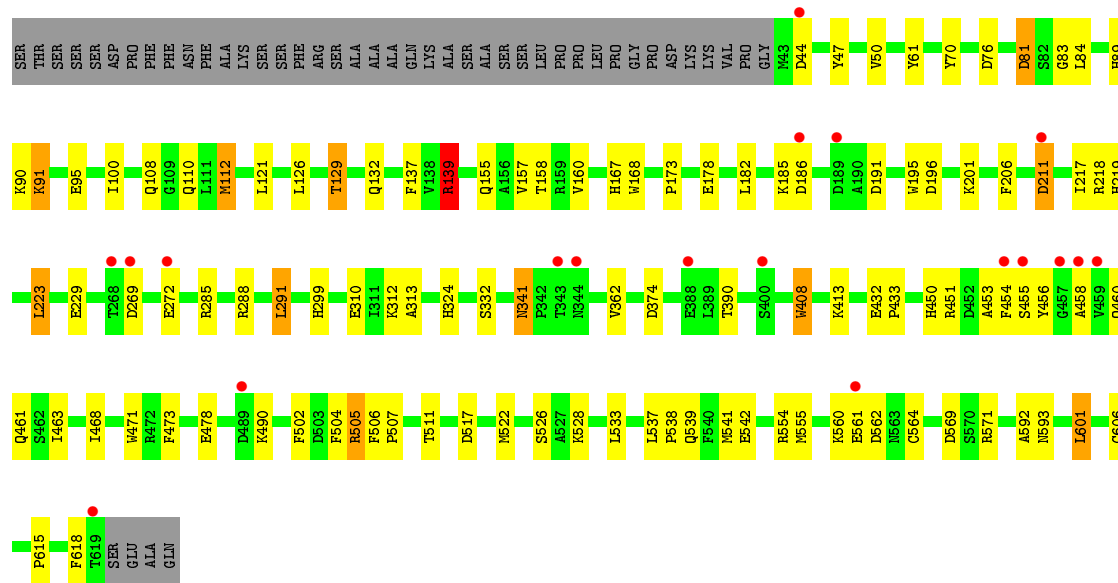
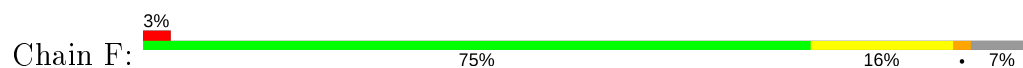


• Molecule 1: pyranose oxidase

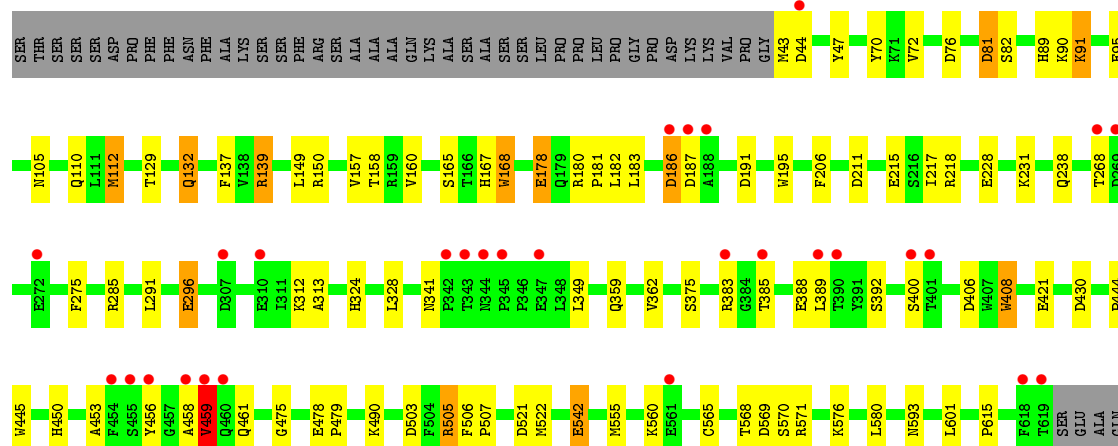
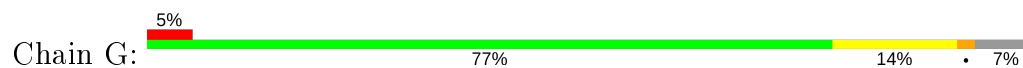





- Molecule 1: pyranose oxidase

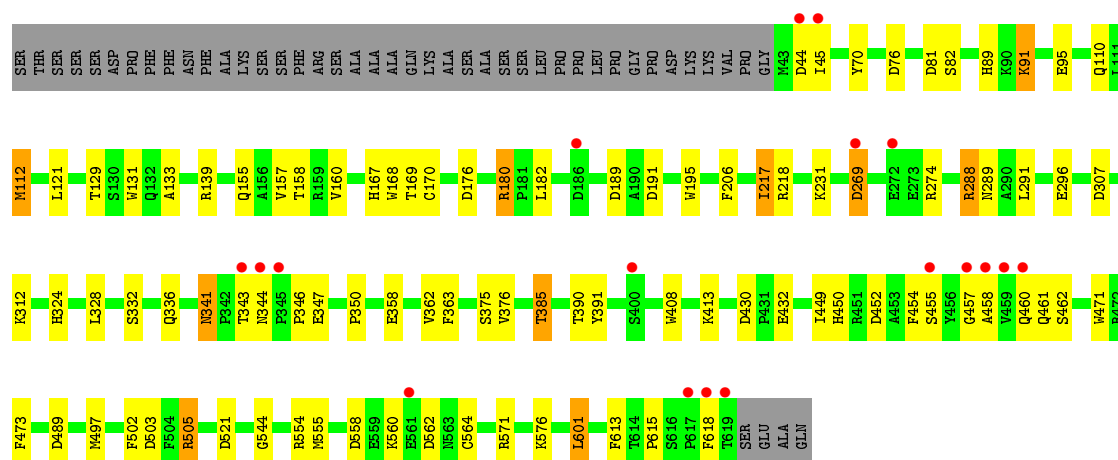


- Molecule 1: pyranose oxidase



- Molecule 1: pyranose oxidase

Chain H: 



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	164.88Å 103.60Å 169.17Å 90.00° 105.25° 90.00°	Depositor
Resolution (Å)	19.70 – 2.35 19.64 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.70-2.35) 100.0 (19.64-2.35)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.96 (at 2.35Å)	Xtrriage
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 <sup>2</sup> )	25.8	Xtrriage
Anisotropy	0.624	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.026 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	38970	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 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.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality i

### 5.1 Standard geometry i

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

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	0.70	0/4650	0.85	12/6298 (0.2%)
1	B	1.20	34/4650 (0.7%)	1.01	23/6298 (0.4%)
1	C	0.68	2/4650 (0.0%)	0.83	19/6298 (0.3%)
1	D	0.59	0/4650	0.80	16/6298 (0.3%)
1	E	0.86	7/4650 (0.2%)	0.87	11/6298 (0.2%)
1	F	0.72	1/4650 (0.0%)	0.85	13/6298 (0.2%)
1	G	0.69	0/4650	0.83	11/6298 (0.2%)
1	H	0.73	0/4650	0.86	18/6298 (0.3%)
All	All	0.79	44/37200 (0.1%)	0.86	123/50384 (0.2%)

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 (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	608	TYR	CG-CD1	15.59	1.59	1.39
1	B	195	TRP	CD2-CE3	13.34	1.60	1.40
1	E	608	TYR	CE2-CZ	13.32	1.55	1.38
1	B	608	TYR	CE2-CZ	12.58	1.54	1.38
1	B	199	TYR	CG-CD1	11.92	1.54	1.39
1	B	199	TYR	CE2-CZ	11.22	1.53	1.38
1	E	608	TYR	CG-CD1	11.18	1.53	1.39
1	B	197	ARG	NE-CZ	10.52	1.46	1.33
1	B	607	GLU	CG-CD	8.70	1.65	1.51
1	B	274	ARG	NE-CZ	8.63	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	203	GLU	N-CA	8.54	1.63	1.46
1	B	48	ASP	CB-CG	8.33	1.69	1.51
1	B	608	TYR	CE1-CZ	8.21	1.49	1.38
1	B	197	ARG	CG-CD	8.18	1.72	1.51
1	B	195	TRP	CZ2-CH2	7.79	1.52	1.37
1	C	136	PHE	CG-CD1	7.20	1.49	1.38
1	B	162	GLY	CA-C	6.95	1.62	1.51
1	B	608	TYR	CG-CD2	6.95	1.48	1.39
1	B	197	ARG	CD-NE	6.93	1.58	1.46
1	B	575	PHE	CG-CD2	6.77	1.49	1.38
1	E	616	SER	CB-OG	6.74	1.51	1.42
1	B	241	LEU	N-CA	6.69	1.59	1.46
1	B	313	ALA	CA-CB	6.60	1.66	1.52
1	B	575	PHE	CE1-CZ	6.42	1.49	1.37
1	B	487	PHE	CE1-CZ	6.09	1.49	1.37
1	C	136	PHE	CE2-CZ	6.05	1.48	1.37
1	B	575	PHE	CG-CD1	6.00	1.47	1.38
1	B	487	PHE	CG-CD2	5.98	1.47	1.38
1	B	478	GLU	CD-OE2	5.94	1.32	1.25
1	B	616	SER	CB-OG	5.91	1.50	1.42
1	B	313	ALA	N-CA	5.71	1.57	1.46
1	B	195	TRP	NE1-CE2	5.67	1.45	1.37
1	B	194	GLU	N-CA	5.58	1.57	1.46
1	E	48	ASP	N-CA	5.55	1.57	1.46
1	B	553	HIS	C-N	5.34	1.46	1.34
1	B	70	TYR	CG-CD2	5.28	1.46	1.39
1	E	487	PHE	CE1-CZ	5.26	1.47	1.37
1	E	487	PHE	CG-CD2	5.26	1.46	1.38
1	E	608	TYR	CE1-CZ	5.24	1.45	1.38
1	B	195	TRP	C-O	5.20	1.33	1.23
1	B	439	PHE	CG-CD2	5.14	1.46	1.38
1	B	514	GLU	CG-CD	5.13	1.59	1.51
1	F	504	PHE	CE1-CZ	5.08	1.47	1.37
1	B	197	ARG	CZ-NH2	5.01	1.39	1.33

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	48	ASP	CB-CG-OD2	9.06	126.45	118.30
1	B	575	PHE	CB-CG-CD1	-8.74	114.68	120.80
1	H	503	ASP	CB-CG-OD2	8.53	125.98	118.30
1	C	288	ARG	NE-CZ-NH2	-8.35	116.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	288	ARG	NE-CZ-NH2	-7.85	116.37	120.30
1	D	76	ASP	CB-CG-OD2	7.54	125.09	118.30
1	B	195	TRP	CE2-CD2-CG	-7.52	101.28	107.30
1	A	503	ASP	CB-CG-OD2	7.45	125.00	118.30
1	B	302	ASP	CB-CG-OD2	7.43	124.99	118.30
1	B	196	ASP	CB-CG-OD2	7.40	124.96	118.30
1	D	503	ASP	CB-CG-OD2	7.27	124.84	118.30
1	D	406	ASP	CB-CG-OD2	6.83	124.45	118.30
1	D	147	ASP	CB-CG-OD1	6.80	124.42	118.30
1	F	76	ASP	CB-CG-OD2	6.79	124.42	118.30
1	F	196	ASP	CB-CG-OD2	6.69	124.33	118.30
1	E	464	ASP	CB-CG-OD2	6.65	124.29	118.30
1	F	139	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	A	191	ASP	CB-CG-OD2	6.56	124.21	118.30
1	A	211	ASP	CB-CG-OD2	6.52	124.17	118.30
1	C	76	ASP	CB-CG-OD2	6.47	124.13	118.30
1	A	76	ASP	CB-CG-OD2	6.45	124.11	118.30
1	C	503	ASP	CB-CG-OD2	6.43	124.09	118.30
1	C	186	ASP	CB-CG-OD2	6.37	124.03	118.30
1	E	186	ASP	CB-CG-OD2	6.34	124.00	118.30
1	G	44	ASP	CB-CG-OD2	6.33	124.00	118.30
1	B	197	ARG	NE-CZ-NH2	6.29	123.45	120.30
1	G	81	ASP	CB-CG-OD2	6.28	123.95	118.30
1	C	452	ASP	CB-CG-OD2	6.23	123.91	118.30
1	G	186	ASP	CB-CG-OD2	6.23	123.91	118.30
1	G	503	ASP	CB-CG-OD2	6.20	123.88	118.30
1	G	191	ASP	CB-CG-OD2	6.20	123.88	118.30
1	C	374	ASP	CB-CG-OD2	6.11	123.80	118.30
1	B	558	ASP	CB-CG-OD2	6.10	123.79	118.30
1	F	562	ASP	CB-CG-OD2	6.08	123.77	118.30
1	H	562	ASP	CB-CG-OD2	6.06	123.76	118.30
1	A	464	ASP	CB-CG-OD2	6.06	123.75	118.30
1	H	489	ASP	CB-CG-OD2	6.04	123.74	118.30
1	H	558	ASP	CB-CG-OD2	6.04	123.73	118.30
1	H	452	ASP	CB-CG-OD2	6.01	123.71	118.30
1	D	186	ASP	CB-CG-OD2	5.99	123.69	118.30
1	E	76	ASP	CB-CG-OD2	5.97	123.67	118.30
1	B	288	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	B	180	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	H	176	ASP	CB-CG-OD2	5.92	123.63	118.30
1	B	503	ASP	CB-CG-OD2	5.90	123.61	118.30
1	B	422	ASP	CB-CG-OD2	5.90	123.61	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	288	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	D	314	ASP	CB-CG-OD2	5.87	123.58	118.30
1	D	430	ASP	CB-CG-OD2	5.85	123.56	118.30
1	D	191	ASP	CB-CG-OD2	5.83	123.55	118.30
1	C	558	ASP	CB-CG-OD2	5.82	123.53	118.30
1	A	422	ASP	CB-CG-OD2	5.79	123.51	118.30
1	D	261	ASP	CB-CG-OD2	5.79	123.51	118.30
1	B	189	ASP	CB-CG-OD2	5.76	123.49	118.30
1	F	139	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	B	76	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A	558	ASP	CB-CG-OD2	5.74	123.47	118.30
1	E	430	ASP	CB-CG-OD2	5.72	123.45	118.30
1	G	406	ASP	CB-CG-OD2	5.61	123.34	118.30
1	B	199	TYR	CG-CD2-CE2	-5.60	116.82	121.30
1	E	517	ASP	CB-CG-OD2	5.59	123.33	118.30
1	B	44	ASP	CB-CG-OD2	5.59	123.33	118.30
1	G	521	ASP	CB-CG-OD2	5.58	123.33	118.30
1	H	44	ASP	CB-CG-OD2	5.57	123.31	118.30
1	C	422	ASP	CB-CG-OD2	5.54	123.29	118.30
1	C	191	ASP	CB-CG-OD2	5.51	123.26	118.30
1	H	81	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	562	ASP	CB-CG-OD2	5.49	123.24	118.30
1	C	192	ASP	CB-CG-OD2	5.48	123.23	118.30
1	E	139	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	B	269	ASP	CB-CG-OD2	5.44	123.19	118.30
1	D	302	ASP	CB-CG-OD2	5.42	123.18	118.30
1	E	422	ASP	CB-CG-OD2	5.42	123.18	118.30
1	C	196	ASP	CB-CG-OD2	5.42	123.18	118.30
1	C	189	ASP	CB-CG-OD2	5.41	123.17	118.30
1	F	186	ASP	CB-CG-OD2	5.39	123.15	118.30
1	F	191	ASP	CB-CG-OD2	5.39	123.15	118.30
1	D	422	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	186	ASP	CB-CG-OD2	5.37	123.14	118.30
1	H	189	ASP	CB-CG-OD2	5.36	123.13	118.30
1	D	464	ASP	CB-CG-OD2	5.34	123.11	118.30
1	F	374	ASP	CB-CG-OD2	5.34	123.10	118.30
1	A	562	ASP	CB-CG-OD2	5.33	123.10	118.30
1	F	569	ASP	CB-CG-OD2	5.33	123.09	118.30
1	H	76	ASP	CB-CG-OD2	5.33	123.09	118.30
1	B	242	ALA	CB-CA-C	5.31	118.07	110.10
1	F	269	ASP	CB-CG-OD2	5.29	123.06	118.30
1	C	562	ASP	CB-CG-OD2	5.28	123.05	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	D	211	ASP	CB-CG-OD2	5.27	123.04	118.30
1	E	307	ASP	CB-CG-OD2	5.27	123.04	118.30
1	G	187	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	81	ASP	CB-CG-OD2	5.27	123.04	118.30
1	E	81	ASP	CB-CG-OD2	5.27	123.04	118.30
1	G	76	ASP	CB-CG-OD2	5.26	123.03	118.30
1	E	503	ASP	CB-CG-OD2	5.25	123.03	118.30
1	C	211	ASP	CB-CG-OD2	5.25	123.03	118.30
1	D	517	ASP	CB-CG-OD2	5.22	123.00	118.30
1	E	269	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	517	ASP	CB-CG-OD2	5.21	122.99	118.30
1	H	288	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	H	139	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	H	191	ASP	CB-CG-OD2	5.18	122.96	118.30
1	C	569	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	608	TYR	CB-CG-CD1	-5.17	117.90	121.00
1	C	430	ASP	CB-CG-OD2	5.17	122.95	118.30
1	H	307	ASP	CB-CG-OD2	5.16	122.94	118.30
1	H	269	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	189	ASP	CB-CG-OD2	5.15	122.94	118.30
1	D	187	ASP	CB-CG-OD2	5.15	122.94	118.30
1	G	569	ASP	CB-CG-OD2	5.14	122.93	118.30
1	H	521	ASP	CB-CG-OD2	5.13	122.92	118.30
1	H	430	ASP	CB-CG-OD2	5.13	122.92	118.30
1	C	269	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	288	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	C	493	ASP	CB-CG-OD1	5.10	122.89	118.30
1	G	430	ASP	CB-CG-OD2	5.09	122.88	118.30
1	B	199	TYR	CD1-CE1-CZ	-5.08	115.22	119.80
1	F	223	LEU	CA-CB-CG	5.08	126.98	115.30
1	B	430	ASP	CB-CG-OD2	5.06	122.86	118.30
1	F	291	LEU	CA-CB-CG	5.06	126.93	115.30
1	F	517	ASP	CB-CG-OD2	5.02	122.82	118.30
1	D	176	ASP	CB-CG-OD2	5.01	122.81	118.30

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	55	0
1	B	4549	0	4395	111	0
1	C	4549	0	4395	40	0
1	D	4549	0	4395	44	0
1	E	4549	0	4395	51	0
1	F	4549	0	4395	63	0
1	G	4549	0	4395	57	0
1	H	4549	0	4395	44	0
2	A	53	0	30	0	0
2	B	53	0	30	6	0
2	C	53	0	30	0	0
2	D	53	0	30	1	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	452	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 6.

All (452) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:71:LYS:HB2	1:E:274:ARG:NH1	1.74	1.01
1:B:167:HIS:NE2	2:B:625:FAD:HM81	1.74	0.99
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:D:513:LYS:HE2	3:D:736:HOH:O	1.99	0.62
1:B:495:TYR:OH	1:D:95:GLU:OE2	2.15	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:B:46:LYS:HE2	1:B:312:LYS:C	2.20	0.62
1:G:555:MSE:HE3	1:G:568:THR:HG22	1.82	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

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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	0.60
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: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: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
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:B:439:PHE:HB2	1:B:445:TRP:C	2.25	0.56
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:ASP:HB2	1:E:71:LYS:O	2.05	0.55
1:G:408:TRP:C	1:G:408:TRP:CD1	2.80	0.55
1:G:453:ALA:O	1:G:456:TYR:CD1	2.57	0.55
1:G:362:VAL:O	1:G:522:MSE:HE1	2.07	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: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:H:460:GLN:C	1:H:462:SER:H	2.10	0.54
1:B:183:LEU:HG	1:B:195:TRP:NE1	2.21	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:CG	1:E:180:ARG:HH11	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:G:505:ARG:NH1	3:G:850:HOH:O	2.42	0.53
1:F:112:MSE:HE2	1:H:95:GLU:HG3	1.89	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:B:439:PHE:HB2	1:B:445:TRP:O	2.09	0.52
1:H:70:TYR:CZ	1:H:615:PRO:HG3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:ASP:HB3	1:D:47:TYR:OH	2.08	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:HE2	1:H:497:MSE:HA	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
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:CG	1:B:594:PRO:HD2	2.44	0.50
1:B:548:HIS:CE1	1:B:593:ASN:HB3	2.46	0.50
1:D:46:LYS:HE3	1:D:312:LYS:HG3	1.92	0.50
1:D:478:GLU:HG2	1:D:511:THR:OG1	2.11	0.50
1:D:70:TYR:CD2	1:D:615:PRO:HB3	2.46	0.50
1:H:110:GLN:NE2	1:H:167:HIS:HD1	1.98	0.50
1:H:432:GLU:CD	1:H:432:GLU:H	2.14	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:A:432:GLU:H	1:A:432:GLU:CD	2.15	0.50
1:B:173:PRO:HG3	1:B:446:HIS:CE1	2.47	0.50
1:A:132:GLN:C	1:A:132:GLN:HE21	2.15	0.50
1:B:570:SER:HB3	1:B:580:LEU:O	2.12	0.50
1:B:293:SER:HA	1:B:574:GLY: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:G:178:GLU:HG3	1:G:178:GLU:O	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:B:158:THR:HG22	1:B:160:VAL:HG22	1.95	0.48
1:B:108:GLN:HE21	1:B:454:PHE:HE2	1.60	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:F:537:LEU:HB3	1:F:538:PRO:HD2	1.94	0.48
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
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
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:G:70:TYR:CZ	1:G:615:PRO:HG3	2.49	0.47
1:D:490:LYS:HG3	3:D:756:HOH:O	2.15	0.47
1:F:463:ILE:HD13	1:F:533:LEU:CD1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:B:201:LYS:HE2	1:B:205:TYR:OH	2.15	0.46
3:A:784:HOH:O	1:C:129:THR:HG21	2.15	0.46
1:E:71:LYS:CB	1:E:274:ARG:NH1	2.63	0.46
1:G:215:GLU:HG2	1:G:215:GLU:O	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:124:ASP:HA	3:B:706:HOH:O	2.16	0.46
1:B:56:PRO:HD3	1:B:165:SER:HB3	1.97	0.46
1:F:432:GLU:CD	1:F:432:GLU:H	2.18	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: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: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:B:231:LYS:HZ3	1:B:231:LYS:HB2	1.82	0.45
1:F:211:ASP:HB2	3:F:862:HOH:O	2.16	0.45
1:C:564:CYS:HG	1:C:573:PHE:HE2	1.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:CG	1:E:180:ARG:NH1	2.78	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:H:358:GLU:HG2	1:H:544:GLY:HA2	2.00	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: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:C:44:ASP:CG	1:C:45:ILE:H	2.22	0.43
1:D:178:GLU:O	1:D:178:GLU:HG3	2.18	0.43
1:D:567:ASN:HD21	1:D:571:ARG:NH1	2.16	0.43
1:F:219:HIS:HB2	1:F:433:PRO:HA	2.00	0.43
1:F:155:GLN:HG2	1:F:502:PHE:CZ	2.53	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:F:541:MSE:HE2	3:F:745:HOH:O	2.18	0.43
1:F:83:GLY:N	3:F:940:HOH:O	2.09	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:195:TRP:CH2	1:F:601:LEU:HD13	2.54	0.43
1:G:459:VAL:C	3:G:840:HOH:O	2.57	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:CA	1:A:132:GLN:NE2	2.81	0.43
1:D:408:TRP:C	1:D:408:TRP:CD1	2.92	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:D:461:GLN:HG3	1:D:461:GLN:H	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:408:TRP:C	1:A:408:TRP:CD1	2.93	0.42
1:B:453:ALA:O	1:B:456:TYR:CD1	2.72	0.42
1:B:446:HIS:NE2	1:B:593:ASN:OD1	2.52	0.42
1:F:70:TYR:CZ	1:F:615:PRO:HG3	2.54	0.42
1:C:124:ASP:N	1:C:124:ASP:OD1	2.52	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:211:ASP:HB2	3:C:730:HOH:O	2.19	0.42
1:C:46:LYS:HE2	1:C:47:TYR:O	2.19	0.42
3:A:850:HOH:O	1:C:81:ASP:C	2.57	0.42
1:D:44:ASP:HB3	1:D:47:TYR:CZ	2.54	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
1:B:383:ARG:NH1	1:B:383:ARG:HG3	2.35	0.42
1:A:132:GLN:CA	1:A:132:GLN:HE21	2.33	0.42
1:H:460:GLN:C	1:H:462:SER:N	2.73	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:HD3	1:E:246:ARG:HA	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:408:TRP:C	1:E:408:TRP:CD1	2.92	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:A:341:ASN:HA	1:A:342:PRO:HD3	1.73	0.41
1:F:408:TRP:CD1	1:F:408:TRP:C	2.92	0.41
1:F:70:TYR:CE1	1:F:615:PRO:HG3	2.55	0.41
1:A:265:ARG:HA	1:A:266:PRO:C	2.41	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: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:HG3	1:B:347:GLU:H	1.67	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:218:ARG:HD2	3:A:640:HOH:O	2.21	0.41
1:A:44:ASP:HB3	1:A:47:TYR:OH	2.20	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:487:PHE:CD1	1:E:500:PRO:HA	2.55	0.41
1:E:50:VAL:HG11	1:E:298:LEU:HD22	2.02	0.41
1:F:229:GLU:HG3	1:F:528:LYS:HG2	2.03	0.41
1:H:363:PHE:HA	1:H:471:TRP:O	2.20	0.41
1:H:89:HIS:CE1	1:H:91:LYS:HB2	2.55	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
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:C:91:LYS:NZ	3:C:853:HOH:O	2.54	0.41
1:E:328:LEU:O	1:E:328:LEU:HD23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:625:FAD:N1	2:E:625:FAD:H2'	2.35	0.41
1:F:137:PHE:O	1:F:139:ARG:HD3	2.21	0.41
1:B:478:GLU:HA	1:B:479:PRO:HD3	1.93	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
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:HG2	1:F:571:ARG:HH11	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: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:A:105:ASN:O	1:C:105:ASN:HB3	2.21	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
1:A:129:THR:HG21	3:C:710:HOH:O	2.21	0.40
2:B:625:FAD:H9	2:B:625:FAD:H1'1	1.91	0.40
1:B:71:LYS:HB2	1:B:274:ARG:CZ	2.52	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%)	47	56
1	C	575/622 (92%)	555 (96%)	18 (3%)	2 (0%)	41	47
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%)	47	56
1	H	575/622 (92%)	551 (96%)	21 (4%)	3 (0%)	29	32
All	All	4600/4976 (92%)	4427 (96%)	166 (4%)	7 (0%)	47	56

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
1	G	459	VAL
1	H	457	GLY
1	C	45	ILE

### 5.3.2 Protein sidechains [i](#)

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

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



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	505/525 (96%)	478 (95%)	27 (5%)	22	26
1	B	505/525 (96%)	474 (94%)	31 (6%)	18	20
1	C	505/525 (96%)	475 (94%)	30 (6%)	19	22
1	D	505/525 (96%)	466 (92%)	39 (8%)	13	12
1	E	505/525 (96%)	474 (94%)	31 (6%)	18	20
1	F	505/525 (96%)	470 (93%)	35 (7%)	15	15
1	G	505/525 (96%)	466 (92%)	39 (8%)	13	12
1	H	505/525 (96%)	478 (95%)	27 (5%)	22	26
All	All	4040/4200 (96%)	3781 (94%)	259 (6%)	17	18

All (259) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	MSE
1	A	81	ASP
1	A	91	LYS
1	A	121	LEU
1	A	129	THR
1	A	132	GLN
1	A	168	TRP
1	A	178	GLU
1	A	180	ARG
1	A	182	LEU
1	A	185	LYS
1	A	206	PHE
1	A	223	LEU
1	A	228	GLU
1	A	285	ARG
1	A	291	LEU
1	A	294	GLU
1	A	341	ASN
1	A	390	THR
1	A	408	TRP
1	A	421	GLU
1	A	450	HIS
1	A	505	ARG
1	A	560	LYS
1	A	593	ASN
1	A	601	LEU
1	A	619	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	44	ASP
1	B	45	ILE
1	B	46	LYS
1	B	91	LYS
1	B	112	MSE
1	B	121	LEU
1	B	129	THR
1	B	168	TRP
1	B	180	ARG
1	B	206	PHE
1	B	217	ILE
1	B	231	LYS
1	B	285	ARG
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	408	TRP
1	B	421	GLU
1	B	439	PHE
1	B	450	HIS
1	B	459	VAL
1	B	490	LYS
1	B	593	ASN
1	B	601	LEU
1	B	616	SER
1	B	619	THR
1	C	46	LYS
1	C	82	SER
1	C	91	LYS
1	C	112	MSE
1	C	121	LEU
1	C	168	TRP
1	C	178	GLU
1	C	180	ARG
1	C	182	LEU
1	C	201	LYS
1	C	206	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	408	TRP
1	C	421	GLU
1	C	439	PHE
1	C	450	HIS
1	C	459	VAL
1	C	505	ARG
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	112	MSE
1	D	121	LEU
1	D	129	THR
1	D	132	GLN
1	D	168	TRP
1	D	180	ARG
1	D	206	PHE
1	D	217	ILE
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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	389	LEU
1	D	400	SER
1	D	413	LYS
1	D	421	GLU
1	D	432	GLU
1	D	450	HIS
1	D	452	ASP
1	D	461	GLN
1	D	462	SER
1	D	505	ARG
1	D	513	LYS
1	D	528	LYS
1	D	576	LYS
1	D	593	ASN
1	D	601	LEU
1	D	619	THR
1	E	45	ILE
1	E	81	ASP
1	E	82	SER
1	E	91	LYS
1	E	112	MSE
1	E	121	LEU
1	E	129	THR
1	E	168	TRP
1	E	178	GLU
1	E	182	LEU
1	E	185	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	389	LEU
1	E	400	SER
1	E	408	TRP
1	E	421	GLU
1	E	450	HIS
1	E	459	VAL
1	E	474	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	561	GLU
1	E	593	ASN
1	E	601	LEU
1	E	615	PRO
1	E	619	THR
1	F	81	ASP
1	F	90	LYS
1	F	91	LYS
1	F	100	ILE
1	F	112	MSE
1	F	121	LEU
1	F	129	THR
1	F	139	ARG
1	F	168	TRP
1	F	178	GLU
1	F	182	LEU
1	F	185	LYS
1	F	201	LYS
1	F	206	PHE
1	F	211	ASP
1	F	217	ILE
1	F	223	LEU
1	F	272	GLU
1	F	285	ARG
1	F	291	LEU
1	F	312	LYS
1	F	341	ASN
1	F	390	THR
1	F	408	TRP
1	F	413	LYS
1	F	450	HIS
1	F	460	GLN
1	F	490	LYS
1	F	505	ARG
1	F	542	GLU
1	F	560	LYS
1	F	561	GLU
1	F	593	ASN
1	F	601	LEU
1	F	618	PHE
1	G	43	MSE
1	G	91	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	G	112	MSE
1	G	129	THR
1	G	132	GLN
1	G	139	ARG
1	G	168	TRP
1	G	178	GLU
1	G	182	LEU
1	G	186	ASP
1	G	206	PHE
1	G	211	ASP
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
1	G	383	ARG
1	G	389	LEU
1	G	392	SER
1	G	400	SER
1	G	408	TRP
1	G	421	GLU
1	G	450	HIS
1	G	459	VAL
1	G	490	LYS
1	G	505	ARG
1	G	542	GLU
1	G	560	LYS
1	G	576	LYS
1	G	593	ASN
1	G	601	LEU
1	H	45	ILE
1	H	82	SER
1	H	91	LYS
1	H	112	MSE
1	H	121	LEU

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Mol	Chain	Res	Type
1	H	129	THR
1	H	168	TRP
1	H	180	ARG
1	H	182	LEU
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	408	TRP
1	H	450	HIS
1	H	505	ARG
1	H	560	LYS
1	H	576	LYS
1	H	601	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	GLN
1	A	155	GLN
1	A	263	GLN
1	A	299	HIS
1	A	324	HIS
1	A	341	ASN
1	A	344	ASN
1	B	108	GLN
1	B	257	ASN
1	B	324	HIS
1	B	404	HIS
1	B	434	GLN
1	B	461	GLN
1	C	110	GLN
1	C	224	ASN
1	C	324	HIS

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Mol	Chain	Res	Type
1	C	418	GLN
1	C	440	GLN
1	C	460	GLN
1	C	461	GLN
1	D	110	GLN
1	D	224	ASN
1	D	324	HIS
1	D	341	ASN
1	D	434	GLN
1	E	155	GLN
1	E	324	HIS
1	E	434	GLN
1	E	440	GLN
1	E	460	GLN
1	E	461	GLN
1	F	108	GLN
1	F	324	HIS
1	F	341	ASN
1	F	434	GLN
1	F	461	GLN
1	G	263	GLN
1	G	324	HIS
1	G	414	ASN
1	G	461	GLN
1	H	224	ASN
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 carbohydrates in this entry.



## 5.6 Ligand geometry

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	H	625	1	51,58,58	1.30	6 (11%)	60,89,89	1.77	10 (16%)
2	FAD	B	625	1	51,58,58	1.42	5 (9%)	60,89,89	1.85	16 (26%)
2	FAD	A	625	1	51,58,58	1.45	6 (11%)	60,89,89	1.82	12 (20%)
2	FAD	D	625	1	51,58,58	1.51	5 (9%)	60,89,89	1.76	10 (16%)
2	FAD	C	625	1	51,58,58	1.58	6 (11%)	60,89,89	1.80	9 (15%)
2	FAD	F	625	1	51,58,58	1.49	6 (11%)	60,89,89	1.61	10 (16%)
2	FAD	E	625	1	51,58,58	1.36	7 (13%)	60,89,89	1.88	9 (15%)
2	FAD	G	625	1	51,58,58	1.40	5 (9%)	60,89,89	1.95	10 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	H	625	1	-	3/30/50/50	0/6/6/6
2	FAD	B	625	1	-	4/30/50/50	0/6/6/6
2	FAD	A	625	1	-	4/30/50/50	0/6/6/6
2	FAD	D	625	1	-	2/30/50/50	0/6/6/6
2	FAD	C	625	1	-	3/30/50/50	0/6/6/6
2	FAD	F	625	1	-	5/30/50/50	0/6/6/6
2	FAD	E	625	1	-	6/30/50/50	0/6/6/6
2	FAD	G	625	1	-	3/30/50/50	0/6/6/6

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	625	FAD	C10-N1	6.22	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	625	FAD	C10-N1	5.64	1.40	1.33
2	D	625	FAD	C10-N1	5.30	1.40	1.33
2	G	625	FAD	C10-N1	5.05	1.39	1.33
2	A	625	FAD	C4-N3	5.03	1.41	1.33
2	F	625	FAD	C10-N1	4.80	1.39	1.33
2	F	625	FAD	C4-N3	4.67	1.41	1.33
2	E	625	FAD	C10-N1	4.62	1.39	1.33
2	H	625	FAD	C10-N1	4.49	1.39	1.33
2	D	625	FAD	C9A-N10	4.40	1.44	1.38
2	A	625	FAD	C10-N1	4.32	1.38	1.33
2	H	625	FAD	C4-N3	4.26	1.40	1.33
2	G	625	FAD	C4-N3	4.24	1.40	1.33
2	D	625	FAD	C4-N3	4.12	1.40	1.33
2	C	625	FAD	C4-N3	4.12	1.40	1.33
2	G	625	FAD	C9A-N10	3.95	1.43	1.38
2	F	625	FAD	C9A-N10	3.71	1.43	1.38
2	E	625	FAD	O4B-C1B	3.66	1.46	1.41
2	C	625	FAD	O4B-C1B	3.54	1.46	1.41
2	D	625	FAD	O4B-C1B	3.43	1.45	1.41
2	E	625	FAD	C4-N3	3.40	1.39	1.33
2	B	625	FAD	C4-N3	3.26	1.38	1.33
2	F	625	FAD	C4X-N5	2.83	1.37	1.33
2	C	625	FAD	C9A-N10	2.82	1.42	1.38
2	C	625	FAD	C8M-C8	2.82	1.56	1.51
2	B	625	FAD	C8M-C8	2.61	1.56	1.51
2	B	625	FAD	C7M-C7	2.60	1.56	1.51
2	B	625	FAD	C2B-C1B	-2.57	1.49	1.53
2	H	625	FAD	C7M-C7	2.53	1.56	1.51
2	E	625	FAD	C8M-C8	2.50	1.56	1.51
2	A	625	FAD	C5'-C4'	2.47	1.55	1.51
2	E	625	FAD	P-O2P	-2.35	1.44	1.55
2	G	625	FAD	C8M-C8	2.31	1.55	1.51
2	D	625	FAD	C1'-N10	2.29	1.50	1.48
2	F	625	FAD	C2-N1	2.27	1.42	1.38
2	A	625	FAD	PA-O5B	2.26	1.68	1.59
2	C	625	FAD	PA-O1A	2.24	1.58	1.50
2	H	625	FAD	C8M-C8	2.23	1.55	1.51
2	E	625	FAD	C9A-N10	2.22	1.41	1.38
2	G	625	FAD	C4X-C10	2.16	1.41	1.38
2	E	625	FAD	C9A-C5X	-2.14	1.38	1.42
2	H	625	FAD	C5A-N7A	-2.11	1.32	1.39
2	F	625	FAD	C4X-C10	2.10	1.40	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	625	FAD	O4B-C4B	-2.07	1.40	1.45
2	A	625	FAD	C8M-C8	2.04	1.55	1.51
2	H	625	FAD	C4X-C10	2.02	1.40	1.38

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	625	FAD	C4-N3-C2	7.04	121.09	115.14
2	A	625	FAD	C4-N3-C2	6.99	121.05	115.14
2	E	625	FAD	C4X-N5-C5X	6.98	123.75	116.77
2	G	625	FAD	C1'-N10-C9A	6.87	123.70	118.29
2	B	625	FAD	C4-N3-C2	6.83	120.91	115.14
2	G	625	FAD	C4-N3-C2	6.81	120.89	115.14
2	C	625	FAD	C4X-N5-C5X	6.53	123.30	116.77
2	C	625	FAD	C4-N3-C2	6.24	120.41	115.14
2	D	625	FAD	C4-N3-C2	6.17	120.35	115.14
2	E	625	FAD	C4-N3-C2	5.84	120.08	115.14
2	D	625	FAD	C1'-N10-C9A	5.78	122.84	118.29
2	F	625	FAD	C4-N3-C2	5.71	119.97	115.14
2	G	625	FAD	N3A-C2A-N1A	-5.46	120.15	128.68
2	A	625	FAD	N3A-C2A-N1A	-5.20	120.56	128.68
2	G	625	FAD	C4X-N5-C5X	4.89	121.66	116.77
2	E	625	FAD	C10-C4X-N5	-4.77	117.96	121.26
2	D	625	FAD	C4X-N5-C5X	4.77	121.54	116.77
2	D	625	FAD	N3A-C2A-N1A	-4.74	121.26	128.68
2	F	625	FAD	C4X-N5-C5X	4.74	121.51	116.77
2	C	625	FAD	N3A-C2A-N1A	-4.72	121.30	128.68
2	E	625	FAD	N3A-C2A-N1A	-4.68	121.36	128.68
2	B	625	FAD	C4X-N5-C5X	4.50	121.27	116.77
2	F	625	FAD	N3A-C2A-N1A	-4.50	121.64	128.68
2	H	625	FAD	C4X-N5-C5X	4.47	121.23	116.77
2	B	625	FAD	C1'-N10-C9A	4.31	121.69	118.29
2	H	625	FAD	N3A-C2A-N1A	-4.13	122.22	128.68
2	C	625	FAD	C1'-N10-C9A	3.71	121.22	118.29
2	A	625	FAD	C4X-N5-C5X	3.64	120.40	116.77
2	B	625	FAD	N3A-C2A-N1A	-3.60	123.06	128.68
2	H	625	FAD	C10-C4X-N5	-3.55	118.80	121.26
2	A	625	FAD	C4-C4X-N5	3.53	122.64	118.60
2	H	625	FAD	C1'-N10-C10	3.53	121.57	118.41
2	A	625	FAD	C1'-N10-C10	3.42	121.47	118.41
2	H	625	FAD	C4-C4X-N5	3.39	122.47	118.60
2	H	625	FAD	C4X-C4-N3	-3.23	119.02	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	625	FAD	C4-C4X-N5	3.22	122.27	118.60
2	C	625	FAD	C10-C4X-N5	-3.21	119.04	121.26
2	F	625	FAD	C1'-N10-C10	3.17	121.25	118.41
2	E	625	FAD	C1'-N10-C9A	3.16	120.78	118.29
2	A	625	FAD	C4-C4X-C10	-3.15	117.86	119.95
2	F	625	FAD	C10-C4X-N5	-3.08	119.13	121.26
2	B	625	FAD	C5'-C4'-C3'	-3.05	106.32	112.20
2	G	625	FAD	C4-C4X-N5	3.02	122.05	118.60
2	G	625	FAD	C4-C4X-C10	-3.01	117.96	119.95
2	E	625	FAD	C4X-C4-N3	-2.98	119.35	123.43
2	D	625	FAD	C9A-N10-C10	-2.95	118.04	121.91
2	B	625	FAD	C4A-C5A-N7A	-2.93	106.35	109.40
2	E	625	FAD	C4A-C5A-N7A	-2.90	106.38	109.40
2	C	625	FAD	C4-C4X-N5	2.78	121.78	118.60
2	D	625	FAD	C4-C4X-C10	-2.74	118.14	119.95
2	G	625	FAD	C4X-C4-N3	-2.72	119.71	123.43
2	B	625	FAD	C8M-C8-C9	-2.69	113.91	120.34
2	F	625	FAD	C4-C4X-N5	2.66	121.64	118.60
2	C	625	FAD	C4A-C5A-N7A	-2.66	106.63	109.40
2	F	625	FAD	O4B-C1B-C2B	-2.65	103.06	106.93
2	A	625	FAD	C10-C4X-N5	-2.63	119.44	121.26
2	C	625	FAD	C4X-C4-N3	-2.60	119.88	123.43
2	A	625	FAD	O4B-C1B-C2B	-2.54	103.21	106.93
2	H	625	FAD	O4B-C1B-C2B	-2.54	103.21	106.93
2	A	625	FAD	N6A-C6A-N1A	2.52	123.81	118.57
2	B	625	FAD	C4-C4X-C10	-2.46	118.32	119.95
2	A	625	FAD	C4X-C4-N3	-2.46	120.07	123.43
2	A	625	FAD	C9A-N10-C10	-2.44	118.72	121.91
2	B	625	FAD	C4X-C4-N3	-2.43	120.11	123.43
2	A	625	FAD	C5A-C6A-N6A	-2.38	116.73	120.35
2	B	625	FAD	C4-C4X-N5	2.38	121.32	118.60
2	H	625	FAD	C9A-N10-C10	-2.37	118.80	121.91
2	E	625	FAD	O3B-C3B-C4B	-2.35	104.24	111.05
2	D	625	FAD	C4-C4X-N5	2.34	121.28	118.60
2	B	625	FAD	O2A-PA-O1A	2.32	123.73	112.24
2	B	625	FAD	C8M-C8-C7	2.31	125.48	120.74
2	B	625	FAD	P-O3P-PA	-2.29	124.98	132.83
2	B	625	FAD	O3B-C3B-C4B	-2.27	104.49	111.05
2	G	625	FAD	C9A-N10-C10	-2.23	118.99	121.91
2	B	625	FAD	O4B-C1B-C2B	-2.22	103.68	106.93
2	H	625	FAD	C5'-C4'-C3'	-2.18	107.99	112.20
2	F	625	FAD	C4X-C4-N3	-2.17	120.46	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	625	FAD	C5A-C6A-N6A	2.12	123.57	120.35
2	G	625	FAD	O3B-C3B-C4B	-2.10	104.96	111.05
2	D	625	FAD	O4B-C1B-C2B	-2.10	103.86	106.93
2	F	625	FAD	O3B-C3B-C4B	-2.10	104.98	111.05
2	F	625	FAD	C4A-C5A-N7A	-2.06	107.25	109.40
2	G	625	FAD	O4B-C1B-C2B	-2.05	103.93	106.93
2	D	625	FAD	C4X-C4-N3	-2.03	120.65	123.43
2	B	625	FAD	C9A-N10-C10	-2.02	119.27	121.91
2	D	625	FAD	P-O3P-PA	-2.01	125.92	132.83

There are no chirality outliers.

All (30) torsion outliers are listed below:

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

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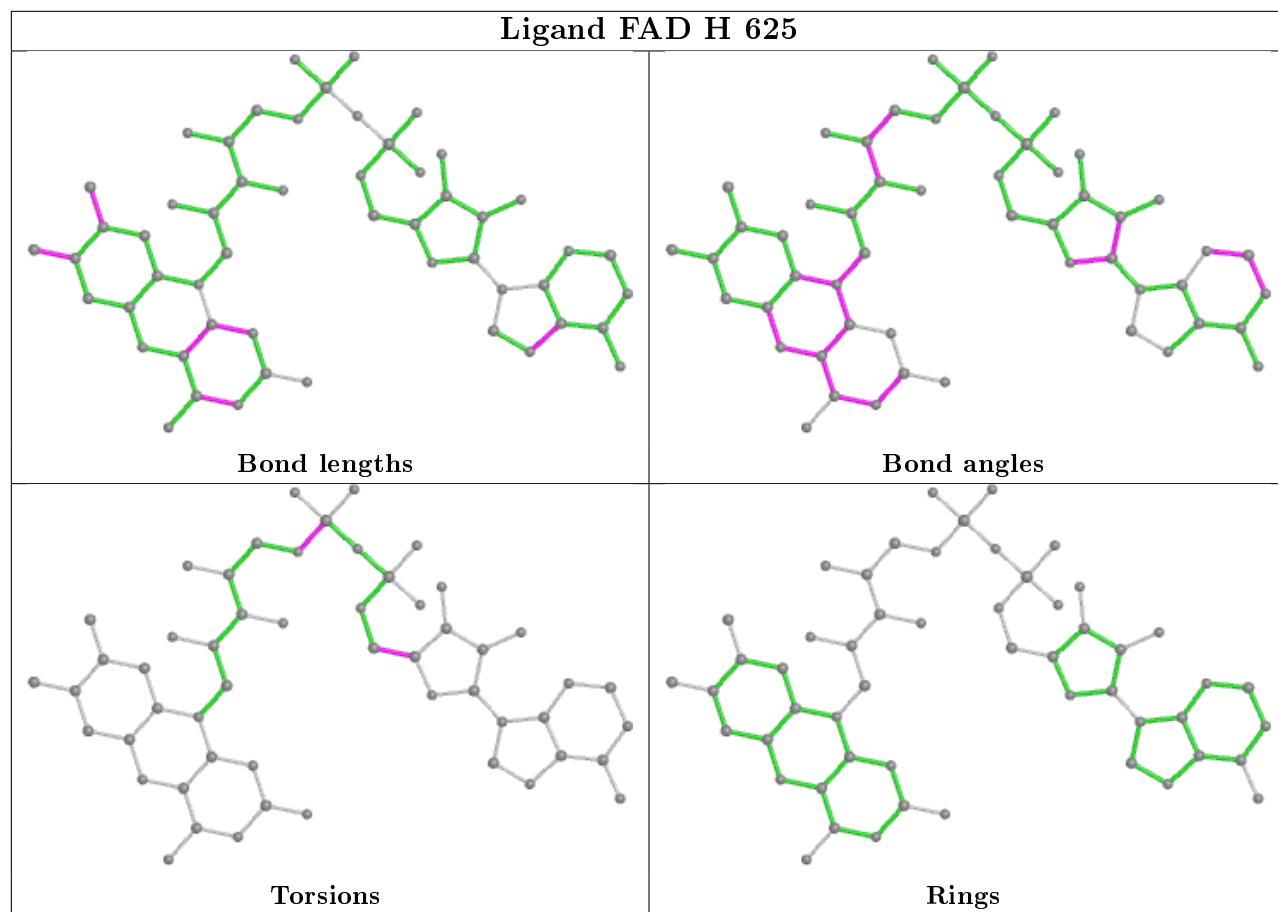
Mol	Chain	Res	Type	Atoms
2	F	625	FAD	O4B-C4B-C5B-O5B
2	G	625	FAD	O4B-C4B-C5B-O5B

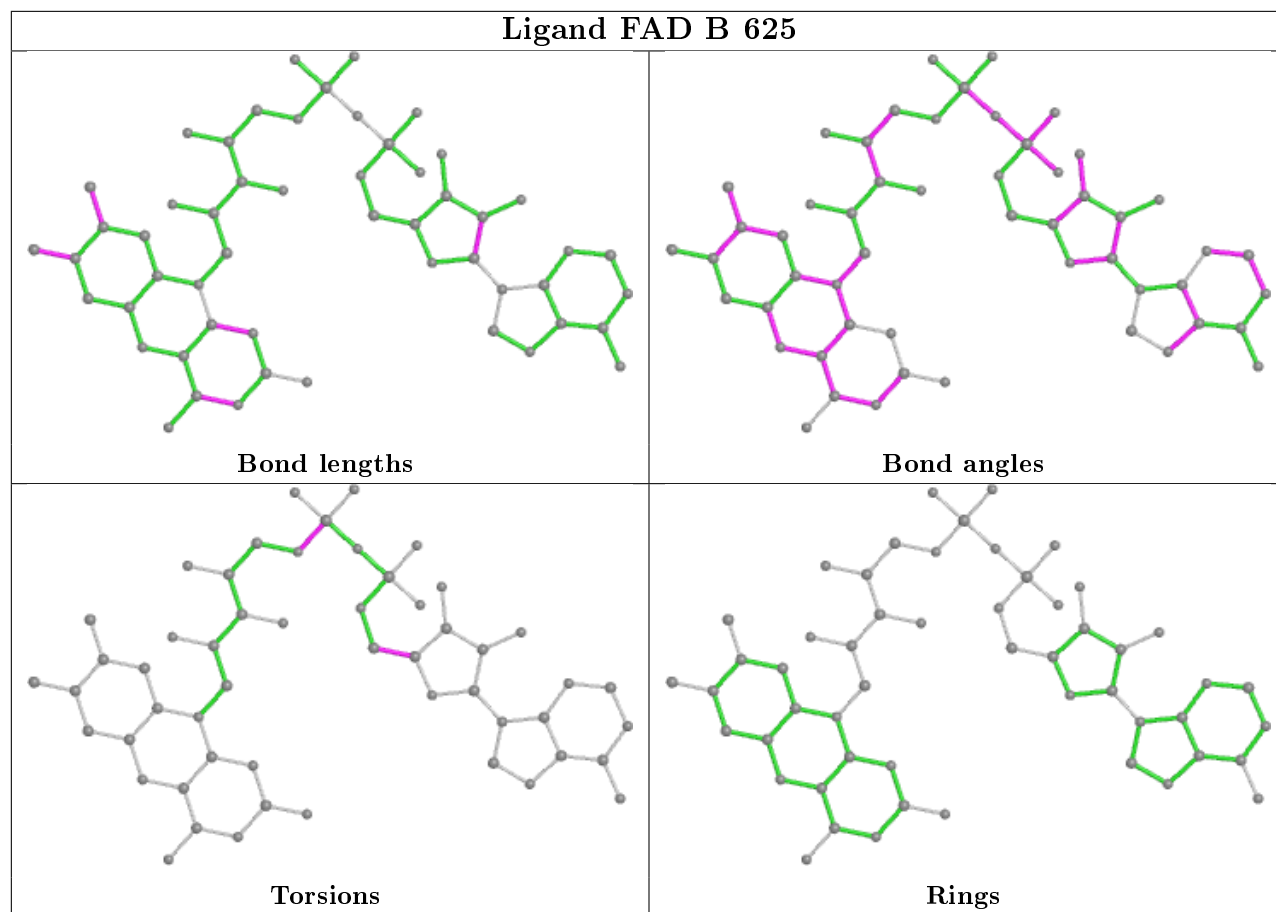
There are no ring outliers.

3 monomers are involved in 8 short contacts:

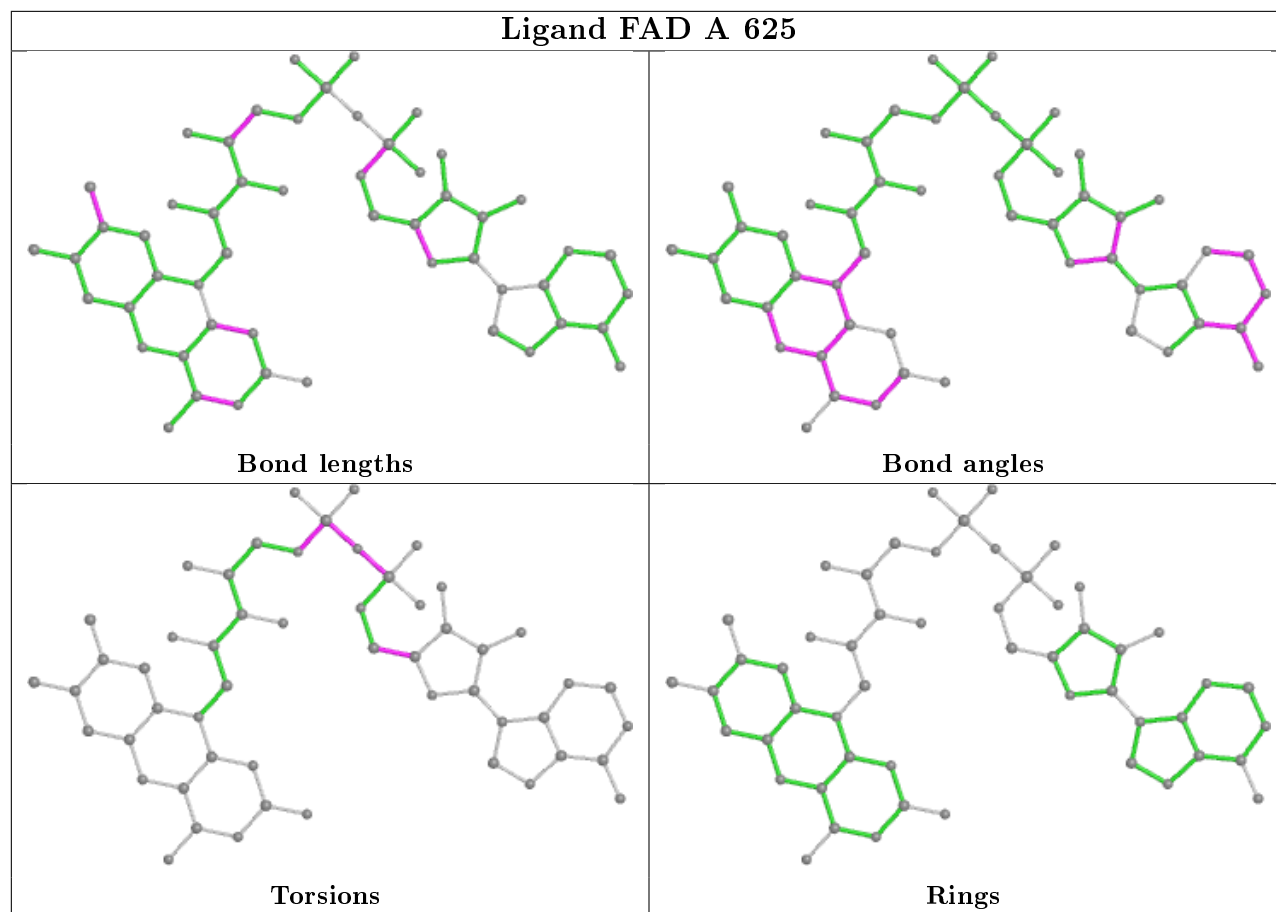
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	625	FAD	6	0
2	D	625	FAD	1	0
2	E	625	FAD	1	0

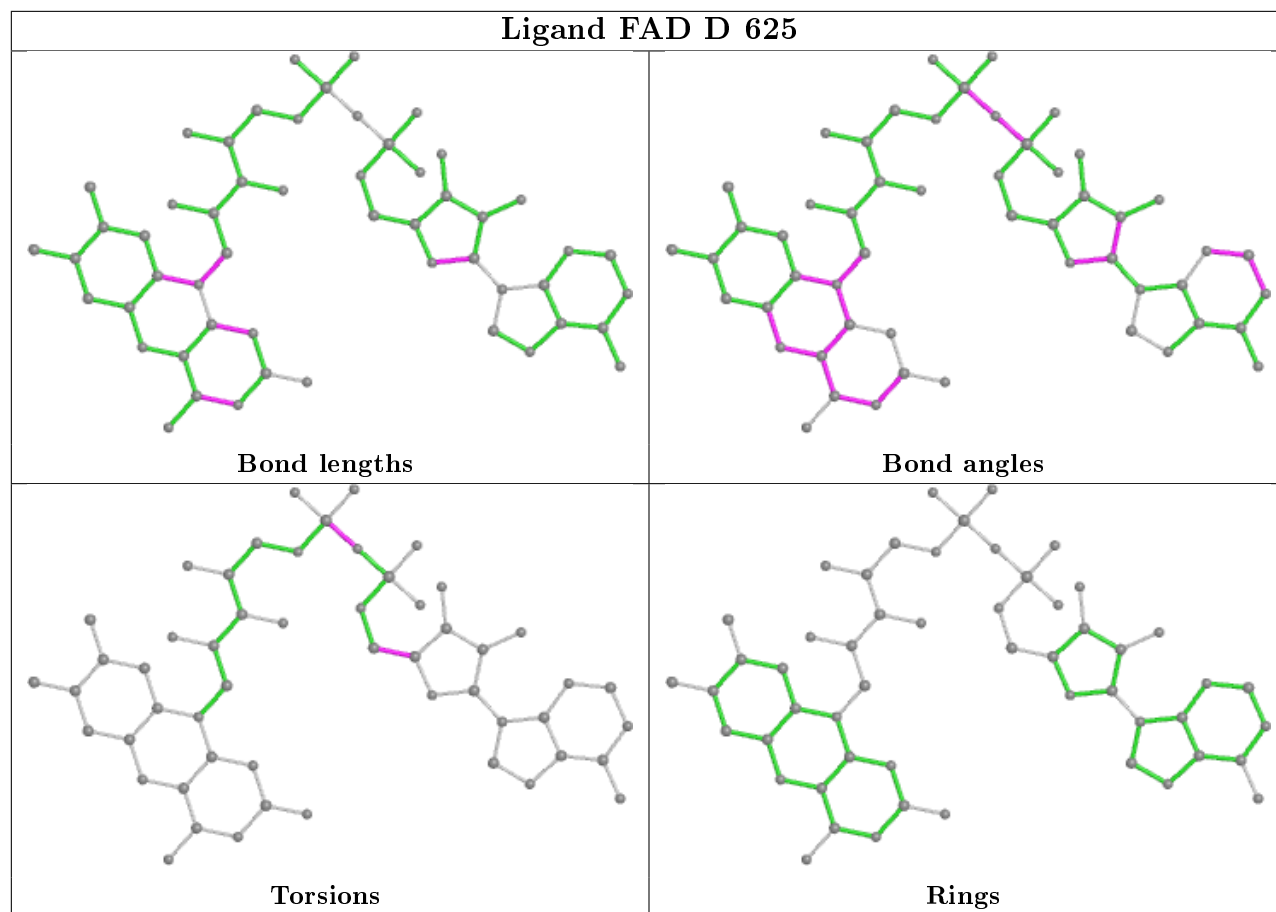
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

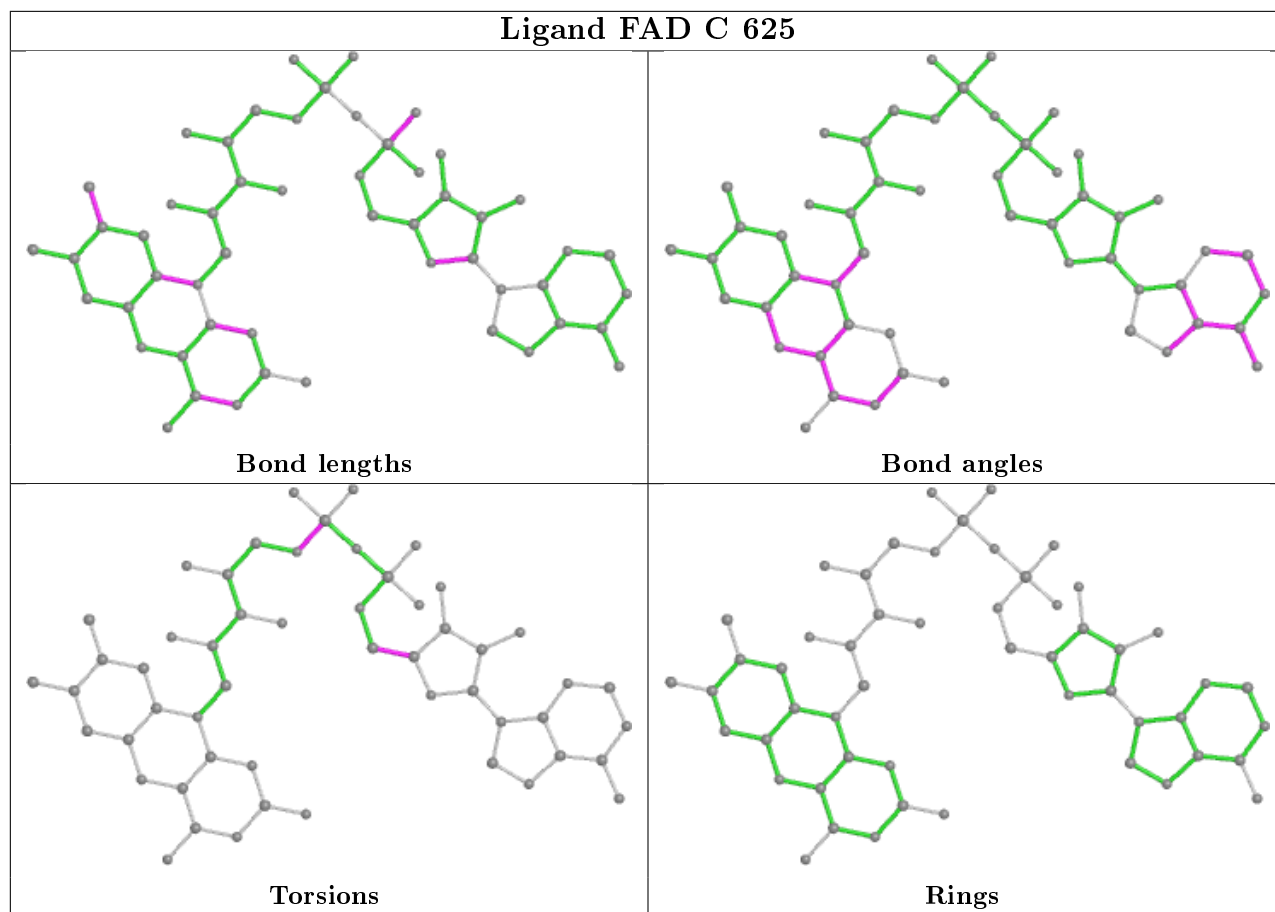


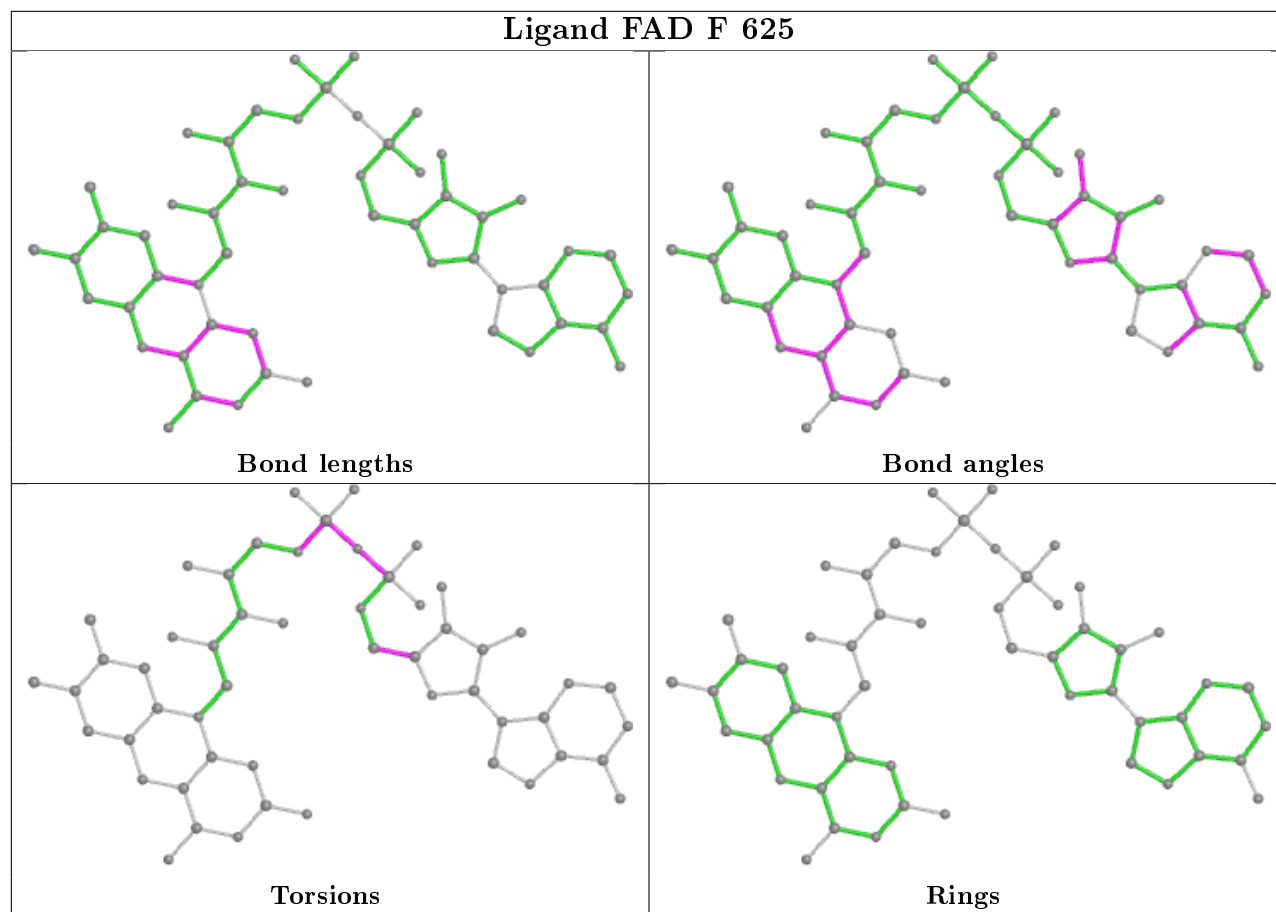


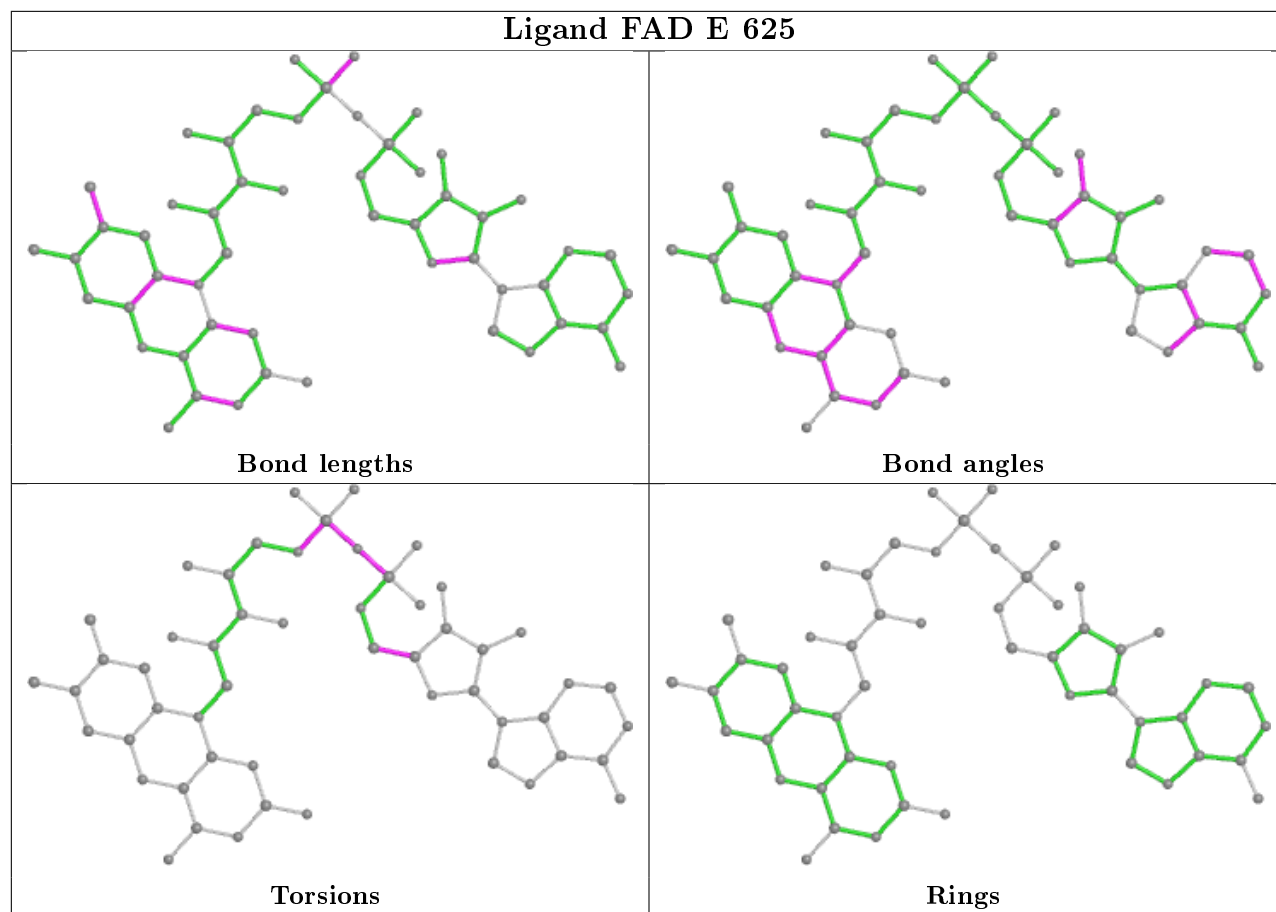


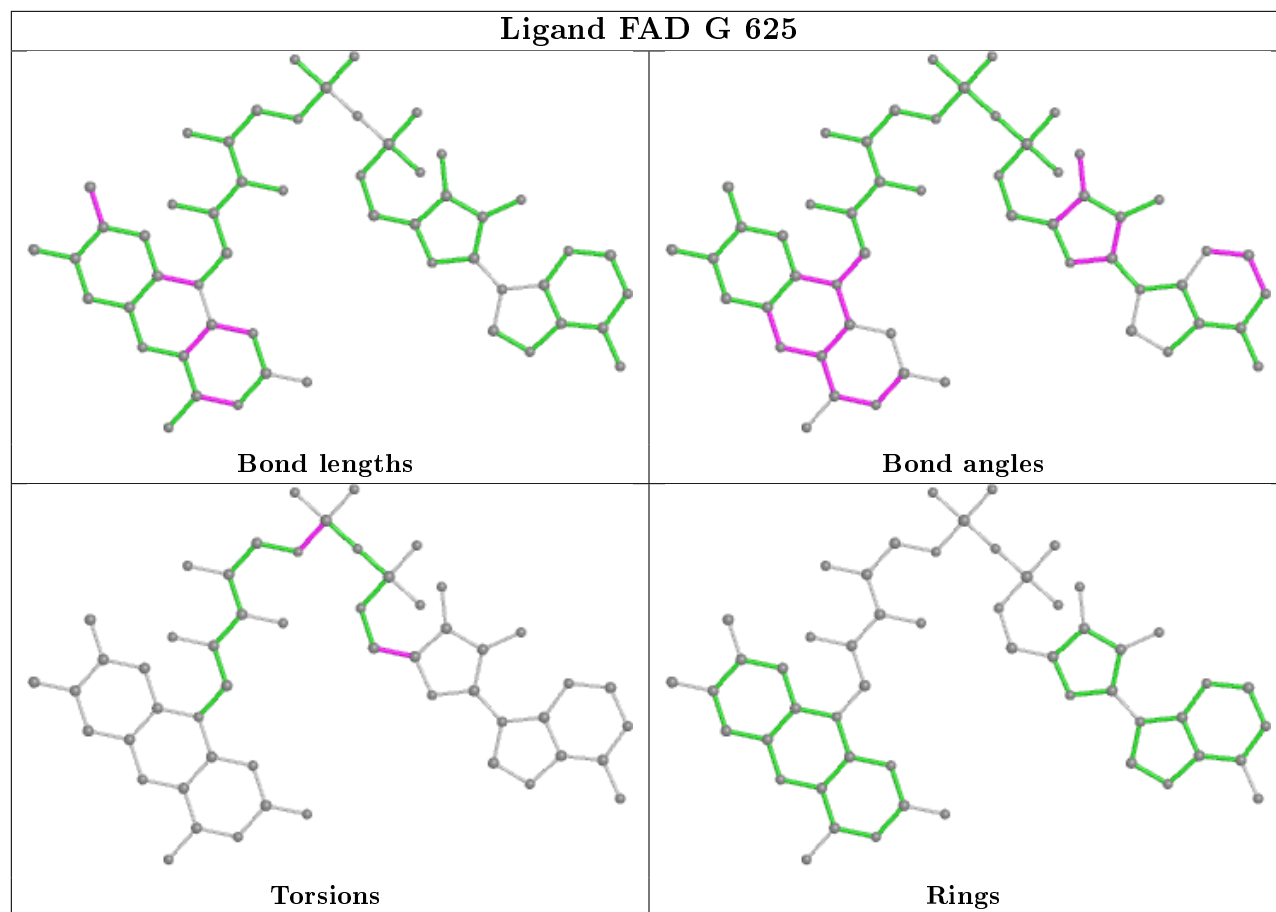












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	561/622 (90%)	-0.01	20 (3%) 42 55	8, 16, 31, 51	0
1	B	561/622 (90%)	0.53	52 (9%) 8 14	12, 23, 38, 58	0
1	C	561/622 (90%)	0.01	25 (4%) 33 46	8, 16, 32, 57	0
1	D	561/622 (90%)	0.29	46 (8%) 11 17	8, 23, 40, 63	0
1	E	561/622 (90%)	0.12	31 (5%) 25 36	5, 16, 36, 56	0
1	F	561/622 (90%)	-0.03	19 (3%) 45 57	4, 14, 31, 50	0
1	G	561/622 (90%)	0.12	29 (5%) 27 39	3, 15, 33, 53	0
1	H	561/622 (90%)	-0.03	18 (3%) 47 59	3, 14, 30, 55	0
All	All	4488/4976 (90%)	0.12	240 (5%) 26 38	3, 17, 36, 63	0

All (240) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	619	THR	8.3
1	D	458	ALA	7.5
1	B	458	ALA	7.2
1	H	459	VAL	7.1
1	G	44	ASP	7.0
1	D	455	SER	6.6
1	F	619	THR	6.1
1	C	459	VAL	6.1
1	E	619	THR	5.9
1	D	459	VAL	5.8
1	H	44	ASP	5.8
1	C	619	THR	5.8
1	C	45	ILE	5.8
1	G	343	THR	5.7
1	F	459	VAL	5.5
1	E	458	ALA	5.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	H	619	THR	5.4
1	D	44	ASP	5.3
1	B	445	TRP	5.3
1	B	459	VAL	5.3
1	G	458	ALA	5.2
1	B	619	THR	5.2
1	G	389	LEU	5.1
1	C	458	ALA	5.1
1	E	47	TYR	5.0
1	D	400	SER	5.0
1	D	389	LEU	4.9
1	G	459	VAL	4.8
1	E	45	ILE	4.7
1	A	459	VAL	4.7
1	E	343	THR	4.7
1	B	45	ILE	4.6
1	E	618	PHE	4.5
1	D	343	THR	4.5
1	G	618	PHE	4.5
1	C	343	THR	4.5
1	D	186	ASP	4.5
1	A	619	THR	4.4
1	D	618	PHE	4.4
1	H	458	ALA	4.4
1	F	186	ASP	4.4
1	B	455	SER	4.3
1	G	619	THR	4.3
1	B	195	TRP	4.3
1	C	44	ASP	4.3
1	E	459	VAL	4.3
1	E	389	LEU	4.2
1	D	45	ILE	4.2
1	E	455	SER	4.2
1	D	290	ALA	4.1
1	B	460	GLN	4.1
1	B	446	HIS	4.1
1	D	390	THR	4.1
1	H	457	GLY	4.0
1	H	186	ASP	4.0
1	C	344	ASN	4.0
1	G	186	ASP	3.9
1	F	458	ALA	3.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	401	THR	3.9
1	D	268	THR	3.9
1	B	343	THR	3.9
1	H	45	ILE	3.9
1	A	455	SER	3.8
1	G	455	SER	3.8
1	E	400	SER	3.7
1	B	473	PHE	3.7
1	B	186	ASP	3.7
1	C	455	SER	3.7
1	B	47	TYR	3.6
1	D	189	ASP	3.6
1	D	344	ASN	3.5
1	D	342	PRO	3.5
1	A	458	ALA	3.5
1	D	401	THR	3.5
1	E	388	GLU	3.5
1	G	400	SER	3.5
1	A	343	THR	3.4
1	B	167	HIS	3.4
1	C	388	GLU	3.4
1	G	454	PHE	3.4
1	E	385	THR	3.3
1	B	269	ASP	3.3
1	A	454	PHE	3.3
1	E	401	THR	3.3
1	D	269	ASP	3.3
1	E	269	ASP	3.3
1	A	307	ASP	3.2
1	E	186	ASP	3.2
1	A	186	ASP	3.2
1	G	187	ASP	3.2
1	B	344	ASN	3.2
1	D	456	TYR	3.2
1	B	44	ASP	3.2
1	G	561	GLU	3.2
1	B	342	PRO	3.2
1	D	384	GLY	3.2
1	F	455	SER	3.1
1	H	344	ASN	3.1
1	D	310	GLU	3.1
1	B	614	THR	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	400	SER	3.1
1	D	460	GLN	3.1
1	C	345	PRO	3.1
1	E	398	GLY	3.1
1	F	457	GLY	3.1
1	G	347	GLU	3.1
1	C	269	ASP	3.0
1	F	454	PHE	3.0
1	D	407	TRP	3.0
1	G	342	PRO	3.0
1	B	618	PHE	2.9
1	G	344	ASN	2.9
1	H	269	ASP	2.9
1	B	592	ALA	2.9
1	G	268	THR	2.9
1	B	561	GLU	2.9
1	E	397	PRO	2.9
1	G	345	PRO	2.9
1	B	345	PRO	2.9
1	E	615	PRO	2.9
1	F	268	THR	2.9
1	C	186	ASP	2.9
1	A	345	PRO	2.8
1	A	44	ASP	2.8
1	D	347	GLU	2.8
1	D	560	LYS	2.8
1	D	561	GLU	2.8
1	H	343	THR	2.8
1	E	44	ASP	2.8
1	F	189	ASP	2.8
1	B	562	ASP	2.7
1	H	460	GLN	2.7
1	D	211	ASP	2.7
1	A	211	ASP	2.7
1	H	400	SER	2.7
1	G	383	ARG	2.7
1	F	44	ASP	2.7
1	G	390	THR	2.7
1	E	617	PRO	2.7
1	A	344	ASN	2.7
1	F	344	ASN	2.7
1	E	460	GLN	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	G	401	THR	2.7
1	B	187	ASP	2.6
1	F	269	ASP	2.6
1	D	617	PRO	2.6
1	B	285	ARG	2.6
1	E	614	THR	2.6
1	B	188	ALA	2.6
1	B	399	ALA	2.6
1	D	345	PRO	2.5
1	B	307	ASP	2.5
1	D	406	ASP	2.5
1	E	344	ASN	2.5
1	C	561	GLU	2.5
1	G	310	GLU	2.5
1	B	548	HIS	2.5
1	B	577	ASN	2.5
1	C	456	TYR	2.5
1	D	442	SER	2.5
1	F	343	THR	2.5
1	E	457	GLY	2.5
1	C	618	PHE	2.5
1	B	456	TYR	2.5
1	C	457	GLY	2.5
1	B	389	LEU	2.5
1	D	305	SER	2.4
1	D	388	GLU	2.4
1	F	388	GLU	2.4
1	D	496	ASN	2.4
1	G	456	TYR	2.4
1	B	400	SER	2.4
1	C	389	LEU	2.4
1	D	187	ASP	2.4
1	B	189	ASP	2.4
1	D	383	ARG	2.4
1	G	307	ASP	2.4
1	D	101	ASP	2.4
1	C	400	SER	2.4
1	E	383	ARG	2.4
1	G	269	ASP	2.4
1	D	385	THR	2.4
1	B	454	PHE	2.4
1	B	305	SER	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	454	PHE	2.3
1	A	457	GLY	2.3
1	B	489	ASP	2.3
1	H	455	SER	2.3
1	D	457	GLY	2.3
1	B	198	LEU	2.3
1	B	272	GLU	2.3
1	C	232	GLY	2.3
1	B	385	THR	2.3
1	G	272	GLU	2.3
1	H	617	PRO	2.3
1	E	390	THR	2.3
1	A	342	PRO	2.3
1	A	456	TYR	2.2
1	D	231	LYS	2.2
1	C	101	ASP	2.2
1	C	442	SER	2.2
1	A	387	GLY	2.2
1	F	561	GLU	2.2
1	E	270	ALA	2.2
1	G	460	GLN	2.2
1	B	309	PHE	2.2
1	B	613	PHE	2.2
1	B	183	LEU	2.2
1	B	560	LYS	2.1
1	C	460	GLN	2.2
1	E	456	TYR	2.1
1	B	268	THR	2.1
1	B	270	ALA	2.1
1	C	342	PRO	2.1
1	E	84	LEU	2.1
1	H	272	GLU	2.1
1	C	270	ALA	2.1
1	B	197	ARG	2.1
1	C	429	GLU	2.1
1	D	291	LEU	2.1
1	F	272	GLU	2.1
1	A	272	GLU	2.1
1	H	618	PHE	2.1
1	F	211	ASP	2.1
1	D	391	TYR	2.1
1	B	178	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	561	GLU	2.1
1	B	308	ARG	2.1
1	A	49	VAL	2.1
1	B	457	GLY	2.1
1	A	453	ALA	2.0
1	G	188	ALA	2.0
1	F	489	ASP	2.0
1	E	272	GLU	2.0
1	D	232	GLY	2.0
1	G	385	THR	2.0
1	A	189	ASP	2.0
1	H	345	PRO	2.0
1	D	341	ASN	2.0
1	E	562	ASP	2.0

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

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

## 6.3 Carbohydrates [i](#)

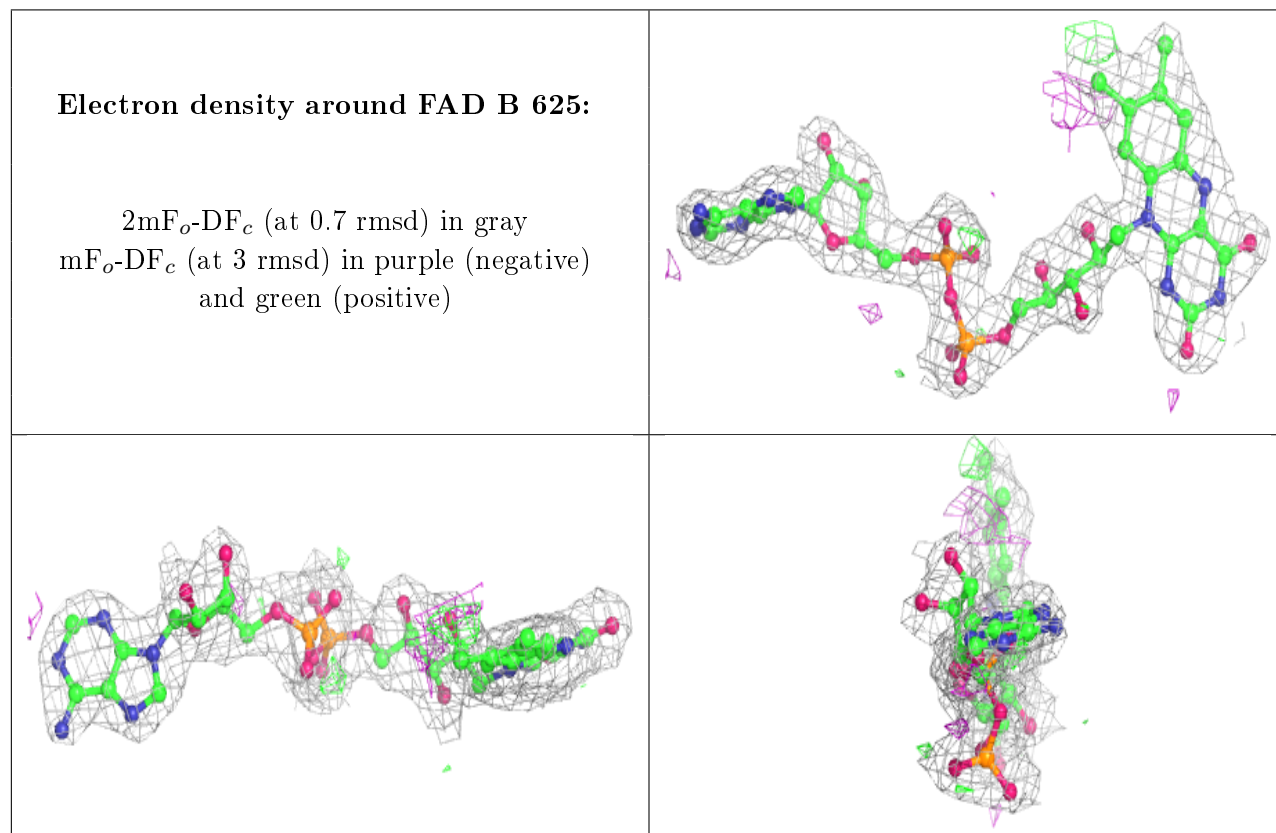
There are no carbohydrates in this entry.

## 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, 95<sup>th</sup> 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.

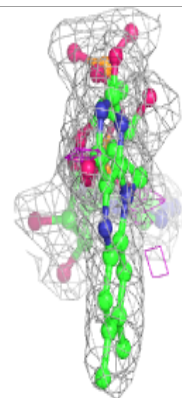
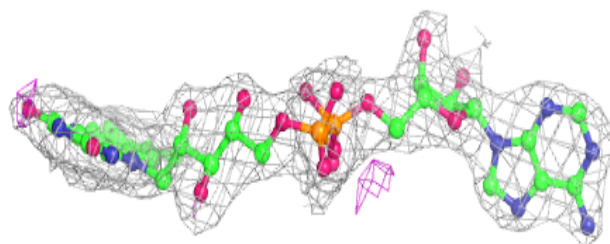
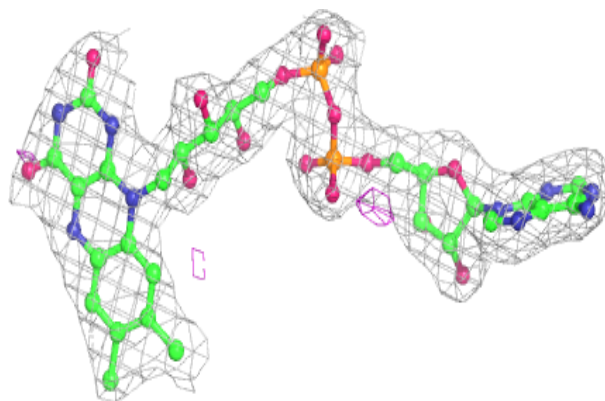
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	FAD	B	625	53/53	0.95	0.11	12,23,28,33	0
2	FAD	D	625	53/53	0.96	0.11	17,21,26,27	0
2	FAD	G	625	53/53	0.96	0.11	10,15,20,22	0
2	FAD	C	625	53/53	0.97	0.10	8,15,18,20	0
2	FAD	E	625	53/53	0.97	0.09	10,16,19,23	0
2	FAD	A	625	53/53	0.97	0.09	6,14,17,19	0
2	FAD	H	625	53/53	0.98	0.10	9,13,16,19	0
2	FAD	F	625	53/53	0.98	0.11	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.

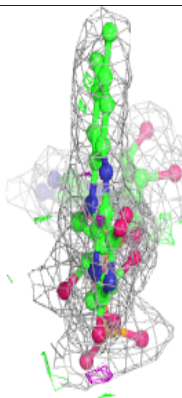
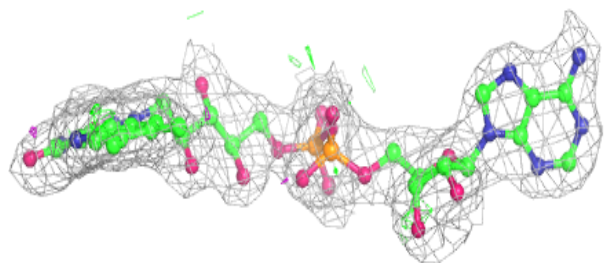
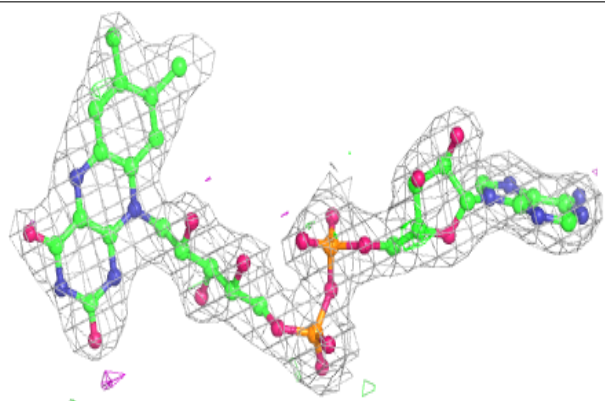


**Electron density around FAD D 625:**

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

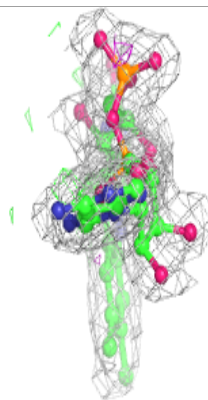
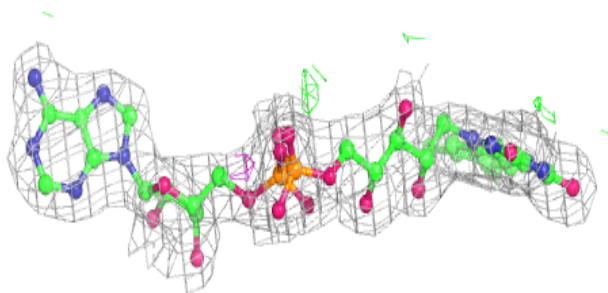
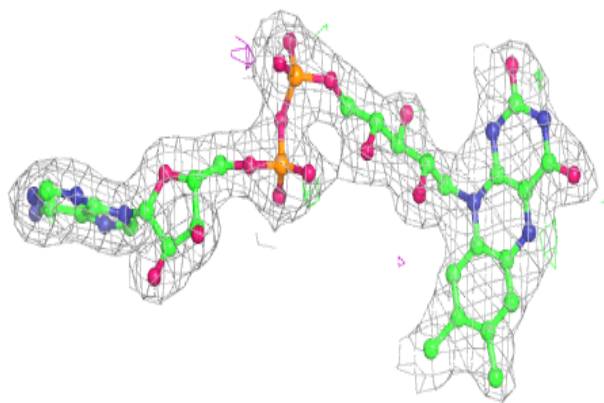
**Electron density around FAD G 625:**

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

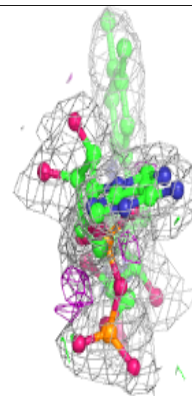
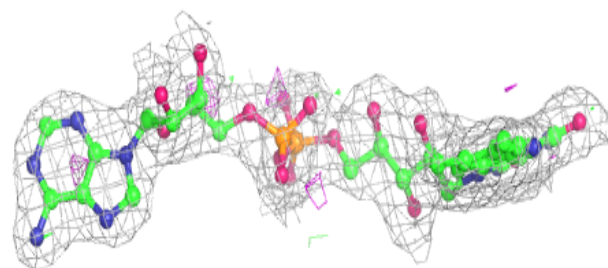
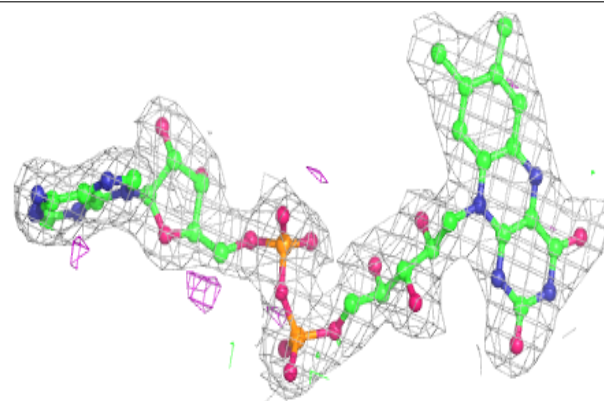


**Electron density around FAD C 625:**

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

**Electron density around FAD E 625:**

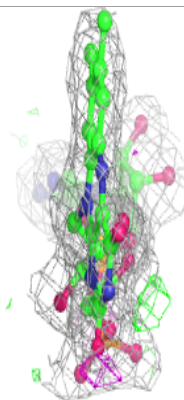
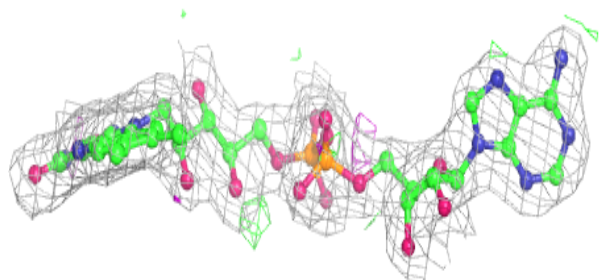
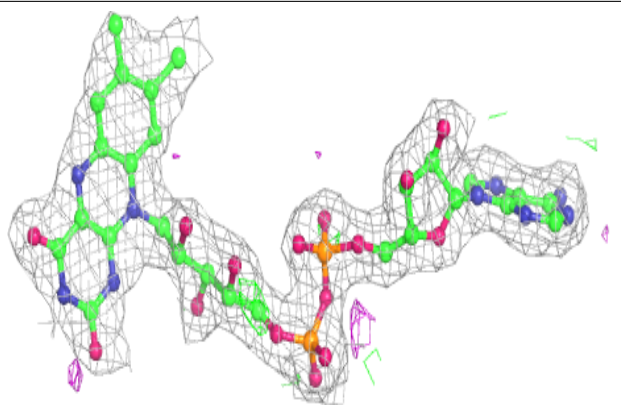
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



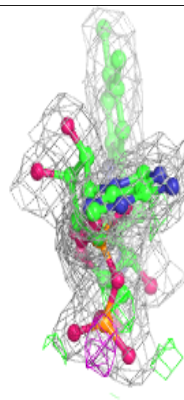
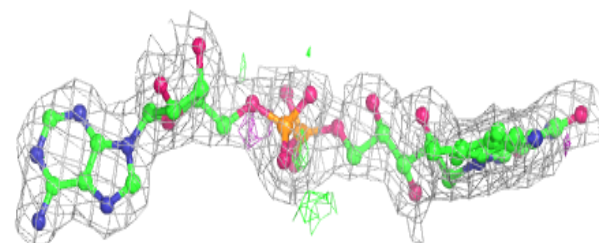
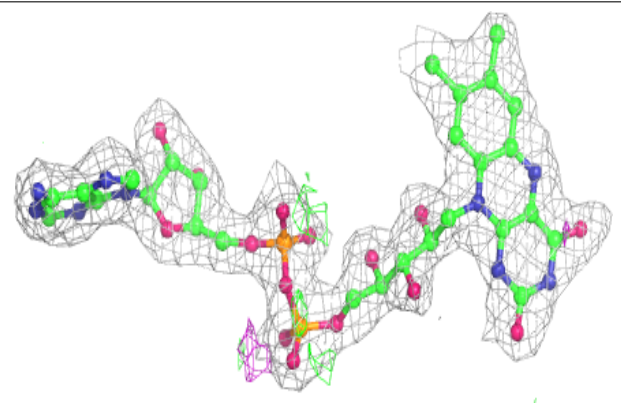


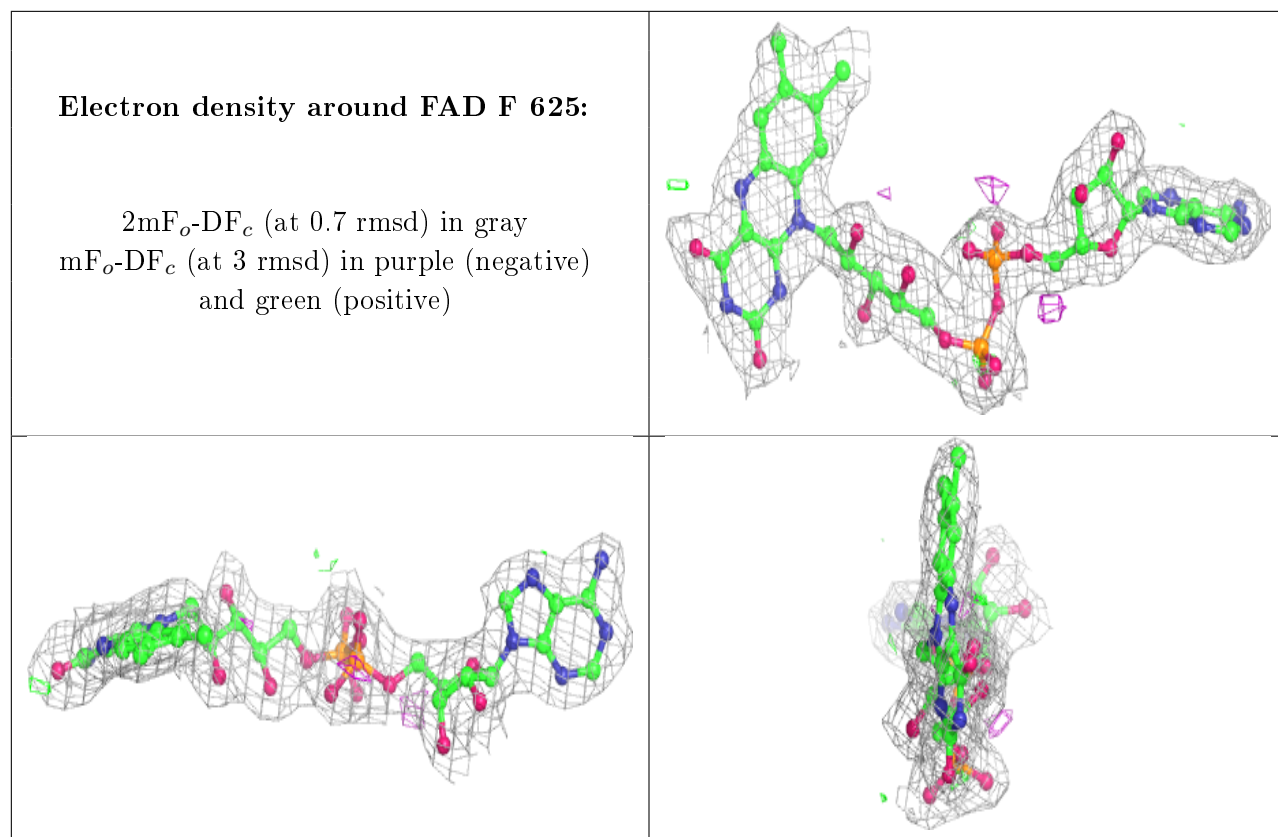
**Electron density around FAD A 625:**

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

**Electron density around FAD 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.