



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 07:48 PM BST

PDB ID : 3NNE  
Title : Crystal structure of choline oxidase S101A mutant  
Authors : Wang, Y.-F.; Finnegan, S.; Yuan, H.; Orville, A.M.; Weber, I.T.; Gadda, G.  
Deposited on : 2010-06-23  
Resolution : 2.47 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 : 2.13.1  
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) : 2.13.1

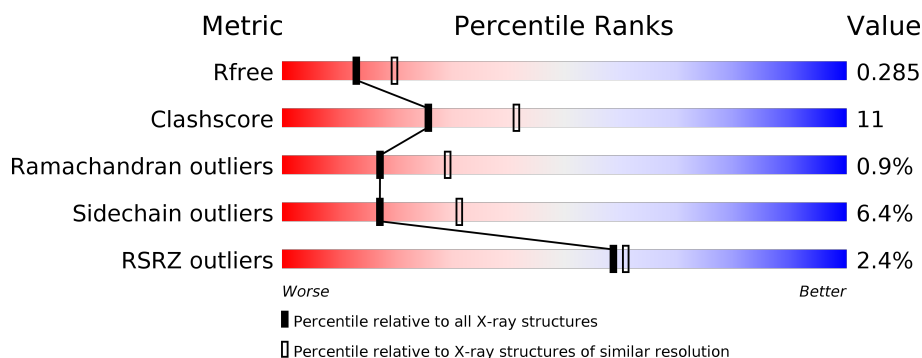
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.47 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	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	546	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>20%</div> <div>• •</div> </div> </div>
1	B	546	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>17%</div> <div>• •</div> </div> </div>
1	C	546	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>21%</div> <div>• •</div> </div> </div>
1	D	546	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>26%</div> <div>• •</div> </div> </div>
1	E	546	<div> <div>4%</div> <div> <div></div> <div>73%</div> <div>21%</div> <div>• •</div> </div> </div>
1	F	546	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>20%</div> <div>• •</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	546	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>22%</div> <div>• •</div> </div> </div>
1	H	546	<div> <div>5%</div> <div> <div></div> <div>63%</div> <div>30%</div> <div>• •</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	A	601	-	-	X	-
3	ACT	F	601	-	-	X	-
3	ACT	H	601	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 33722 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.

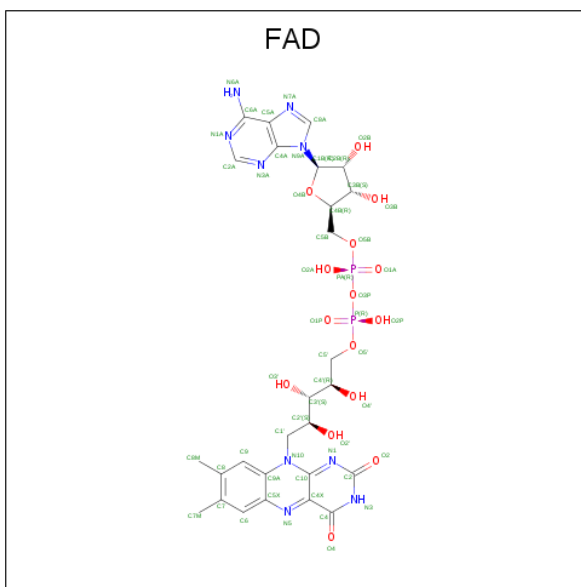
- Molecule 1 is a protein called Choline oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	530	Total	C	N	O	S	0	3	0
			4119	2561	743	791	24			
1	B	530	Total	C	N	O	S	0	4	0
			4122	2562	739	797	24			
1	C	528	Total	C	N	O	S	0	3	0
			4097	2547	736	790	24			
1	D	530	Total	C	N	O	S	0	3	0
			4121	2561	745	791	24			
1	E	530	Total	C	N	O	S	0	6	0
			4136	2571	749	792	24			
1	F	530	Total	C	N	O	S	0	3	0
			4118	2559	742	793	24			
1	G	529	Total	C	N	O	S	0	4	0
			4108	2554	737	793	24			
1	H	530	Total	C	N	O	S	0	3	0
			4120	2561	744	791	24			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	101	ALA	SER	ENGINEERED MUTATION	UNP Q7X2H8
B	101	ALA	SER	ENGINEERED MUTATION	UNP Q7X2H8
C	101	ALA	SER	ENGINEERED MUTATION	UNP Q7X2H8
D	101	ALA	SER	ENGINEERED MUTATION	UNP Q7X2H8
E	101	ALA	SER	ENGINEERED MUTATION	UNP Q7X2H8
F	101	ALA	SER	ENGINEERED MUTATION	UNP Q7X2H8
G	101	ALA	SER	ENGINEERED MUTATION	UNP Q7X2H8
H	101	ALA	SER	ENGINEERED MUTATION	UNP Q7X2H8

- 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 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 ACETATE ION (three-letter code: ACT) (formula:  $\text{C}_2\text{H}_3\text{O}_2$ ).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	20	Total	O	0	0
			20	20		
4	B	38	Total	O	0	0
			38	38		
4	C	47	Total	O	0	0
			47	47		
4	D	39	Total	O	0	0
			39	39		

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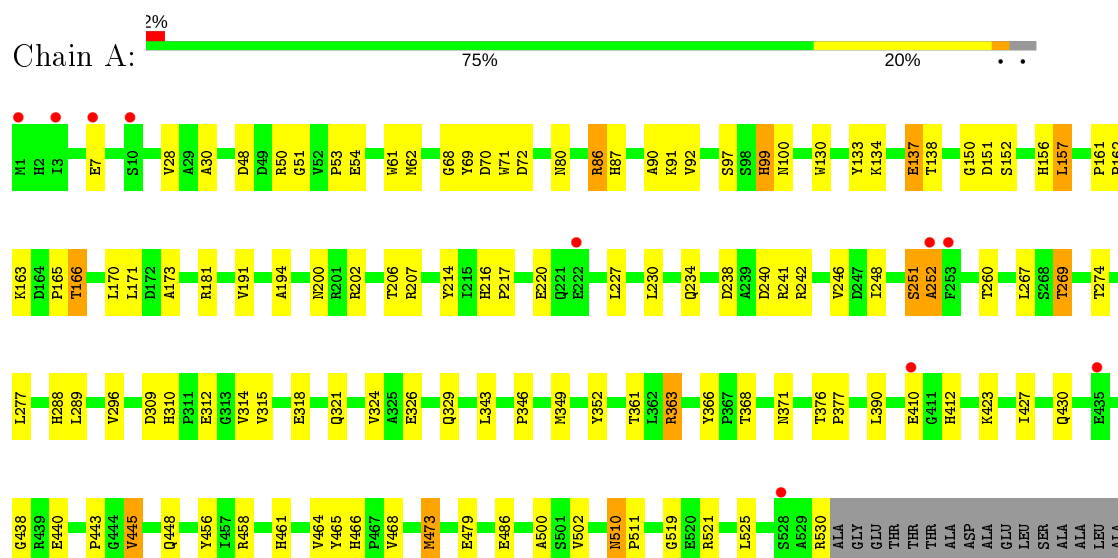
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	38	Total 38	O 38	0	0
4	F	58	Total 58	O 58	0	0
4	G	47	Total 47	O 47	0	0
4	H	38	Total 38	O 38	0	0

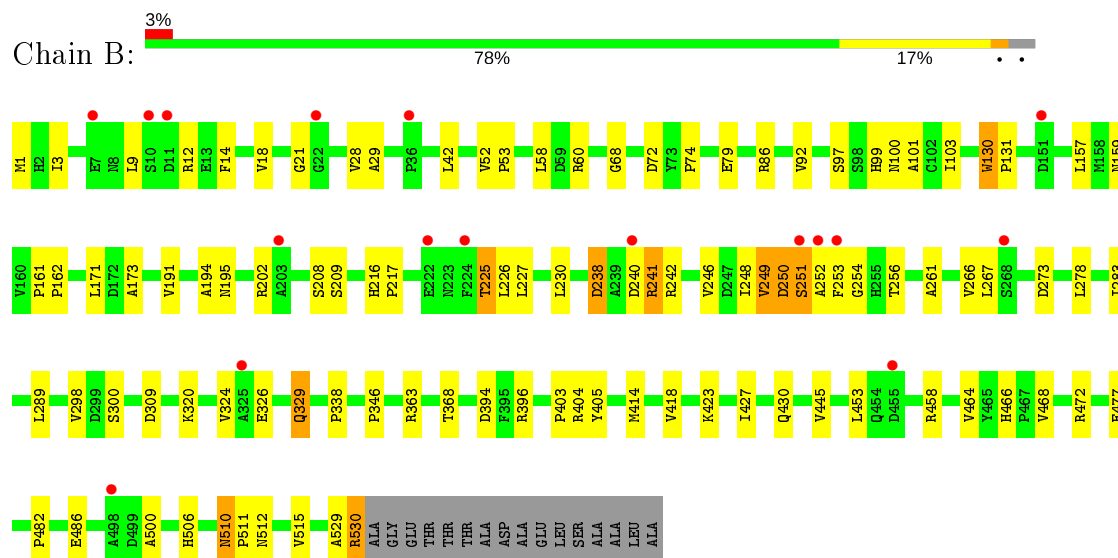
### 3 Residue-property plots [i](#)

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.

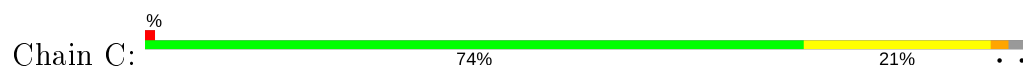
- Molecule 1: Choline oxidase



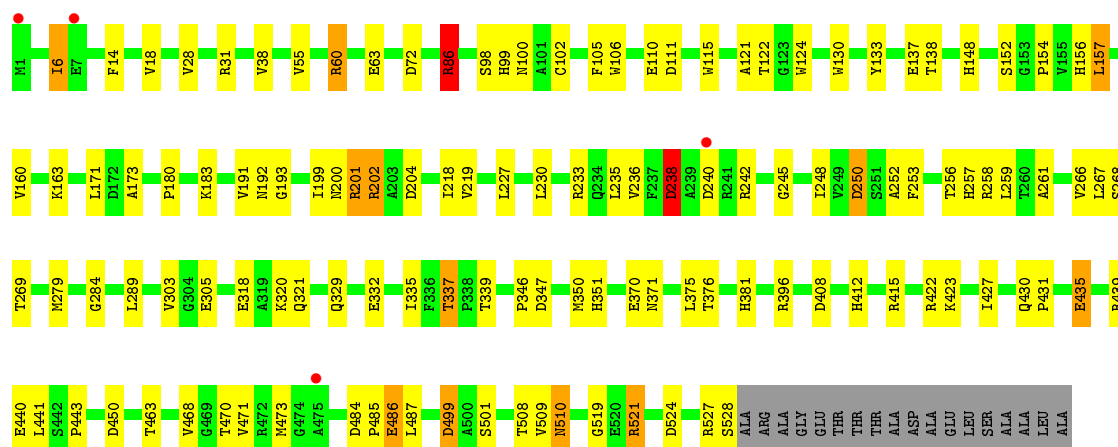
- Molecule 1: Choline oxidase



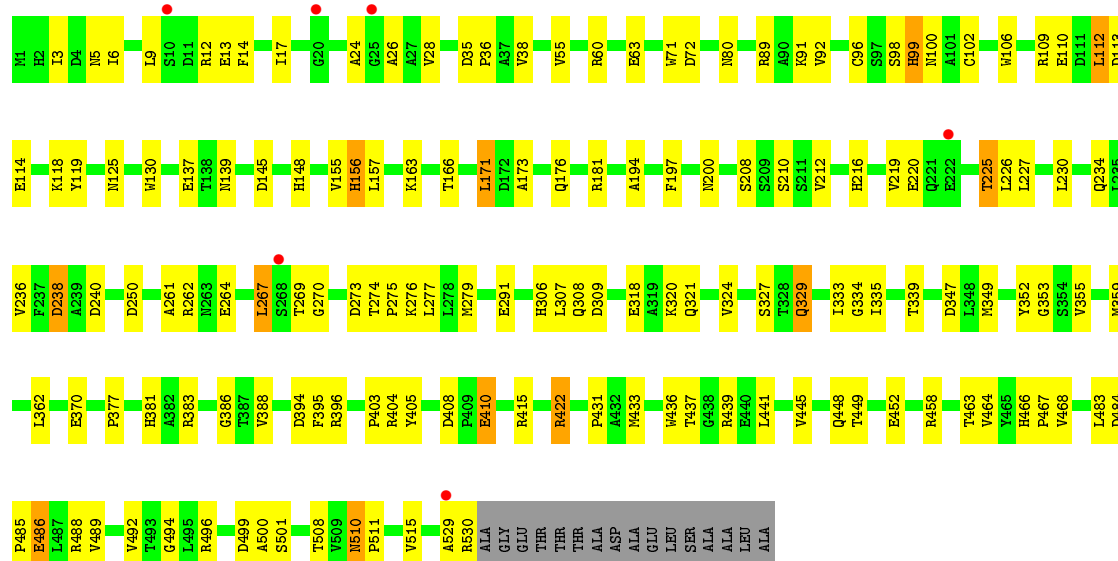
- Molecule 1: Choline oxidase



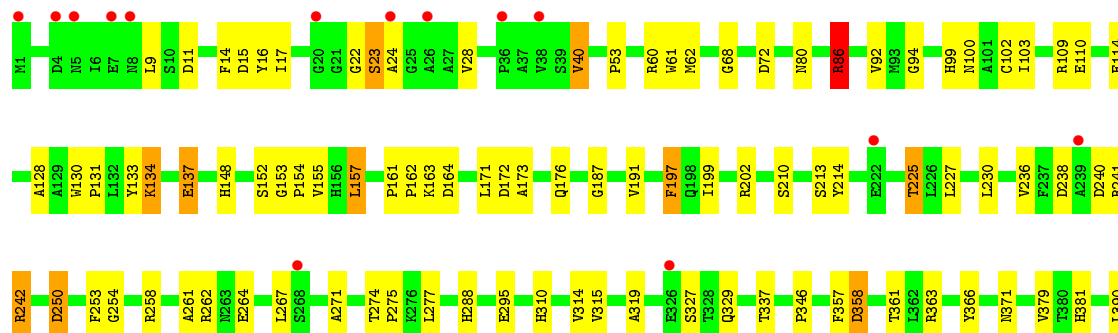


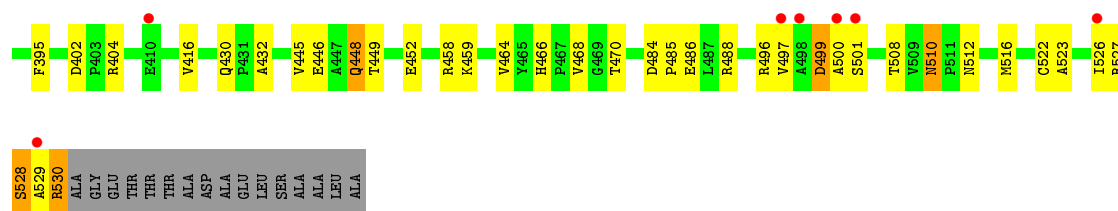


• Molecule 1: Choline oxidase

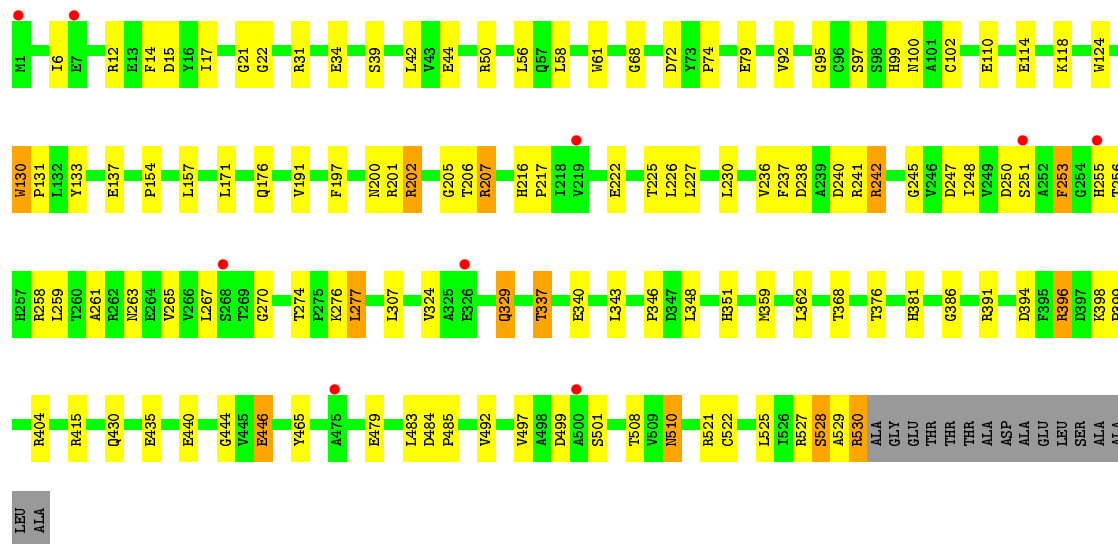
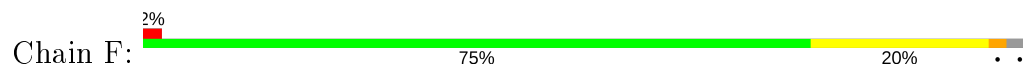


• Molecule 1: Choline oxidase

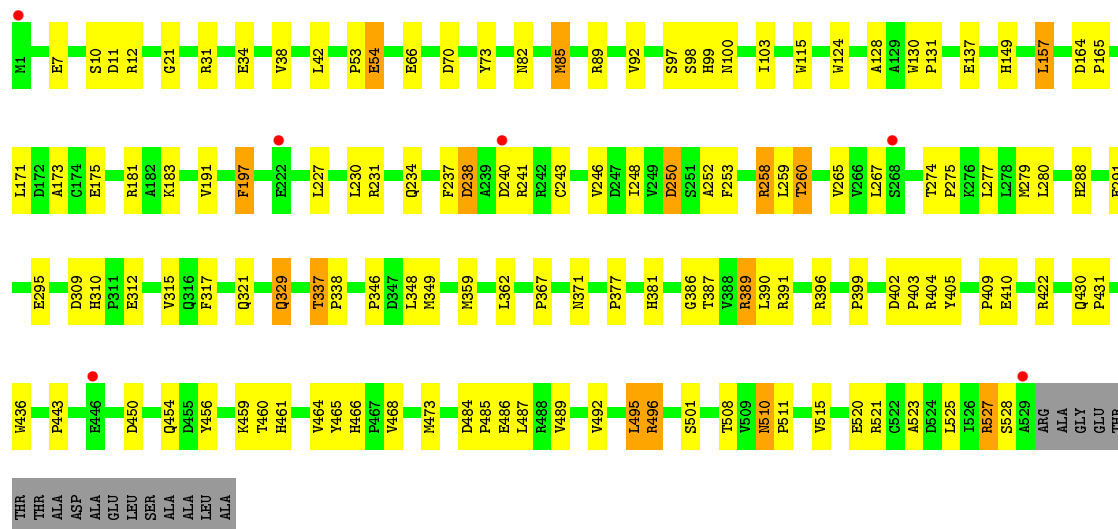




• Molecule 1: Choline oxidase

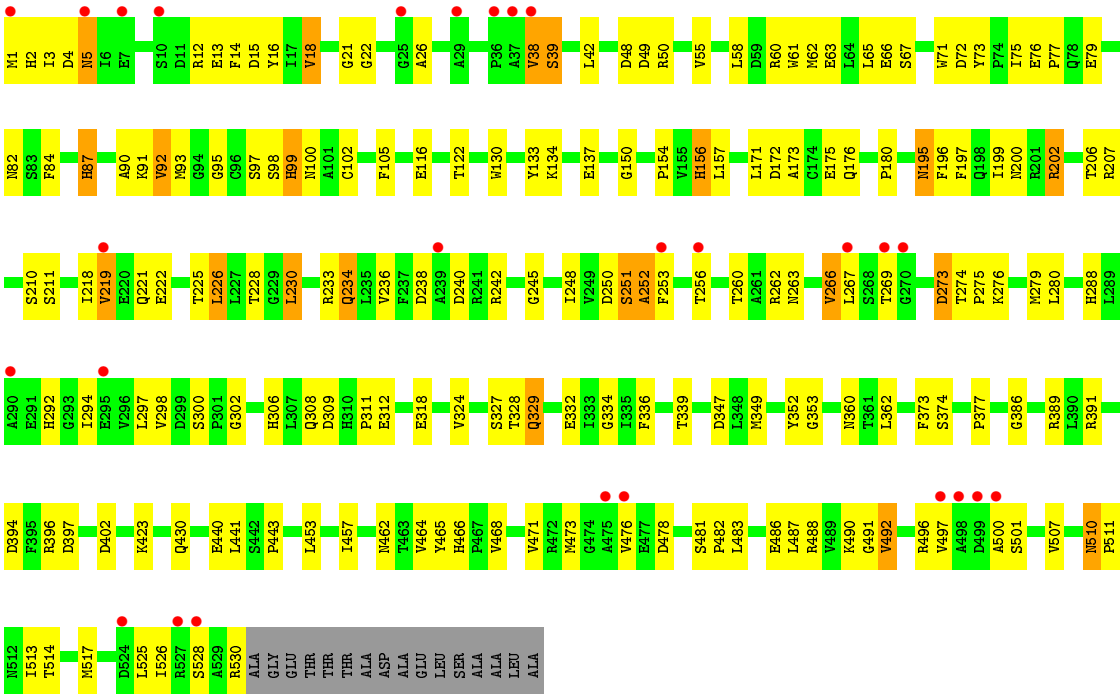


• Molecule 1: Choline oxidase



• Molecule 1: Choline oxidase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.26Å 346.03Å 105.92Å 90.00° 94.33° 90.00°	Depositor
Resolution (Å)	29.99 – 2.47 29.99 – 2.47	Depositor EDS
% Data completeness (in resolution range)	90.8 (29.99-2.47) 89.8 (29.99-2.47)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.47 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.228 , 0.293 0.225 , 0.285	Depositor DCC
$R_{free}$ test set	7966 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.6	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 33.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	33722	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.49% of the height of the origin peak. No significant pseudotranslation is detected.*

<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

### 5.1 Standard geometry

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

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	0.64	0/4229	0.73	1/5757 (0.0%)
1	B	0.68	0/4233	0.82	2/5761 (0.0%)
1	C	0.74	2/4208 (0.0%)	0.82	3/5728 (0.1%)
1	D	0.70	1/4228 (0.0%)	0.80	1/5751 (0.0%)
1	E	0.64	0/4257	0.77	6/5792 (0.1%)
1	F	0.78	0/4226	0.86	3/5751 (0.1%)
1	G	0.73	0/4222	0.79	3/5747 (0.1%)
1	H	0.64	0/4229	0.77	1/5755 (0.0%)
All	All	0.70	3/33832 (0.0%)	0.79	20/46042 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	E	0	2
1	F	0	1
1	G	0	1
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	435	GLU	CG-CD	6.03	1.60	1.51
1	C	370	GLU	CG-CD	5.60	1.60	1.51
1	D	102	CYS	CB-SG	-5.04	1.73	1.81

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	86	ARG	NE-CZ-NH2	-9.09	115.75	120.30
1	E	86	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	G	496	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	H	396	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	G	157	LEU	CA-CB-CG	6.27	129.73	115.30
1	E	363	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	C	157	LEU	CA-CB-CG	6.02	129.14	115.30
1	C	86	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	F	207	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	A	363	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	C	201	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	F	343	LEU	CA-CB-CG	5.63	128.25	115.30
1	F	277	LEU	CA-CB-CG	5.52	128.00	115.30
1	E	157	LEU	CA-CB-CG	5.41	127.75	115.30
1	E	363	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	B	363	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	B	289	LEU	CA-CB-CG	5.17	127.20	115.30
1	E	358	ASP	CB-CG-OD2	5.14	122.92	118.30
1	D	109	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	G	496	ARG	NE-CZ-NH1	5.06	122.83	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	GLU	Peptide
1	B	250	ASP	Peptide
1	E	137	GLU	Peptide
1	E	197	PHE	Peptide
1	F	197	PHE	Peptide
1	G	197	PHE	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	4119	0	3956	75	0
1	B	4122	0	3958	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4097	0	3932	78	0
1	D	4121	0	3968	92	0
1	E	4136	0	3983	85	0
1	F	4118	0	3959	82	0
1	G	4108	0	3943	88	0
1	H	4120	0	3962	128	0
2	A	53	0	29	6	0
2	B	53	0	30	6	0
2	C	53	0	29	7	0
2	D	53	0	30	4	0
2	E	53	0	30	6	0
2	F	53	0	30	7	0
2	G	53	0	29	3	0
2	H	53	0	30	7	0
3	A	4	0	3	3	0
3	B	4	0	3	1	0
3	C	4	0	3	1	0
3	D	4	0	3	0	0
3	E	4	0	3	0	0
3	F	4	0	3	2	0
3	G	4	0	3	0	0
3	H	4	0	3	2	0
4	A	20	0	0	1	0
4	B	38	0	0	1	0
4	C	47	0	0	0	0
4	D	39	0	0	1	0
4	E	38	0	0	0	0
4	F	58	0	0	2	0
4	G	47	0	0	1	0
4	H	38	0	0	1	0
All	All	33722	0	31922	688	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 11.

All (688) 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)
3:F:601:ACT:H1	4:F:611:HOH:O	1.03	1.18
1:B:241:ARG:HG3	1:B:241:ARG:HH11	1.14	1.13
1:F:415[B]:ARG:CG	1:F:415[B]:ARG:HH11	1.65	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:415[B]:ARG:HH11	1:F:415[B]:ARG:HG2	1.12	1.06
1:H:230:LEU:HD13	1:H:248:ILE:CD1	1.86	1.04
1:H:230:LEU:HD13	1:H:248:ILE:HD13	1.39	1.04
1:E:530:ARG:HG2	1:E:530:ARG:HH11	1.27	0.98
3:F:601:ACT:CH3	4:F:611:HOH:O	1.64	0.97
1:D:227:LEU:HB3	1:D:230:LEU:HD12	1.53	0.90
1:B:241:ARG:NH1	1:B:241:ARG:HG3	1.81	0.88
1:D:267:LEU:HD13	1:D:274:THR:HG23	1.57	0.87
1:B:238:ASP:HB3	1:B:240:ASP:H	1.40	0.87
1:D:275:PRO:O	1:D:279:MET:HG3	1.75	0.86
1:B:249:VAL:HG13	1:B:249:VAL:O	1.76	0.86
1:G:265:VAL:HG23	1:G:495:LEU:HD23	1.59	0.85
1:H:195:ASN:HD22	1:H:196:PHE:H	1.22	0.84
1:G:389:ARG:HH11	1:G:389:ARG:HG3	1.41	0.83
1:B:191:VAL:HA	1:B:346:PRO:HD3	1.60	0.83
1:B:529:ALA:O	1:B:530:ARG:HB2	1.78	0.83
1:F:100:ASN:HB2	2:F:547:FAD:C5X	2.08	0.83
1:B:510:ASN:H	1:B:510:ASN:HD22	1.28	0.82
1:F:415[B]:ARG:HG2	1:F:415[B]:ARG:NH1	1.93	0.81
1:H:488:ARG:HG3	1:H:496:ARG:HD3	1.62	0.81
1:D:100:ASN:HB2	2:D:547:FAD:C5X	2.09	0.81
1:H:230:LEU:CD1	1:H:248:ILE:HD13	2.10	0.81
1:A:510:ASN:H	1:A:510:ASN:ND2	1.80	0.79
1:E:267:LEU:HD11	1:E:277:LEU:HD23	1.65	0.79
1:E:238:ASP:HB3	1:E:240:ASP:H	1.50	0.77
1:D:14:PHE:HE2	1:D:225:THR:HG21	1.49	0.77
1:E:510:ASN:H	1:E:510:ASN:HD22	1.32	0.77
1:A:227:LEU:HB3	1:A:230:LEU:HD12	1.67	0.76
1:F:337:THR:HG22	1:F:348:LEU:HD23	1.67	0.76
1:B:241:ARG:HH11	1:B:241:ARG:CG	1.98	0.75
1:C:510:ASN:H	1:C:510:ASN:HD22	1.35	0.75
1:D:238:ASP:HB3	1:D:240:ASP:H	1.51	0.75
1:B:252:ALA:HA	1:B:253:PHE:C	2.08	0.74
1:C:72:ASP:OD1	1:C:86:ARG:HD3	1.86	0.74
1:D:176:GLN:OE1	1:D:431:PRO:HD2	1.86	0.74
1:H:230:LEU:HD13	1:H:248:ILE:HD12	1.70	0.74
1:C:154:PRO:O	1:C:202:ARG:NH2	2.21	0.74
1:F:415[B]:ARG:CG	1:F:415[B]:ARG:NH1	2.38	0.73
1:F:510:ASN:H	1:F:510:ASN:HD22	1.34	0.73
1:B:252:ALA:HA	1:B:254:GLY:N	2.04	0.73
1:E:510:ASN:ND2	1:E:510:ASN:H	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:510:ASN:HD22	1:G:510:ASN:H	1.34	0.72
1:F:240:ASP:O	1:F:241:ARG:HB2	1.88	0.72
1:D:529:ALA:O	1:D:530[A]:ARG:HB2	1.89	0.71
1:E:80:ASN:OD1	1:E:458:ARG:NH1	2.23	0.71
1:E:173:ALA:HB1	1:E:430:GLN:HB2	1.72	0.70
1:H:230:LEU:CD1	1:H:248:ILE:CD1	2.66	0.70
1:C:100:ASN:HB2	2:C:547:FAD:N5	2.06	0.70
1:D:449:THR:OG1	1:D:452:GLU:HG3	1.91	0.70
1:B:100:ASN:HB2	2:B:547:FAD:C4X	2.21	0.70
1:A:138:THR:HB	1:A:156:HIS:HD2	1.57	0.70
1:A:267:LEU:HD11	1:A:277:LEU:HD23	1.73	0.69
1:C:233:ARG:NH1	1:C:256:THR:OG1	2.24	0.69
1:G:267:LEU:CD1	1:G:277:LEU:HD23	2.22	0.69
1:A:510:ASN:HD22	1:A:510:ASN:H	1.40	0.69
1:B:238:ASP:HB2	1:B:242:ARG:H	1.58	0.69
1:D:464:VAL:HG12	1:D:466:HIS:CE1	2.27	0.69
1:E:288:HIS:HE1	1:E:390:LEU:H	1.41	0.69
1:G:267:LEU:HD11	1:G:277:LEU:HD23	1.75	0.69
1:F:499:ASP:OD1	1:F:501:SER:HB2	1.92	0.68
1:G:100:ASN:HB2	2:G:547:FAD:N5	2.08	0.68
1:C:227:LEU:HB3	1:C:230:LEU:HD12	1.75	0.68
1:F:191:VAL:HA	1:F:346:PRO:HD3	1.75	0.68
1:E:445:VAL:O	1:E:448:GLN:NE2	2.27	0.68
1:F:100:ASN:HB2	2:F:547:FAD:N5	2.09	0.68
1:F:227:LEU:HB3	1:F:230:LEU:HD12	1.75	0.67
1:B:510:ASN:ND2	1:B:510:ASN:H	1.91	0.67
1:C:235:LEU:HD11	1:C:267:LEU:HD22	1.75	0.67
1:E:530:ARG:HG2	1:E:530:ARG:NH1	2.04	0.66
1:B:100:ASN:HB2	2:B:547:FAD:N5	2.09	0.66
1:D:529:ALA:O	1:D:530[B]:ARG:HB2	1.94	0.66
1:G:422:ARG:NH2	1:G:450:ASP:OD2	2.28	0.66
1:C:124:TRP:CH2	1:C:521:ARG:HG2	2.31	0.66
1:G:489:VAL:HG21	1:G:495:LEU:HD13	1.78	0.66
1:G:237:PHE:CE2	1:G:243:CYS:HB2	2.31	0.66
1:D:173:ALA:HB2	1:D:433:MET:HG2	1.78	0.65
1:H:195:ASN:HD22	1:H:196:PHE:N	1.92	0.65
1:H:13:GLU:HA	1:H:260:THR:O	1.96	0.65
1:H:292:HIS:HB2	1:H:294:ILE:CD1	2.27	0.65
1:A:464:VAL:HG12	3:A:601:ACT:H3	1.79	0.65
1:G:381[B]:HIS:HE1	1:G:508:THR:OG1	1.80	0.65
1:G:359:MET:HE2	1:H:253:PHE:HZ	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:464:VAL:HG12	3:H:601:ACT:H3	1.77	0.65
1:B:191:VAL:O	1:B:338:PRO:HD3	1.96	0.64
1:H:510:ASN:ND2	1:H:510:ASN:H	1.95	0.64
1:E:238:ASP:HB2	1:E:242:ARG:H	1.61	0.64
1:H:197:PHE:CZ	1:H:334:GLY:HA3	2.32	0.64
1:H:100:ASN:HB2	2:H:547:FAD:N5	2.13	0.64
1:G:464:VAL:CG1	1:G:466:HIS:CE1	2.81	0.64
1:C:100:ASN:HB2	2:C:547:FAD:C5X	2.28	0.64
1:E:468:VAL:HG12	1:E:500:ALA:HB1	1.79	0.64
1:G:252:ALA:O	1:G:396:ARG:HD3	1.97	0.64
1:C:440:GLU:OE2	1:C:443:PRO:HD2	1.98	0.64
1:H:471:VAL:HG23	1:H:501:SER:HB3	1.80	0.64
1:G:100:ASN:HB2	2:G:547:FAD:C5X	2.28	0.63
1:G:258:ARG:HG2	1:G:260:THR:HG22	1.79	0.63
1:F:15:ASP:H	1:F:39:SER:HB3	1.61	0.63
1:D:318:GLU:HG2	1:D:441:LEU:HD21	1.80	0.63
1:F:110:GLU:O	1:F:114:GLU:HG3	1.98	0.63
1:H:318:GLU:HG3	1:H:441:LEU:HD21	1.81	0.63
1:B:464:VAL:CG1	1:B:466:HIS:CE1	2.82	0.62
1:G:137:GLU:OE1	1:G:149[A]:HIS:HD2	1.81	0.62
1:H:440:GLU:OE2	1:H:443:PRO:HD2	2.00	0.62
1:D:510:ASN:H	1:D:510:ASN:HD22	1.45	0.62
1:G:227:LEU:HB3	1:G:230:LEU:HD12	1.82	0.62
1:A:230:LEU:HD22	1:A:248:ILE:HD12	1.80	0.62
1:F:238:ASP:HB3	1:F:240:ASP:H	1.64	0.62
1:C:396:ARG:HH11	1:D:362:LEU:HD23	1.63	0.62
1:H:15:ASP:OD2	1:H:39:SER:N	2.26	0.62
1:A:468:VAL:HG12	1:A:500:ALA:HB1	1.82	0.61
1:E:449:THR:OG1	1:E:452:GLU:HG3	2.00	0.61
1:D:381[B]:HIS:HE1	1:D:508:THR:OG1	1.83	0.61
1:G:523:ALA:O	1:G:527:ARG:HG3	1.99	0.61
1:C:408:ASP:OD2	1:C:412:HIS:N	2.32	0.61
1:F:230:LEU:HD13	1:F:248:ILE:CD1	2.30	0.61
1:E:238:ASP:HB3	1:E:240:ASP:N	2.14	0.61
1:C:192:ASN:ND2	1:C:337:THR:OG1	2.34	0.61
1:G:409:PRO:HD2	4:G:614:HOH:O	2.00	0.61
1:E:72:ASP:OD1	1:E:86:ARG:HD3	2.01	0.60
1:F:79:GLU:OE2	1:F:404:ARG:HD2	2.00	0.60
1:G:82:ASN:O	1:G:85:MET:HB2	2.01	0.60
1:C:381[B]:HIS:HE1	1:C:508:THR:OG1	1.82	0.60
1:G:337:THR:HG22	1:G:348:LEU:HD23	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:496:ARG:HH21	1:H:526:ILE:HG12	1.66	0.60
1:F:267:LEU:HD13	1:F:274:THR:HG23	1.83	0.60
1:H:100:ASN:HB2	2:H:547:FAD:C5X	2.31	0.60
1:C:250:ASP:N	1:C:250:ASP:OD1	2.35	0.60
1:F:230:LEU:HD13	1:F:248:ILE:HD12	1.83	0.60
1:D:510:ASN:H	1:D:510:ASN:ND2	1.99	0.60
1:H:491:GLY:O	1:H:492:VAL:HG23	2.02	0.60
1:B:468:VAL:HG12	1:B:500:ALA:HB1	1.83	0.60
1:C:422:ARG:NH2	1:C:450:ASP:OD2	2.33	0.60
1:C:321:GLN:O	1:C:371:ASN:ND2	2.28	0.59
1:D:14:PHE:HE2	1:D:225:THR:CG2	2.15	0.59
1:F:236:VAL:HG21	1:F:258:ARG:NH1	2.15	0.59
1:H:100:ASN:HB2	2:H:547:FAD:C4X	2.33	0.59
1:G:359:MET:CE	1:H:253:PHE:HZ	2.16	0.59
1:B:216:HIS:HB2	1:B:217:PRO:HD3	1.83	0.59
1:H:487:LEU:O	1:H:496:ARG:HA	2.01	0.59
1:D:422:ARG:NH2	1:D:448:GLN:O	2.35	0.59
1:E:271:ALA:HA	1:E:501:SER:HB3	1.83	0.59
1:G:511:PRO:O	1:G:515:VAL:HG23	2.03	0.59
1:B:28:VAL:HG11	1:B:266:VAL:HG11	1.84	0.59
1:B:403:PRO:HG2	1:B:405:TYR:CE1	2.38	0.59
1:G:288:HIS:CE1	1:G:389:ARG:HB3	2.38	0.59
1:B:14:PHE:HE2	1:B:225:THR:HG1	1.51	0.59
1:D:35:ASP:C	1:D:35:ASP:OD1	2.40	0.58
1:F:381[B]:HIS:HE1	1:F:508:THR:OG1	1.87	0.58
1:B:394:ASP:OD1	1:B:396:ARG:HD3	2.03	0.58
1:H:267:LEU:HD13	1:H:274:THR:HG23	1.86	0.58
1:E:236:VAL:HG11	1:E:258:ARG:NH1	2.18	0.58
1:A:445:VAL:O	1:A:448:GLN:NE2	2.37	0.58
1:B:464:VAL:HG12	1:B:466:HIS:NE2	2.19	0.58
1:A:267:LEU:HD23	1:A:274:THR:HG23	1.86	0.58
1:G:359:MET:CE	1:H:253:PHE:CZ	2.87	0.58
1:C:252:ALA:O	1:C:396:ARG:HD3	2.03	0.57
2:B:547:FAD:N5	3:B:601:ACT:H2	2.19	0.57
1:E:267:LEU:HD23	1:E:274:THR:HG23	1.85	0.57
1:E:310:HIS:O	1:E:464:VAL:HG23	2.03	0.57
1:H:58:LEU:HD13	1:H:102:CYS:SG	2.44	0.57
1:H:13:GLU:HB2	1:H:260:THR:HG22	1.87	0.57
1:H:238:ASP:OD1	1:H:242:ARG:HB3	2.04	0.57
1:F:133:TYR:O	1:F:137:GLU:HG2	2.04	0.57
1:B:173:ALA:HB1	1:B:430:GLN:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:253:PHE:HD2	1:G:396:ARG:NH2	2.03	0.57
1:D:100:ASN:HB2	2:D:547:FAD:N5	2.19	0.57
1:H:105:PHE:O	1:H:513:ILE:HB	2.04	0.57
1:H:468:VAL:HG12	1:H:500:ALA:HB1	1.85	0.57
1:A:410:GLU:O	1:A:410:GLU:HG2	2.05	0.57
1:C:160:VAL:HG11	1:C:332:GLU:HB3	1.86	0.57
1:C:191:VAL:HA	1:C:346:PRO:HD3	1.87	0.57
1:H:478:ASP:OD2	1:H:481:SER:OG	2.17	0.57
1:E:240:ASP:O	1:E:241:ARG:HB2	2.05	0.56
1:H:100:ASN:C	1:H:100:ASN:OD1	2.43	0.56
1:D:307:LEU:HD22	1:D:388:VAL:HG23	1.88	0.56
1:F:14:PHE:HE2	1:F:225:THR:HG1	1.53	0.56
1:H:514:THR:O	1:H:517:MET:HB3	2.05	0.56
1:C:173:ALA:HB1	1:C:430:GLN:HB2	1.87	0.56
1:E:23:SER:OG	1:E:512:ASN:ND2	2.38	0.56
1:E:100:ASN:HB2	2:E:547:FAD:C5X	2.36	0.56
1:H:22:GLY:HA3	2:H:547:FAD:O5B	2.06	0.56
1:E:288:HIS:CE1	1:E:390:LEU:H	2.24	0.56
1:B:458:ARG:HH11	1:B:458:ARG:HG3	1.71	0.56
1:D:264:GLU:HG2	1:D:494:GLY:HA2	1.87	0.56
1:A:310[B]:HIS:HD2	1:A:466:HIS:ND1	2.04	0.56
1:F:15:ASP:O	1:F:263:ASN:HB2	2.05	0.56
1:F:22:GLY:HA2	1:F:95:GLY:HA3	1.88	0.56
1:H:92:VAL:HG22	1:H:93:MET:N	2.21	0.56
1:D:100:ASN:OD1	1:D:100:ASN:C	2.45	0.56
1:D:113:ASP:OD1	1:D:125:ASN:HB2	2.06	0.56
1:G:359:MET:HE2	1:H:253:PHE:CZ	2.41	0.56
1:A:312:GLU:O	1:A:461:HIS:HB2	2.06	0.55
1:A:466:HIS:HB3	1:A:511:PRO:HG3	1.88	0.55
1:C:110:GLU:OE1	1:C:110:GLU:N	2.37	0.55
1:F:415[B]:ARG:HH11	1:F:415[B]:ARG:HG3	1.67	0.55
1:G:31:ARG:NH2	1:G:520:GLU:OE2	2.30	0.55
1:B:238:ASP:HB3	1:B:240:ASP:N	2.15	0.55
1:E:16:TYR:HE2	1:E:264:GLU:HB2	1.71	0.55
1:A:157:LEU:HD22	1:A:200:ASN:HB3	1.87	0.55
1:E:137:GLU:O	1:E:153:GLY:N	2.39	0.55
1:C:236:VAL:HG11	1:C:258:ARG:CZ	2.37	0.55
1:D:383:ARG:NH1	1:D:410:GLU:OE1	2.40	0.55
1:C:486:GLU:O	1:C:487:LEU:HB2	2.05	0.55
1:D:14:PHE:CE2	1:D:225:THR:CG2	2.90	0.55
1:E:530:ARG:CG	1:E:530:ARG:HH11	2.10	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:115:TRP:CE3	1:G:473:MET:CE	2.89	0.55
1:F:17:ILE:HG13	1:F:261:ALA:HB2	1.88	0.55
1:D:6:ILE:O	1:D:12:ARG:NH2	2.39	0.55
1:D:484:ASP:HB2	1:D:485:PRO:CD	2.37	0.55
1:F:510:ASN:H	1:F:510:ASN:ND2	2.02	0.55
1:H:60:ARG:O	1:H:63:GLU:HG3	2.06	0.55
1:H:525:LEU:O	1:H:528:SER:HB3	2.07	0.55
1:F:484:ASP:HB2	1:F:485:PRO:HD2	1.88	0.54
1:B:249:VAL:CG1	1:B:249:VAL:O	2.47	0.54
1:C:423:LYS:O	1:C:427:ILE:HG13	2.07	0.54
1:G:510:ASN:H	1:G:510:ASN:ND2	2.04	0.54
1:H:26:ALA:HB3	1:H:210:SER:HB2	1.90	0.54
1:A:138:THR:HG23	1:A:151:ASP:O	2.08	0.54
1:F:510:ASN:HB3	2:F:547:FAD:C2	2.37	0.54
1:D:118:LYS:HD2	1:D:119:TYR:CZ	2.41	0.54
1:G:34:GLU:OE1	1:G:527:ARG:NH2	2.40	0.54
1:F:248:ILE:HD13	1:F:259:LEU:HD11	1.90	0.54
1:H:483:LEU:HD11	1:H:497:VAL:HB	1.90	0.54
1:D:483:LEU:HD23	1:D:489:VAL:HA	1.88	0.54
1:A:61:TRP:CE2	1:A:62:MET:HG3	2.43	0.54
1:B:472:ARG:O	1:B:482:PRO:HD2	2.07	0.54
1:D:270:GLY:O	1:D:274:THR:HB	2.07	0.54
1:G:243:CYS:SG	1:G:265:VAL:HG21	2.47	0.54
1:B:130:TRP:N	1:B:131:PRO:CD	2.70	0.53
1:D:60:ARG:HD2	1:D:63:GLU:OE2	2.09	0.53
1:C:133:TYR:O	1:C:137:GLU:HG2	2.08	0.53
1:B:18:VAL:HG21	1:B:29:ALA:HB2	1.91	0.53
1:E:191:VAL:HA	1:E:346:PRO:HD3	1.89	0.53
1:H:175:GLU:HG2	1:H:180:PRO:HA	1.89	0.53
1:G:321:GLN:O	1:G:371:ASN:ND2	2.37	0.53
1:E:24:ALA:O	1:E:28:VAL:HG23	2.09	0.53
1:D:306:HIS:O	1:D:308:GLN:HG3	2.09	0.53
1:H:251:SER:O	1:H:253:PHE:N	2.42	0.53
1:D:403:PRO:HG2	1:D:405:TYR:CE1	2.44	0.52
1:F:440:GLU:OE2	1:F:444:GLY:N	2.41	0.52
1:G:73:TYR:CE1	1:G:399:PRO:HD2	2.44	0.52
1:A:466:HIS:HE2	3:A:601:ACT:H3	1.74	0.52
1:H:98:SER:HA	1:H:207:ARG:CD	2.40	0.52
1:H:133:TYR:O	1:H:137:GLU:HG2	2.09	0.52
1:H:236:VAL:HG12	1:H:245:GLY:O	2.09	0.52
1:A:423:LYS:O	1:A:427:ILE:HD12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:GLY:HA3	1:B:68:GLY:HA3	1.91	0.52
1:F:484:ASP:HB2	1:F:485:PRO:CD	2.40	0.52
1:G:486:GLU:HA	1:G:525:LEU:HD13	1.91	0.52
1:B:246:VAL:HG13	1:B:248:ILE:HG23	1.91	0.52
1:D:464:VAL:CG1	1:D:466:HIS:CE1	2.92	0.52
1:E:133:TYR:O	1:E:137:GLU:HG2	2.10	0.52
1:F:238:ASP:HB3	1:F:240:ASP:N	2.25	0.52
1:F:483:LEU:HD11	1:F:497:VAL:HB	1.92	0.52
1:H:292:HIS:HB2	1:H:294:ILE:HD12	1.91	0.52
1:D:14:PHE:CE2	1:D:225:THR:HG21	2.36	0.52
1:H:73:TYR:OH	1:H:273:ASP:OD2	2.21	0.52
1:E:109:ARG:NH2	1:E:187:GLY:O	2.38	0.51
1:E:379:VAL:HG22	1:E:416:VAL:HG12	1.90	0.51
1:H:394:ASP:O	1:H:397:ASP:HB2	2.09	0.51
1:A:133:TYR:O	1:A:137:GLU:HG2	2.11	0.51
1:F:157:LEU:HD22	1:F:200:ASN:HB3	1.92	0.51
1:A:191:VAL:HA	1:A:346:PRO:HD3	1.93	0.51
1:C:115:TRP:CE3	1:C:473:MET:HE1	2.45	0.51
1:B:100:ASN:HB2	2:B:547:FAD:C5X	2.40	0.51
1:F:247:ASP:HB3	1:F:256:THR:CG2	2.40	0.51
1:D:110:GLU:O	1:D:114:GLU:HG3	2.11	0.51
1:A:54:GLU:H	1:A:54:GLU:CD	2.13	0.51
1:B:79:GLU:OE2	1:B:404:ARG:NH1	2.40	0.51
1:D:24:ALA:O	1:D:28:VAL:HG23	2.10	0.51
1:D:386:GLY:HA2	1:D:404:ARG:HG3	1.93	0.51
1:G:234:GLN:O	1:G:246:VAL:HG23	2.11	0.51
1:G:191:VAL:HA	1:G:346:PRO:HD3	1.93	0.51
1:G:315:VAL:HG12	1:G:317:PHE:CE1	2.45	0.51
1:A:440:GLU:OE2	1:A:443:PRO:HD2	2.10	0.51
1:F:267:LEU:HD21	1:F:277:LEU:HD12	1.93	0.51
1:A:288:HIS:HE1	1:A:390:LEU:H	1.58	0.50
1:G:53:PRO:HD2	1:G:54:GLU:OE1	2.11	0.50
1:C:111:ASP:OD1	1:C:381[A]:HIS:HE1	1.94	0.50
1:E:527:ARG:O	1:E:528:SER:HB2	2.12	0.50
1:G:238:ASP:HB3	1:G:240:ASP:H	1.76	0.50
1:H:510:ASN:H	1:H:510:ASN:HD22	1.60	0.50
1:C:121:ALA:O	1:C:122:THR:C	2.49	0.50
1:D:276:LYS:NZ	1:D:395:PHE:O	2.39	0.50
1:H:386:GLY:HA3	1:H:402:ASP:O	2.11	0.50
1:F:236:VAL:HG12	1:F:245:GLY:C	2.32	0.50
1:F:50:ARG:HG3	1:F:216:HIS:CE1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:14:PHE:O	1:H:262:ARG:N	2.39	0.50
1:E:100:ASN:HB2	2:E:547:FAD:N5	2.26	0.50
1:E:14:PHE:HE2	1:E:225:THR:HG1	1.60	0.50
1:E:16:TYR:HB2	1:E:40:VAL:HG13	1.94	0.50
1:D:309:ASP:OD2	1:D:463:THR:OG1	2.21	0.50
1:D:3:ILE:HD13	1:D:9:LEU:HD13	1.93	0.50
1:G:464:VAL:HG11	1:G:466:HIS:CE1	2.47	0.50
1:E:267:LEU:HB3	1:E:497:VAL:HG22	1.92	0.50
1:H:238:ASP:HB3	1:H:240:ASP:H	1.77	0.50
1:D:321:GLN:HB2	1:D:436:TRP:CZ3	2.47	0.49
1:G:12:ARG:HB3	1:G:259:LEU:HD23	1.94	0.49
1:G:288:HIS:HE1	1:G:390:LEU:H	1.58	0.49
1:C:115:TRP:CE3	1:C:473:MET:CE	2.95	0.49
1:H:50:ARG:NH1	1:H:219:VAL:HG11	2.28	0.49
1:E:227:LEU:HB3	1:E:230:LEU:HD12	1.93	0.49
1:F:391:ARG:NE	1:F:398:LYS:O	2.46	0.49
1:B:309:ASP:OD2	1:B:405:TYR:OH	2.26	0.49
1:A:80:ASN:OD1	1:A:458:ARG:NH1	2.45	0.49
1:C:199:ILE:HD12	1:C:201:ARG:HB2	1.95	0.49
1:F:130:TRP:N	1:F:131:PRO:HD2	2.28	0.49
1:F:17:ILE:HB	1:F:265:VAL:HG22	1.93	0.49
1:G:115:TRP:CE3	1:G:473:MET:HE1	2.48	0.49
1:H:97:SER:O	1:H:207:ARG:NH1	2.44	0.49
1:H:453:LEU:O	1:H:457:ILE:HD12	2.13	0.49
1:D:488:ARG:HA	1:D:496:ARG:HG2	1.95	0.49
1:E:510:ASN:HB3	2:E:547:FAD:C2	2.43	0.49
1:F:72:ASP:O	1:F:74:PRO:HD3	2.13	0.49
1:H:478:ASP:O	1:H:490:LYS:NZ	2.45	0.49
1:C:157:LEU:HD22	1:C:200:ASN:HB3	1.94	0.49
1:D:145:ASP:OD1	1:D:145:ASP:C	2.51	0.49
1:D:26:ALA:HB3	1:D:210:SER:HB2	1.94	0.49
1:D:220:GLU:OE1	1:D:220:GLU:HA	2.12	0.49
1:G:456:TYR:O	1:G:460:THR:OG1	2.20	0.49
1:B:283:ILE:HG23	1:B:298:VAL:HB	1.94	0.49
1:G:359:MET:HE3	1:H:253:PHE:CZ	2.47	0.49
1:G:464:VAL:HG12	1:G:466:HIS:CE1	2.48	0.49
1:H:134:LYS:O	1:H:150:GLY:HA3	2.12	0.49
1:H:202:ARG:HG3	1:H:206:THR:HB	1.95	0.49
1:C:351:HIS:HB2	1:C:376:THR:OG1	2.12	0.49
1:D:484:ASP:HB2	1:D:485:PRO:HD2	1.95	0.49
1:C:499:ASP:HB2	2:C:547:FAD:O2P	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:473:MET:HA	1:H:483:LEU:HB2	1.94	0.48
1:C:180:PRO:O	1:C:193:GLY:HA2	2.13	0.48
1:H:275:PRO:O	1:H:279:MET:HG3	2.12	0.48
1:E:16:TYR:CE2	1:E:264:GLU:HB2	2.48	0.48
1:A:30:ALA:HB2	1:A:214:TYR:HB3	1.95	0.48
1:C:524:ASP:O	1:C:528:SER:HA	2.12	0.48
1:D:216:HIS:O	1:D:219:VAL:HG23	2.13	0.48
1:A:473:MET:HG2	1:A:502:VAL:O	2.14	0.48
1:B:510:ASN:ND2	1:B:510:ASN:N	2.60	0.48
1:C:321:GLN:OE1	1:C:435:GLU:HG3	2.14	0.48
1:C:100:ASN:HB2	2:C:547:FAD:C4X	2.44	0.48
1:F:362:LEU:HD13	1:F:368:THR:HG21	1.94	0.48
1:A:289:LEU:HD12	1:A:296:VAL:HG22	1.95	0.48
1:D:80:ASN:OD1	1:D:458:ARG:HD3	2.14	0.48
1:E:358:ASP:H	1:F:253:PHE:HZ	1.61	0.48
1:F:21:GLY:CA	1:F:42:LEU:HD11	2.44	0.48
2:A:547:FAD:N5	3:A:601:ACT:H2	2.29	0.48
1:G:321:GLN:HB2	1:G:436:TRP:CZ3	2.49	0.48
1:E:103:ILE:HG12	1:E:197:PHE:CD1	2.48	0.48
1:H:13:GLU:HB2	1:H:260:THR:CG2	2.43	0.48
1:H:298:VAL:HG12	1:H:300:SER:HB2	1.95	0.48
1:A:100:ASN:HB2	2:A:547:FAD:C4X	2.43	0.48
1:H:292:HIS:HB2	1:H:294:ILE:HD11	1.95	0.48
1:H:312:GLU:HB2	1:H:464:VAL:HG22	1.96	0.48
1:D:112:LEU:HD12	1:D:112:LEU:HA	1.67	0.48
1:D:55:VAL:HG13	1:D:98:SER:HB3	1.96	0.47
1:E:172:ASP:HB2	1:E:432:ALA:HB1	1.96	0.47
1:G:387:THR:N	1:G:402:ASP:O	2.41	0.47
1:H:465:TYR:HB3	2:H:547:FAD:C8	2.44	0.47
1:A:361:THR:HB	1:A:366:TYR:HB2	1.95	0.47
1:H:233:ARG:O	1:H:234:GLN:HG3	2.14	0.47
1:A:318:GLU:O	1:A:438:GLY:HA3	2.14	0.47
1:D:333:ILE:HB	1:D:352:TYR:HB3	1.97	0.47
1:H:13:GLU:CB	1:H:260:THR:HB	2.44	0.47
1:A:321:GLN:O	1:A:371:ASN:ND2	2.44	0.47
1:G:267:LEU:HD13	1:G:277:LEU:HD23	1.95	0.47
1:A:97:SER:HA	1:A:100:ASN:ND2	2.29	0.47
1:F:154:PRO:O	1:F:202:ARG:NH2	2.42	0.47
1:A:443:PRO:HB3	1:A:456:TYR:CG	2.49	0.47
1:B:72:ASP:O	1:B:74:PRO:HD3	2.14	0.47
1:E:154:PRO:HB2	1:E:213:SER:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:23:SER:HB2	2:E:547:FAD:O5'	2.15	0.47
1:D:212:VAL:HG22	1:D:216:HIS:CE1	2.50	0.47
1:C:253:PHE:CE2	1:D:359:MET:HG3	2.50	0.47
1:E:210:SER:O	1:E:214:TYR:HB2	2.14	0.47
1:H:18:VAL:HG22	1:H:42:LEU:CD1	2.44	0.47
1:A:216:HIS:HB2	1:A:217:PRO:HD3	1.96	0.47
1:A:90:ALA:HB2	1:A:99:HIS:CG	2.50	0.47
1:E:464:VAL:CG1	1:E:466:HIS:CE1	2.98	0.47
1:F:446:GLU:CD	1:F:446:GLU:H	2.18	0.47
1:G:274:THR:N	1:G:275:PRO:HD2	2.30	0.47
1:H:251:SER:O	1:H:252:ALA:C	2.52	0.47
1:B:464:VAL:HG11	1:B:466:HIS:CE1	2.49	0.47
1:B:464:VAL:HG12	1:B:466:HIS:CE1	2.50	0.47
1:H:327:SER:OG	1:H:328:THR:N	2.48	0.47
1:H:73:TYR:O	1:H:87:HIS:N	2.40	0.47
1:A:61:TRP:HA	4:A:613:HOH:O	2.14	0.47
1:G:253:PHE:HD2	1:G:396:ARG:HH21	1.61	0.47
1:H:353:GLY:O	1:H:373:PHE:HB2	2.15	0.47
1:C:138:THR:HB	1:C:156:HIS:CD2	2.51	0.46
1:C:510:ASN:ND2	1:C:510:ASN:H	2.06	0.46
1:E:530:ARG:HD3	1:E:530:ARG:HA	1.66	0.46
1:D:529:ALA:O	1:D:530[A]:ARG:CB	2.60	0.46
1:F:522:CYS:HA	1:F:525:LEU:HD12	1.96	0.46
1:A:50:ARG:HG2	1:A:216:HIS:CE1	2.50	0.46
1:F:238:ASP:HB2	1:F:242:ARG:H	1.81	0.46
1:E:314:VAL:HG22	1:E:315:VAL:N	2.30	0.46
1:F:510:ASN:N	1:F:510:ASN:ND2	2.64	0.46
1:G:175:GLU:OE1	1:G:181:ARG:NH1	2.39	0.46
1:G:253:PHE:CE2	1:G:396:ARG:HD2	2.51	0.46
1:G:391:ARG:HG2	1:H:84:PHE:HE2	1.81	0.46
1:A:240:ASP:O	1:A:241:ARG:HB2	2.15	0.46
1:A:251:SER:O	1:A:252:ALA:CB	2.63	0.46
1:B:21:GLY:HA2	1:B:42:LEU:HD11	1.97	0.46
1:E:529:ALA:O	1:E:530:ARG:HB2	2.15	0.46
1:H:302:GLY:HA3	1:H:482:PRO:HD3	1.97	0.46
1:H:92:VAL:CG2	1:H:93:MET:N	2.78	0.46
2:A:547:FAD:H9	2:A:547:FAD:H1'	1.68	0.46
1:A:100:ASN:HB2	2:A:547:FAD:N5	2.31	0.46
1:D:166:THR:HB	1:D:352:TYR:OH	2.15	0.46
1:D:269:THR:HG22	2:D:547:FAD:C4A	2.45	0.46
1:E:172:ASP:O	1:E:176:GLN:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:ASP:HB3	1:C:240:ASP:N	2.31	0.46
1:D:267:LEU:CD2	1:D:269:THR:OG1	2.63	0.46
1:E:488:ARG:HA	1:E:496:ARG:HG2	1.97	0.46
1:H:236:VAL:HG12	1:H:245:GLY:C	2.36	0.46
1:C:396:ARG:NH1	1:D:362:LEU:HD23	2.30	0.46
1:E:530:ARG:CG	1:E:530:ARG:NH1	2.74	0.46
1:G:430:GLN:OE1	1:G:431:PRO:HD2	2.16	0.46
1:G:70:ASP:HA	1:G:89:ARG:O	2.16	0.46
1:A:238:ASP:HB2	1:A:242:ARG:H	1.81	0.46
1:A:251:SER:O	1:A:252:ALA:HB3	2.16	0.46
1:A:464:VAL:CG1	1:A:466:HIS:CE1	2.99	0.46
1:C:60:ARG:HD2	1:C:63:GLU:OE2	2.16	0.46
1:F:237:PHE:HE2	1:F:492:VAL:CG1	2.29	0.46
1:H:269:THR:HG22	2:H:547:FAD:C4A	2.46	0.46
1:H:309:ASP:O	1:H:311:PRO:HD3	2.16	0.46
1:B:58:LEU:C	1:B:60:ARG:H	2.20	0.46
1:C:245:GLY:HA3	1:C:259:LEU:O	2.15	0.46
1:E:253:PHE:CZ	1:F:359:MET:HE2	2.51	0.46
1:A:521:ARG:O	1:A:521:ARG:HG3	2.15	0.45
1:D:194:ALA:HB1	1:D:335:ILE:HG12	1.98	0.45
1:F:362:LEU:CD1	1:F:368:THR:HG21	2.46	0.45
1:A:100:ASN:HB2	2:A:547:FAD:C5X	2.46	0.45
1:A:166:THR:HB	1:A:352:TYR:OH	2.16	0.45
1:A:163:LYS:O	1:A:165:PRO:HD3	2.16	0.45
1:A:173:ALA:HB1	1:A:430:GLN:HB2	1.99	0.45
1:D:35:ASP:HA	1:D:36:PRO:HD2	1.73	0.45
1:A:70:ASP:OD2	1:A:72:ASP:N	2.44	0.45
1:C:100:ASN:CB	2:C:547:FAD:C5X	2.93	0.45
1:F:270:GLY:O	1:F:274:THR:HB	2.16	0.45
1:H:18:VAL:HB	1:H:266:VAL:HG13	1.98	0.45
1:A:71:TRP:CH2	1:A:91:LYS:HE3	2.52	0.45
1:G:279:MET:HE3	1:G:390:LEU:HG	1.98	0.45
1:H:173:ALA:HB1	1:H:430:GLN:HB2	1.98	0.45
1:C:124:TRP:CZ2	1:C:521:ARG:HG2	2.52	0.45
1:G:31:ARG:HE	1:G:520:GLU:CD	2.20	0.45
1:H:252:ALA:HB3	1:H:253:PHE:HD1	1.82	0.45
2:H:547:FAD:C4X	3:H:601:ACT:H2	2.46	0.45
1:B:512:ASN:HB2	2:B:547:FAD:C2	2.46	0.45
1:D:89[B]:ARG:HA	1:D:89[B]:ARG:HD2	1.82	0.45
1:F:124:TRP:CH2	1:F:521:ARG:HG2	2.51	0.45
1:G:124:TRP:CH2	1:G:521:ARG:HG2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:511:PRO:O	1:B:515:VAL:HG23	2.17	0.45
1:D:137:GLU:CD	1:D:139:ASN:HB2	2.37	0.45
1:D:156:HIS:O	1:D:200:ASN:HA	2.17	0.45
1:D:99:HIS:CD2	1:D:99:HIS:C	2.90	0.45
1:F:58:LEU:HD13	1:F:102:CYS:SG	2.57	0.45
1:A:227:LEU:N	1:A:227:LEU:HD12	2.31	0.45
1:D:511:PRO:O	1:D:515:VAL:HG23	2.16	0.45
1:G:312:GLU:O	1:G:461:HIS:HB2	2.17	0.45
1:H:306[A]:HIS:HD2	4:H:647:HOH:O	2.00	0.45
1:C:31:ARG:O	1:C:527:ARG:NH1	2.49	0.44
1:D:197:PHE:CZ	1:D:334:GLY:HA3	2.52	0.44
1:H:90:ALA:HB2	1:H:99:HIS:CG	2.52	0.44
1:B:249:VAL:O	1:B:250:ASP:C	2.54	0.44
1:B:278:LEU:HB3	1:B:283:ILE:HB	1.99	0.44
1:D:267:LEU:HD22	1:D:269:THR:OG1	2.18	0.44
1:D:307:LEU:HD22	1:D:388:VAL:CG2	2.47	0.44
1:E:68:GLY:HA2	1:F:68:GLY:HA2	2.00	0.44
1:D:100:ASN:HB2	2:D:547:FAD:C9A	2.46	0.44
1:H:5:ASN:H	1:H:5:ASN:ND2	2.16	0.44
1:B:159:ASN:O	1:B:161:PRO:HD3	2.18	0.44
1:G:510:ASN:N	1:G:510:ASN:ND2	2.66	0.44
1:H:154:PRO:O	1:H:202:ARG:NH2	2.51	0.44
1:B:52:VAL:HA	1:B:53:PRO:HD2	1.83	0.44
1:C:510:ASN:HB3	2:C:547:FAD:C2	2.48	0.44
1:E:527:ARG:O	1:E:528:SER:CB	2.66	0.44
1:G:164:ASP:HA	1:G:165:PRO:HD2	1.83	0.44
1:G:265:VAL:HG23	1:G:495:LEU:CD2	2.38	0.44
1:H:15:ASP:HA	1:H:262:ARG:HB2	2.00	0.44
1:B:466:HIS:HB3	1:B:511:PRO:HG3	1.98	0.44
1:D:17:ILE:HD12	1:D:261:ALA:HB2	1.99	0.44
1:E:361:THR:HB	1:E:366:TYR:HB2	1.98	0.44
1:G:510:ASN:HB3	2:G:547:FAD:C2	2.48	0.44
1:H:48:ASP:OD1	1:H:49:ASP:N	2.51	0.44
1:A:72:ASP:OD1	1:A:86:ARG:HD3	2.18	0.44
1:A:87[A]:HIS:HE1	1:A:309:ASP:OD2	2.01	0.44
1:B:250:ASP:HB3	1:B:251:SER:H	1.74	0.44
1:E:14:PHE:O	1:E:261:ALA:HA	2.18	0.44
1:F:31:ARG:O	1:F:34:GLU:HB2	2.18	0.44
1:C:14:PHE:O	1:C:261:ALA:HA	2.17	0.43
1:C:105:PHE:HB3	1:C:509:VAL:HG21	2.00	0.43
1:E:191:VAL:O	1:E:346:PRO:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:402:ASP:OD2	1:E:404:ARG:HG2	2.17	0.43
1:A:465:TYR:C	1:A:466:HIS:CD2	2.92	0.43
1:D:386:GLY:HA3	1:D:403:PRO:HA	2.00	0.43
1:E:381[B]:HIS:HE1	1:E:508:THR:OG1	2.01	0.43
1:F:351:HIS:HB2	1:F:376:THR:OG1	2.18	0.43
1:G:128:ALA:O	1:G:131:PRO:HD2	2.18	0.43
1:H:360:ASN:ND2	1:H:462:ASN:OD1	2.51	0.43
1:A:71:TRP:CZ3	1:A:91:LYS:HE3	2.53	0.43
1:C:284:GLY:HA2	1:C:303:VAL:HB	2.00	0.43
1:D:394:ASP:OD1	1:D:396:ARG:CD	2.67	0.43
1:A:269:THR:HG22	2:A:547:FAD:C4A	2.48	0.43
1:E:523:ALA:O	1:E:527:ARG:HG2	2.18	0.43
1:H:116:GLU:HG3	1:H:122:THR:HA	2.01	0.43
1:F:394:ASP:OD1	1:F:396:ARG:CD	2.66	0.43
1:F:394:ASP:OD1	1:F:396:ARG:HD3	2.18	0.43
1:G:21:GLY:HA2	1:G:42:LEU:HD11	2.00	0.43
1:G:484:ASP:HB2	1:G:485:PRO:CD	2.49	0.43
1:C:18:VAL:HG22	1:C:266:VAL:HB	2.00	0.43
1:D:415:ARG:NH1	4:D:644:HOH:O	2.51	0.43
1:D:89[A]:ARG:CZ	1:D:96:CYS:SG	3.07	0.43
1:E:163:LYS:NZ	1:E:327:SER:HA	2.34	0.43
1:H:248:ILE:O	1:H:256:THR:HA	2.18	0.43
1:A:238:ASP:HB3	1:A:240:ASP:H	1.82	0.43
1:C:218:ILE:O	1:C:219:VAL:C	2.56	0.43
1:D:13:GLU:OE1	1:D:262:ARG:NH1	2.51	0.43
1:H:13:GLU:HB3	1:H:260:THR:HB	2.00	0.43
1:B:3:ILE:HB	1:B:227:LEU:HD23	2.01	0.43
1:E:17:ILE:HG12	1:E:261:ALA:HB2	2.01	0.43
1:F:6:ILE:HG13	1:F:12:ARG:NH2	2.34	0.43
1:A:28:VAL:HG22	1:A:519:GLY:O	2.19	0.43
1:G:238:ASP:HB3	1:G:240:ASP:N	2.34	0.43
1:G:82:ASN:C	1:G:82:ASN:OD1	2.57	0.43
1:H:102:CYS:O	1:H:199:ILE:HA	2.19	0.43
1:H:93:MET:SD	1:H:226:LEU:HD21	2.59	0.43
1:A:363:ARG:HG2	4:B:643:HOH:O	2.19	0.43
1:C:238:ASP:OD2	1:C:240:ASP:HB2	2.18	0.43
1:E:250:ASP:N	1:E:250:ASP:OD1	2.52	0.43
1:H:349:MET:O	1:H:377:PRO:HA	2.19	0.43
1:H:391:ARG:HB3	1:H:397:ASP:HB3	2.00	0.43
1:D:394:ASP:OD1	1:D:396:ARG:HD2	2.18	0.42
1:D:466:HIS:HB3	1:D:511:PRO:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:319:ALA:HB3	1:E:371:ASN:ND2	2.34	0.42
1:E:275:PRO:HG3	1:E:470:THR:HB	2.01	0.42
1:G:10:SER:OG	1:G:11:ASP:N	2.52	0.42
1:G:487:LEU:O	1:G:496:ARG:HA	2.19	0.42
1:H:71:TRP:CZ2	1:H:91:LYS:HG3	2.54	0.42
1:C:6:ILE:HG21	1:C:257:HIS:CD2	2.54	0.42
1:H:197:PHE:CZ	1:H:334:GLY:CA	3.01	0.42
1:H:157:LEU:HD22	1:H:200:ASN:HB3	2.02	0.42
1:A:238:ASP:HB3	1:A:240:ASP:N	2.34	0.42
1:C:138:THR:HB	1:C:156:HIS:HD2	1.84	0.42
1:C:318:GLU:HG3	1:C:441:LEU:HD21	2.01	0.42
1:D:349:MET:O	1:D:377:PRO:HA	2.19	0.42
1:E:15:ASP:OD1	1:E:262:ARG:NE	2.50	0.42
1:F:530:ARG:HB2	1:F:530:ARG:HE	1.49	0.42
1:G:362:LEU:HD12	1:G:362:LEU:HA	1.83	0.42
1:C:471:VAL:HB	1:C:501:SER:HB3	2.01	0.42
1:C:510:ASN:ND2	1:C:510:ASN:N	2.66	0.42
1:H:65:LEU:O	1:H:66:GLU:HB2	2.19	0.42
1:A:51:GLY:O	1:A:53:PRO:HD3	2.19	0.42
1:B:414:MET:O	1:B:418:VAL:HG23	2.20	0.42
1:D:486:GLU:HG3	1:D:488:ARG:CZ	2.49	0.42
1:H:16:TYR:HE1	1:H:38:VAL:HG21	1.85	0.42
1:C:102:CYS:O	1:C:199:ILE:HA	2.20	0.42
1:G:403:PRO:HG2	1:G:405:TYR:CE1	2.54	0.42
1:H:276:LYS:HE3	1:H:280:LEU:HD11	2.01	0.42
1:H:339:THR:OG1	1:H:347:ASP:OD2	2.37	0.42
1:A:486:GLU:HB3	1:A:525:LEU:HD22	2.02	0.42
1:C:111:ASP:OD1	1:C:381[A]:HIS:CE1	2.72	0.42
1:C:305:GLU:O	1:C:470:THR:HA	2.20	0.42
1:F:230:LEU:HB3	1:F:248:ILE:HD12	2.00	0.42
1:F:44:GLU:OE1	2:F:547:FAD:H1B	2.20	0.42
1:H:362:LEU:HD12	1:H:362:LEU:HA	1.78	0.42
1:B:14:PHE:HE2	1:B:225:THR:OG1	2.01	0.42
1:C:484:ASP:HB2	1:C:485:PRO:HD2	2.02	0.42
1:D:71:TRP:CE2	1:D:91:LYS:HG3	2.55	0.42
1:G:103:ILE:HG12	1:G:197:PHE:CD1	2.55	0.42
1:G:191:VAL:HG12	1:G:338:PRO:HG3	2.02	0.42
1:G:349:MET:O	1:G:377:PRO:HA	2.19	0.42
1:H:2[A]:HIS:CD2	1:H:50:ARG:HH21	2.38	0.42
1:H:76:GLU:O	1:H:77:PRO:C	2.58	0.42
1:A:134:LYS:O	1:A:150:GLY:HA3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:PHE:O	1:B:261:ALA:HA	2.20	0.42
1:C:279:MET:O	1:C:289:LEU:CD2	2.68	0.42
1:E:499:ASP:HB2	2:E:547:FAD:O2P	2.20	0.42
1:E:526:ILE:O	1:E:529:ALA:HB3	2.20	0.42
1:F:176:GLN:OE1	1:F:430:GLN:HB3	2.20	0.42
1:H:156:HIS:O	1:H:200:ASN:HA	2.20	0.42
1:A:170:LEU:HD22	1:A:352:TYR:CD1	2.55	0.42
1:A:220:GLU:HA	1:A:220:GLU:OE1	2.19	0.42
1:H:15:ASP:OD2	1:H:39:SER:OG	2.36	0.42
1:H:466:HIS:HB3	1:H:511:PRO:HG3	2.02	0.42
1:A:206:THR:HG22	1:A:207:ARG:O	2.20	0.41
1:C:238:ASP:HB2	1:C:242:ARG:N	2.35	0.41
1:C:28:VAL:HG22	1:C:519:GLY:O	2.19	0.41
1:D:349:MET:HE1	1:D:510:ASN:HD21	1.85	0.41
1:E:102:CYS:O	1:E:199:ILE:HA	2.20	0.41
1:H:288:HIS:CE1	1:H:389:ARG:HB3	2.55	0.41
1:H:528:SER:O	1:H:530:ARG:HG3	2.20	0.41
1:E:522:CYS:O	1:E:523:ALA:C	2.59	0.41
1:F:201:ARG:HD2	1:F:205:GLY:HA2	2.01	0.41
1:F:276:LYS:HD2	1:F:399:PRO:HB3	2.02	0.41
1:F:56:LEU:O	1:F:206:THR:HA	2.20	0.41
1:C:339:THR:OG1	1:C:415:ARG:NH2	2.53	0.41
1:C:527:ARG:O	1:C:527:ARG:HG3	2.20	0.41
2:C:547:FAD:N5	3:C:601:ACT:H2	2.36	0.41
1:F:528:SER:C	1:F:530:ARG:N	2.73	0.41
1:A:69:TYR:O	1:A:91:LYS:N	2.53	0.41
1:B:173:ALA:O	1:B:430:GLN:HG3	2.20	0.41
1:C:230:LEU:HD13	1:C:248:ILE:HD12	2.02	0.41
1:C:55:VAL:HG13	1:C:98:SER:HB3	2.03	0.41
1:E:9:LEU:HD11	1:E:11:ASP:O	2.20	0.41
1:E:484:ASP:HB2	1:E:485:PRO:HD2	2.02	0.41
1:F:61:TRP:HB3	1:F:207:ARG:NH2	2.35	0.41
1:H:423:LYS:HA	1:H:423:LYS:HD3	1.86	0.41
1:H:71:TRP:CH2	1:H:91:LYS:HE3	2.56	0.41
1:B:250:ASP:HB2	1:B:254:GLY:HA3	2.02	0.41
1:E:155:VAL:HG21	1:E:516:MET:SD	2.60	0.41
1:E:22:GLY:HA3	2:E:547:FAD:O5B	2.21	0.41
1:F:337:THR:CG2	1:F:348:LEU:HD23	2.43	0.41
1:A:464:VAL:HG12	1:A:466:HIS:CE1	2.55	0.41
1:B:423:LYS:O	1:B:427:ILE:HG13	2.21	0.41
1:E:134:LYS:HG3	1:E:148:HIS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:309:ASP:OD1	1:G:310:HIS:N	2.54	0.41
1:G:443:PRO:HB3	1:G:456:TYR:CG	2.55	0.41
1:H:15:ASP:HB3	1:H:263:ASN:HD22	1.86	0.41
1:B:453:LEU:HA	1:B:453:LEU:HD23	1.78	0.41
1:D:106:TRP:CH2	1:D:148:HIS:HD2	2.39	0.41
1:E:358:ASP:HA	1:E:361:THR:OG1	2.20	0.41
1:F:307:LEU:HB3	1:F:386:GLY:C	2.41	0.41
1:F:58:LEU:HG	1:F:329:GLN:HB3	2.02	0.41
1:G:250:ASP:OD1	1:G:250:ASP:N	2.54	0.41
1:G:386:GLY:HA2	1:G:404:ARG:HG3	2.03	0.41
1:B:100:ASN:CB	2:B:547:FAD:C5X	2.99	0.41
1:E:161:PRO:HA	1:E:162:PRO:HD3	1.75	0.41
1:F:100:ASN:HB2	2:F:547:FAD:C9A	2.50	0.41
1:H:218:ILE:O	1:H:221:GLN:HB3	2.21	0.41
1:H:71:TRP:CE2	1:H:91:LYS:HG3	2.55	0.41
1:A:349:MET:O	1:A:377:PRO:HA	2.21	0.41
1:E:110:GLU:O	1:E:114:GLU:HG3	2.21	0.41
1:E:61:TRP:CE2	1:E:62:MET:HG2	2.56	0.41
1:G:267:LEU:HD11	1:G:277:LEU:CD2	2.49	0.41
1:H:21:GLY:HA2	1:H:42:LEU:HD11	2.02	0.41
1:A:181:ARG:HA	1:A:194:ALA:O	2.21	0.41
1:C:268:SER:HA	1:C:499:ASP:OD2	2.21	0.41
1:C:339:THR:OG1	1:C:347:ASP:OD2	2.31	0.41
1:C:335:ILE:HD12	1:C:350:MET:HE2	2.03	0.41
1:D:466:HIS:N	1:D:467:PRO:CD	2.84	0.41
1:D:468:VAL:HG12	1:D:500:ALA:HB1	2.02	0.41
1:F:216:HIS:N	1:F:217:PRO:CD	2.84	0.41
1:E:357:PHE:HA	1:F:253:PHE:CZ	2.56	0.41
1:H:196:PHE:HA	1:H:332:GLU:O	2.21	0.41
1:H:336:PHE:CE2	1:H:349:MET:SD	3.14	0.41
1:H:61:TRP:CE2	1:H:62:MET:HG3	2.55	0.41
1:B:101:ALA:HB3	1:B:103:ILE:HD12	2.02	0.41
1:D:353:GLY:C	1:D:355:VAL:H	2.24	0.41
1:F:15:ASP:HB2	1:F:39:SER:H	1.85	0.41
1:G:337:THR:HA	1:G:338:PRO:HD3	1.88	0.41
1:G:450:ASP:O	1:G:454:GLN:HG3	2.21	0.41
1:A:161:PRO:HA	1:A:162:PRO:HD3	1.87	0.40
1:A:234:GLN:O	1:A:246:VAL:HG23	2.21	0.40
1:A:314:VAL:HG23	1:A:376:THR:HG22	2.03	0.40
1:B:530:ARG:HG3	1:B:530:ARG:HH11	1.85	0.40
1:C:106:TRP:CH2	1:C:148:HIS:HD2	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:GLU:HA	1:D:155:VAL:O	2.20	0.40
1:D:171:LEU:HB3	1:D:181:ARG:CZ	2.51	0.40
1:B:194:ALA:O	1:B:195:ASN:HB2	2.20	0.40
1:B:227:LEU:HB3	1:B:230:LEU:HD12	2.02	0.40
1:E:163:LYS:CG	1:E:164:ASP:N	2.83	0.40
1:G:527:ARG:O	1:G:528:SER:HB3	2.21	0.40
1:H:172:ASP:O	1:H:176:GLN:HG3	2.21	0.40
1:H:22:GLY:HA2	1:H:95:GLY:HA3	2.03	0.40
1:B:267:LEU:HD23	1:B:267:LEU:HA	1.90	0.40
1:B:74:PRO:HG3	1:B:86:ARG:NH2	2.36	0.40
1:D:499:ASP:OD1	1:D:501:SER:CB	2.69	0.40
1:E:53:PRO:HB2	1:E:60:ARG:HH21	1.86	0.40
1:E:22:GLY:HA2	1:E:94:GLY:C	2.42	0.40
1:F:510:ASN:HB3	2:F:547:FAD:O2	2.22	0.40
1:G:253:PHE:CD2	1:G:396:ARG:NH2	2.87	0.40
1:C:351:HIS:O	1:C:375:LEU:HA	2.21	0.40
1:D:320:LYS:HD2	1:D:437:THR:O	2.21	0.40
1:E:128:ALA:O	1:E:131:PRO:HD2	2.22	0.40
1:G:231:ARG:O	1:G:248:ILE:HA	2.22	0.40
1:H:157:LEU:CD2	1:H:200:ASN:HB3	2.52	0.40
1:H:488:ARG:CG	1:H:496:ARG:HD3	2.40	0.40
1:H:75:ILE:HD11	1:H:82:ASN:O	2.22	0.40
1:B:1:MET:HG3	1:B:225:THR:HG23	2.02	0.40
1:B:458:ARG:HG3	1:B:458:ARG:NH1	2.36	0.40
1:C:258:ARG:CG	1:C:259:LEU:N	2.84	0.40
1:C:31:ARG:HA	1:C:31:ARG:HD3	1.91	0.40
1:F:22:GLY:HA3	2:F:547:FAD:O5B	2.22	0.40
1:G:173:ALA:HB1	1:G:430:GLN:HB2	2.03	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	531/546 (97%)	496 (93%)	31 (6%)	4 (1%)	19	33
1	B	532/546 (97%)	485 (91%)	42 (8%)	5 (1%)	17	29
1	C	529/546 (97%)	487 (92%)	40 (8%)	2 (0%)	34	52
1	D	530/546 (97%)	494 (93%)	32 (6%)	4 (1%)	19	33
1	E	534/546 (98%)	497 (93%)	32 (6%)	5 (1%)	17	29
1	F	531/546 (97%)	497 (94%)	31 (6%)	3 (1%)	25	40
1	G	531/546 (97%)	492 (93%)	34 (6%)	5 (1%)	17	29
1	H	531/546 (97%)	488 (92%)	35 (7%)	8 (2%)	10	16
All	All	4249/4368 (97%)	3936 (93%)	277 (6%)	36 (1%)	17	33

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	VAL
1	A	252	ALA
1	B	238	ASP
1	G	92	VAL
1	A	48	ASP
1	B	256	THR
1	D	72	ASP
1	D	92	VAL
1	E	92	VAL
1	E	528	SER
1	H	92	VAL
1	H	252	ALA
1	H	329	GLN
1	H	476	VAL
1	A	445	VAL
1	B	329	GLN
1	F	92	VAL
1	F	465	TYR
1	F	529	ALA
1	G	238	ASP
1	G	280	LEU
1	G	329	GLN
1	H	72	ASP
1	H	251	SER
1	C	238	ASP
1	C	499	ASP
1	D	291	GLU

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Mol	Chain	Res	Type
1	D	329	GLN
1	E	499	ASP
1	G	465	TYR
1	B	209	SER
1	E	395	PHE
1	H	67	SER
1	E	254	GLY
1	H	492	VAL
1	B	92	VAL

### 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	439/445 (99%)	416 (95%)	23 (5%)	23	41
1	B	440/445 (99%)	411 (93%)	29 (7%)	16	30
1	C	438/445 (98%)	413 (94%)	25 (6%)	20	37
1	D	439/445 (99%)	406 (92%)	33 (8%)	13	24
1	E	442/445 (99%)	420 (95%)	22 (5%)	24	43
1	F	439/445 (99%)	414 (94%)	25 (6%)	20	37
1	G	439/445 (99%)	409 (93%)	30 (7%)	16	28
1	H	439/445 (99%)	403 (92%)	36 (8%)	11	20
All	All	3515/3560 (99%)	3292 (94%)	223 (6%)	17	32

All (223) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	86	ARG
1	A	99	HIS
1	A	130	TRP
1	A	152	SER
1	A	157	LEU

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Mol	Chain	Res	Type
1	A	166	THR
1	A	171	LEU
1	A	202	ARG
1	A	251	SER
1	A	260	THR
1	A	269	THR
1	A	315	VAL
1	A	324	VAL
1	A	326	GLU
1	A	329	GLN
1	A	343	LEU
1	A	368	THR
1	A	412	HIS
1	A	473	MET
1	A	479	GLU
1	A	510	ASN
1	A	530	ARG
1	B	9	LEU
1	B	12	ARG
1	B	97	SER
1	B	99	HIS
1	B	130	TRP
1	B	157	LEU
1	B	162	PRO
1	B	171	LEU
1	B	202	ARG
1	B	208	SER
1	B	225	THR
1	B	226	LEU
1	B	241	ARG
1	B	249	VAL
1	B	251	SER
1	B	273	ASP
1	B	300	SER
1	B	320	LYS
1	B	324	VAL
1	B	326	GLU
1	B	329	GLN
1	B	368	THR
1	B	445	VAL
1	B	477[A]	GLU
1	B	477[B]	GLU

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Mol	Chain	Res	Type
1	B	486	GLU
1	B	506	HIS
1	B	510	ASN
1	B	530	ARG
1	C	6	ILE
1	C	38	VAL
1	C	60	ARG
1	C	86	ARG
1	C	99	HIS
1	C	130	TRP
1	C	152	SER
1	C	163	LYS
1	C	171	LEU
1	C	183	LYS
1	C	202	ARG
1	C	204	ASP
1	C	238	ASP
1	C	250	ASP
1	C	269	THR
1	C	320	LYS
1	C	329	GLN
1	C	337	THR
1	C	431	PRO
1	C	439	ARG
1	C	463	THR
1	C	468	VAL
1	C	486	GLU
1	C	510	ASN
1	C	521	ARG
1	D	5	ASN
1	D	38	VAL
1	D	99	HIS
1	D	112	LEU
1	D	130	TRP
1	D	156	HIS
1	D	157	LEU
1	D	163	LYS
1	D	171	LEU
1	D	208	SER
1	D	225	THR
1	D	226	LEU
1	D	234	GLN

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Mol	Chain	Res	Type
1	D	236	VAL
1	D	238	ASP
1	D	250	ASP
1	D	267	LEU
1	D	273	ASP
1	D	277	LEU
1	D	324	VAL
1	D	327	SER
1	D	329	GLN
1	D	339	THR
1	D	347	ASP
1	D	370	GLU
1	D	408	ASP
1	D	410	GLU
1	D	422	ARG
1	D	439	ARG
1	D	445	VAL
1	D	486	GLU
1	D	492	VAL
1	D	510	ASN
1	E	23	SER
1	E	40	VAL
1	E	86	ARG
1	E	99	HIS
1	E	130	TRP
1	E	134	LYS
1	E	152	SER
1	E	157	LEU
1	E	171	LEU
1	E	202	ARG
1	E	225	THR
1	E	242	ARG
1	E	250	ASP
1	E	295	GLU
1	E	329	GLN
1	E	337	THR
1	E	446	GLU
1	E	448	GLN
1	E	459	LYS
1	E	486	GLU
1	E	510	ASN
1	E	530	ARG

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Mol	Chain	Res	Type
1	F	97	SER
1	F	99	HIS
1	F	118	LYS
1	F	130	TRP
1	F	171	LEU
1	F	202	ARG
1	F	222	GLU
1	F	226	LEU
1	F	242	ARG
1	F	250	ASP
1	F	251	SER
1	F	253	PHE
1	F	255	HIS
1	F	324	VAL
1	F	329	GLN
1	F	337	THR
1	F	340	GLU
1	F	396	ARG
1	F	435	GLU
1	F	446	GLU
1	F	479	GLU
1	F	510	ASN
1	F	527	ARG
1	F	528	SER
1	F	530	ARG
1	G	7	GLU
1	G	38	VAL
1	G	54	GLU
1	G	66	GLU
1	G	85	MET
1	G	97	SER
1	G	98	SER
1	G	99	HIS
1	G	130	TRP
1	G	157	LEU
1	G	171	LEU
1	G	183	LYS
1	G	241	ARG
1	G	250	ASP
1	G	258	ARG
1	G	260	THR
1	G	291	GLU

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Mol	Chain	Res	Type
1	G	295	GLU
1	G	329	GLN
1	G	337	THR
1	G	367	PRO
1	G	389	ARG
1	G	410	GLU
1	G	459	LYS
1	G	468	VAL
1	G	492	VAL
1	G	495	LEU
1	G	501	SER
1	G	510	ASN
1	G	527	ARG
1	H	1	MET
1	H	3	ILE
1	H	4	ASP
1	H	5	ASN
1	H	12	ARG
1	H	18	VAL
1	H	38	VAL
1	H	39	SER
1	H	55	VAL
1	H	79	GLU
1	H	87	HIS
1	H	99	HIS
1	H	130	TRP
1	H	156	HIS
1	H	171	LEU
1	H	195	ASN
1	H	202	ARG
1	H	211	SER
1	H	219	VAL
1	H	222	GLU
1	H	225	THR
1	H	226	LEU
1	H	228	THR
1	H	230	LEU
1	H	234	GLN
1	H	250	ASP
1	H	266	VAL
1	H	273	ASP
1	H	297	LEU

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Mol	Chain	Res	Type
1	H	324	VAL
1	H	329	GLN
1	H	352	TYR
1	H	374	SER
1	H	486	GLU
1	H	507	VAL
1	H	510	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	HIS
1	A	216	HIS
1	A	288	HIS
1	A	448	GLN
1	A	510	ASN
1	A	512	ASN
1	B	8	ASN
1	B	263	ASN
1	B	316	GLN
1	B	510	ASN
1	B	512	ASN
1	C	192	ASN
1	C	448	GLN
1	C	510	ASN
1	C	512	ASN
1	D	510	ASN
1	D	512	ASN
1	E	288	HIS
1	E	448	GLN
1	E	510	ASN
1	E	512	ASN
1	F	192	ASN
1	F	292	HIS
1	F	316	GLN
1	F	510	ASN
1	F	512	ASN
1	G	288	HIS
1	G	378	ASN
1	G	510	ASN
1	G	512	ASN
1	H	5	ASN

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Mol	Chain	Res	Type
1	H	8	ASN
1	H	148	HIS
1	H	192	ASN
1	H	195	ASN
1	H	234	GLN
1	H	263	ASN
1	H	292	HIS
1	H	329	GLN
1	H	412	HIS
1	H	510	ASN
1	H	512	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	ACT	G	601	-	1,3,3	1.20	0	0,3,3	0.00	-
3	ACT	F	601	-	1,3,3	2.03	1 (100%)	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ACT	E	601	-	1,3,3	2.02	1 (100%)	0,3,3	0.00	-
3	ACT	D	601	-	1,3,3	1.33	0	0,3,3	0.00	-
2	FAD	C	547	1	51,58,58	1.39	6 (11%)	60,89,89	2.21	16 (26%)
2	FAD	A	547	1	51,58,58	1.49	6 (11%)	60,89,89	1.80	12 (20%)
2	FAD	G	547	1	51,58,58	1.56	7 (13%)	60,89,89	2.75	18 (30%)
2	FAD	E	547	1	51,58,58	1.51	8 (15%)	60,89,89	1.77	10 (16%)
3	ACT	C	601	-	1,3,3	1.71	0	0,3,3	0.00	-
3	ACT	H	601	-	1,3,3	1.09	0	0,3,3	0.00	-
2	FAD	B	547	1	51,58,58	1.41	7 (13%)	60,89,89	2.09	15 (25%)
3	ACT	B	601	-	1,3,3	1.79	0	0,3,3	0.00	-
2	FAD	F	547	1	51,58,58	1.38	6 (11%)	60,89,89	1.86	9 (15%)
2	FAD	D	547	1	51,58,58	1.72	9 (17%)	60,89,89	1.94	12 (20%)
2	FAD	H	547	1	51,58,58	1.48	6 (11%)	60,89,89	1.84	7 (11%)
3	ACT	A	601	-	1,3,3	1.06	0	0,3,3	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	C	547	1	-	7/30/50/50	0/6/6/6
2	FAD	A	547	1	-	4/30/50/50	0/6/6/6
2	FAD	G	547	1	-	5/30/50/50	0/6/6/6
2	FAD	E	547	1	-	3/30/50/50	0/6/6/6
2	FAD	B	547	1	-	11/30/50/50	0/6/6/6
2	FAD	F	547	1	-	5/30/50/50	0/6/6/6
2	FAD	D	547	1	-	5/30/50/50	0/6/6/6
2	FAD	H	547	1	-	3/30/50/50	0/6/6/6

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	547	FAD	C2A-N3A	5.18	1.40	1.32
2	D	547	FAD	C4X-N5	5.05	1.40	1.33
2	G	547	FAD	C10-N1	5.00	1.39	1.33
2	G	547	FAD	C4X-N5	4.78	1.40	1.33
2	H	547	FAD	C2A-N3A	4.51	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	547	FAD	C2A-N3A	4.38	1.39	1.32
2	A	547	FAD	C2A-N3A	4.37	1.39	1.32
2	D	547	FAD	C10-N1	4.36	1.38	1.33
2	F	547	FAD	C2A-N3A	4.29	1.39	1.32
2	E	547	FAD	C1'-N10	4.25	1.52	1.48
2	E	547	FAD	C2A-N3A	4.24	1.38	1.32
2	C	547	FAD	C10-N1	4.21	1.38	1.33
2	A	547	FAD	C4X-N5	4.15	1.39	1.33
2	E	547	FAD	C10-N1	4.14	1.38	1.33
2	A	547	FAD	C10-N1	4.14	1.38	1.33
2	C	547	FAD	C4X-N5	4.07	1.39	1.33
2	H	547	FAD	C4-N3	3.98	1.40	1.33
2	D	547	FAD	C4-N3	3.80	1.39	1.33
2	F	547	FAD	C10-N1	3.42	1.37	1.33
2	D	547	FAD	C5X-N5	3.40	1.41	1.35
2	G	547	FAD	C4-N3	3.39	1.38	1.33
2	H	547	FAD	C4X-N5	3.37	1.38	1.33
2	H	547	FAD	C1'-N10	3.32	1.51	1.48
2	F	547	FAD	C4X-N5	3.31	1.38	1.33
2	A	547	FAD	C5X-N5	3.30	1.40	1.35
2	H	547	FAD	C5X-N5	3.30	1.40	1.35
2	E	547	FAD	C4X-N5	3.20	1.37	1.33
2	D	547	FAD	C8M-C8	-3.12	1.44	1.51
2	B	547	FAD	C4-N3	3.05	1.38	1.33
2	G	547	FAD	C2A-N3A	3.00	1.36	1.32
2	C	547	FAD	C2A-N3A	2.93	1.36	1.32
2	H	547	FAD	C10-N1	2.92	1.37	1.33
2	E	547	FAD	C4-N3	2.90	1.38	1.33
2	C	547	FAD	C4-N3	2.82	1.38	1.33
2	D	547	FAD	C6-C5X	-2.82	1.37	1.41
2	G	547	FAD	C5X-N5	2.74	1.39	1.35
2	G	547	FAD	C1'-N10	2.73	1.51	1.48
2	B	547	FAD	C10-N1	2.72	1.36	1.33
2	B	547	FAD	C9A-C5X	-2.62	1.37	1.42
2	A	547	FAD	C8M-C8	2.57	1.56	1.51
2	A	547	FAD	C4-N3	2.56	1.37	1.33
2	B	547	FAD	C6-C5X	-2.51	1.37	1.41
2	F	547	FAD	C5X-N5	2.50	1.39	1.35
2	B	547	FAD	C2A-N1A	2.47	1.38	1.33
2	C	547	FAD	C5X-N5	2.38	1.39	1.35
2	E	547	FAD	C5X-N5	2.35	1.39	1.35
2	D	547	FAD	C2A-N1A	2.34	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	547	FAD	C2B-C1B	-2.34	1.50	1.53
2	E	547	FAD	C2A-N1A	2.27	1.38	1.33
2	B	547	FAD	C4X-N5	2.27	1.36	1.33
2	G	547	FAD	O4B-C1B	2.20	1.44	1.41
2	C	547	FAD	C1'-N10	2.17	1.50	1.48
2	F	547	FAD	C4-C4X	-2.09	1.37	1.41
2	D	547	FAD	C2B-C1B	-2.04	1.50	1.53
3	F	601	ACT	CH3-C	2.03	1.51	1.48
3	E	601	ACT	CH3-C	2.02	1.51	1.48
2	E	547	FAD	C6-C5X	-2.00	1.38	1.41

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	547	FAD	C8M-C8-C7	-8.99	102.31	120.74
2	G	547	FAD	C4-N3-C2	8.98	122.73	115.14
2	F	547	FAD	C4-N3-C2	7.23	121.25	115.14
2	G	547	FAD	C8M-C8-C9	-6.93	103.77	120.34
2	B	547	FAD	C10-C4X-N5	-6.86	116.51	121.26
2	D	547	FAD	C4-N3-C2	6.82	120.90	115.14
2	G	547	FAD	C1'-N10-C9A	6.80	123.64	118.29
2	A	547	FAD	C4-N3-C2	6.78	120.87	115.14
2	G	547	FAD	N3A-C2A-N1A	-6.67	118.26	128.68
2	C	547	FAD	C4-N3-C2	6.66	120.77	115.14
2	E	547	FAD	C4-N3-C2	6.23	120.40	115.14
2	C	547	FAD	C8M-C8-C9	-5.99	106.01	120.34
2	H	547	FAD	N3A-C2A-N1A	-5.96	119.36	128.68
2	D	547	FAD	N3A-C2A-N1A	-5.95	119.38	128.68
2	D	547	FAD	C8M-C8-C9	-5.90	106.23	120.34
2	H	547	FAD	C4-N3-C2	5.62	119.88	115.14
2	B	547	FAD	C4-N3-C2	5.60	119.87	115.14
2	E	547	FAD	N3A-C2A-N1A	-5.30	120.39	128.68
2	F	547	FAD	N3A-C2A-N1A	-5.24	120.48	128.68
2	B	547	FAD	C4X-N5-C5X	5.22	121.99	116.77
2	C	547	FAD	N3A-C2A-N1A	-5.14	120.64	128.68
2	A	547	FAD	N3A-C2A-N1A	-5.13	120.66	128.68
2	E	547	FAD	C1'-N10-C9A	5.02	122.25	118.29
2	H	547	FAD	C10-C4X-N5	-5.01	117.80	121.26
2	H	547	FAD	C8M-C8-C9	-4.93	108.55	120.34
2	C	547	FAD	C5X-C9A-N10	4.88	121.25	117.72
2	F	547	FAD	C1'-N10-C9A	4.82	122.08	118.29
2	B	547	FAD	N3A-C2A-N1A	-4.63	121.44	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	547	FAD	C4A-C5A-N7A	-4.52	104.69	109.40
2	C	547	FAD	C1'-N10-C9A	4.33	121.70	118.29
2	B	547	FAD	C4X-C4-N3	-4.28	117.57	123.43
2	A	547	FAD	C8M-C8-C9	-4.25	110.17	120.34
2	C	547	FAD	C5A-C6A-N6A	4.02	126.46	120.35
2	C	547	FAD	C8M-C8-C7	3.94	128.81	120.74
2	B	547	FAD	O4B-C1B-C2B	-3.88	101.26	106.93
2	E	547	FAD	C4X-N5-C5X	3.86	120.63	116.77
2	H	547	FAD	C4X-N5-C5X	3.86	120.63	116.77
2	H	547	FAD	C4X-C4-N3	-3.83	118.19	123.43
2	G	547	FAD	C4X-N5-C5X	3.81	120.58	116.77
2	G	547	FAD	C1B-N9A-C4A	-3.61	120.31	126.64
2	F	547	FAD	C4X-C4-N3	-3.53	118.61	123.43
2	G	547	FAD	C5X-C9A-N10	3.42	120.19	117.72
2	A	547	FAD	C5X-C9A-N10	3.38	120.16	117.72
2	D	547	FAD	C1'-N10-C10	3.33	121.39	118.41
2	B	547	FAD	C4A-C5A-N7A	-3.28	105.98	109.40
2	E	547	FAD	C10-C4X-N5	-3.28	118.99	121.26
2	G	547	FAD	C4-C4X-C10	-3.26	117.79	119.95
2	G	547	FAD	C4A-C5A-N7A	-3.24	106.02	109.40
2	D	547	FAD	C10-C4X-N5	-3.23	119.02	121.26
2	B	547	FAD	C4'-C3'-C2'	-3.18	106.75	113.36
2	G	547	FAD	C4X-C4-N3	-3.09	119.21	123.43
2	F	547	FAD	O4B-C1B-C2B	-3.06	102.46	106.93
2	F	547	FAD	C4X-N5-C5X	3.04	119.81	116.77
2	C	547	FAD	C4-C4X-C10	-3.01	117.96	119.95
2	D	547	FAD	C4-C4X-N5	3.00	122.03	118.60
2	F	547	FAD	C5X-C9A-N10	2.99	119.88	117.72
2	G	547	FAD	C5A-C6A-N6A	2.96	124.84	120.35
2	G	547	FAD	C4-C4X-N5	2.94	121.96	118.60
2	D	547	FAD	C8M-C8-C7	2.89	126.65	120.74
2	A	547	FAD	C4A-C5A-N7A	-2.88	106.40	109.40
2	C	547	FAD	C9A-N10-C10	-2.87	118.15	121.91
2	E	547	FAD	P-O3P-PA	-2.83	123.13	132.83
2	B	547	FAD	C8M-C8-C9	-2.77	113.71	120.34
2	F	547	FAD	C4A-C5A-N7A	-2.75	106.53	109.40
2	A	547	FAD	C4X-N5-C5X	2.70	119.47	116.77
2	C	547	FAD	C1B-N9A-C4A	-2.65	121.99	126.64
2	A	547	FAD	C4-C4X-N5	2.63	121.60	118.60
2	B	547	FAD	C4-C4X-N5	2.59	121.56	118.60
2	H	547	FAD	C4-C4X-N5	2.56	121.52	118.60
2	G	547	FAD	C1'-N10-C10	-2.55	116.12	118.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	547	FAD	C4X-C4-N3	-2.55	119.95	123.43
2	D	547	FAD	C4X-C4-N3	-2.52	119.98	123.43
2	E	547	FAD	C8M-C8-C9	-2.50	114.37	120.34
2	E	547	FAD	C4X-C4-N3	-2.50	120.02	123.43
2	C	547	FAD	C4-C4X-N5	2.48	121.43	118.60
2	C	547	FAD	O3B-C3B-C4B	-2.47	103.90	111.05
2	G	547	FAD	C9A-C5X-N5	-2.46	118.51	122.36
2	A	547	FAD	P-O3P-PA	-2.45	124.41	132.83
2	D	547	FAD	C4X-N5-C5X	2.44	119.20	116.77
2	G	547	FAD	C6-C5X-N5	2.43	121.72	119.05
2	B	547	FAD	C1'-N10-C9A	2.43	120.20	118.29
2	D	547	FAD	O3'-C3'-C4'	2.42	114.66	108.81
2	C	547	FAD	C4X-C4-N3	-2.35	120.22	123.43
2	C	547	FAD	P-O3P-PA	-2.34	124.78	132.83
2	A	547	FAD	C8M-C8-C7	2.32	125.49	120.74
2	B	547	FAD	C4-C4X-C10	2.31	121.48	119.95
2	F	547	FAD	C10-C4X-N5	-2.28	119.68	121.26
2	A	547	FAD	O4'-C4'-C3'	-2.28	103.54	109.10
2	G	547	FAD	C2A-N1A-C6A	2.26	122.62	118.75
2	A	547	FAD	C4-C4X-C10	-2.24	118.47	119.95
2	C	547	FAD	O3'-C3'-C4'	-2.21	103.48	108.81
2	B	547	FAD	C5B-C4B-C3B	-2.17	107.06	115.18
2	B	547	FAD	P-O3P-PA	-2.13	125.51	132.83
2	D	547	FAD	C9A-N10-C10	-2.11	119.14	121.91
2	D	547	FAD	O4B-C1B-C2B	-2.09	103.86	106.93
2	G	547	FAD	O3B-C3B-C4B	-2.06	105.08	111.05
2	E	547	FAD	C4-C4X-N5	2.05	120.94	118.60
2	B	547	FAD	C9A-C5X-N5	-2.05	119.16	122.36
2	E	547	FAD	O2'-C2'-C3'	2.01	113.98	109.10

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	547	FAD	O4B-C4B-C5B-O5B
2	C	547	FAD	C2'-C1'-N10-C9A
2	C	547	FAD	O4'-C4'-C5'-O5'
2	A	547	FAD	C2'-C1'-N10-C9A
2	A	547	FAD	PA-O3P-P-O5'
2	E	547	FAD	N10-C1'-C2'-O2'
2	B	547	FAD	C5B-O5B-PA-O2A
2	B	547	FAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	B	547	FAD	C3'-C4'-C5'-O5'
2	B	547	FAD	O4'-C4'-C5'-O5'
2	B	547	FAD	C5'-O5'-P-O1P
2	B	547	FAD	C5'-O5'-P-O2P
2	B	547	FAD	PA-O3P-P-O5'
2	F	547	FAD	N10-C1'-C2'-O2'
2	D	547	FAD	C5B-O5B-PA-O2A
2	H	547	FAD	C2'-C1'-N10-C9A
2	D	547	FAD	O4B-C4B-C5B-O5B
2	H	547	FAD	O4B-C4B-C5B-O5B
2	C	547	FAD	C3B-C4B-C5B-O5B
2	A	547	FAD	O4B-C4B-C5B-O5B
2	B	547	FAD	C3B-C4B-C5B-O5B
2	D	547	FAD	C3B-C4B-C5B-O5B
2	H	547	FAD	C3B-C4B-C5B-O5B
2	G	547	FAD	O4B-C4B-C5B-O5B
2	A	547	FAD	C3B-C4B-C5B-O5B
2	E	547	FAD	O4B-C4B-C5B-O5B
2	G	547	FAD	PA-O3P-P-O5'
2	F	547	FAD	PA-O3P-P-O5'
2	F	547	FAD	O4B-C4B-C5B-O5B
2	B	547	FAD	C5'-O5'-P-O3P
2	D	547	FAD	C5B-O5B-PA-O3P
2	C	547	FAD	C5B-O5B-PA-O1A
2	C	547	FAD	C5B-O5B-PA-O2A
2	D	547	FAD	C5B-O5B-PA-O1A
2	G	547	FAD	N10-C1'-C2'-O2'
2	B	547	FAD	N10-C1'-C2'-O2'
2	F	547	FAD	C3B-C4B-C5B-O5B
2	F	547	FAD	O4'-C4'-C5'-O5'
2	E	547	FAD	C3B-C4B-C5B-O5B
2	G	547	FAD	P-O3P-PA-O2A
2	G	547	FAD	C3B-C4B-C5B-O5B
2	C	547	FAD	C5B-O5B-PA-O3P
2	B	547	FAD	C5B-O5B-PA-O1A

There are no ring outliers.

13 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	601	ACT	2	0
2	C	547	FAD	7	0

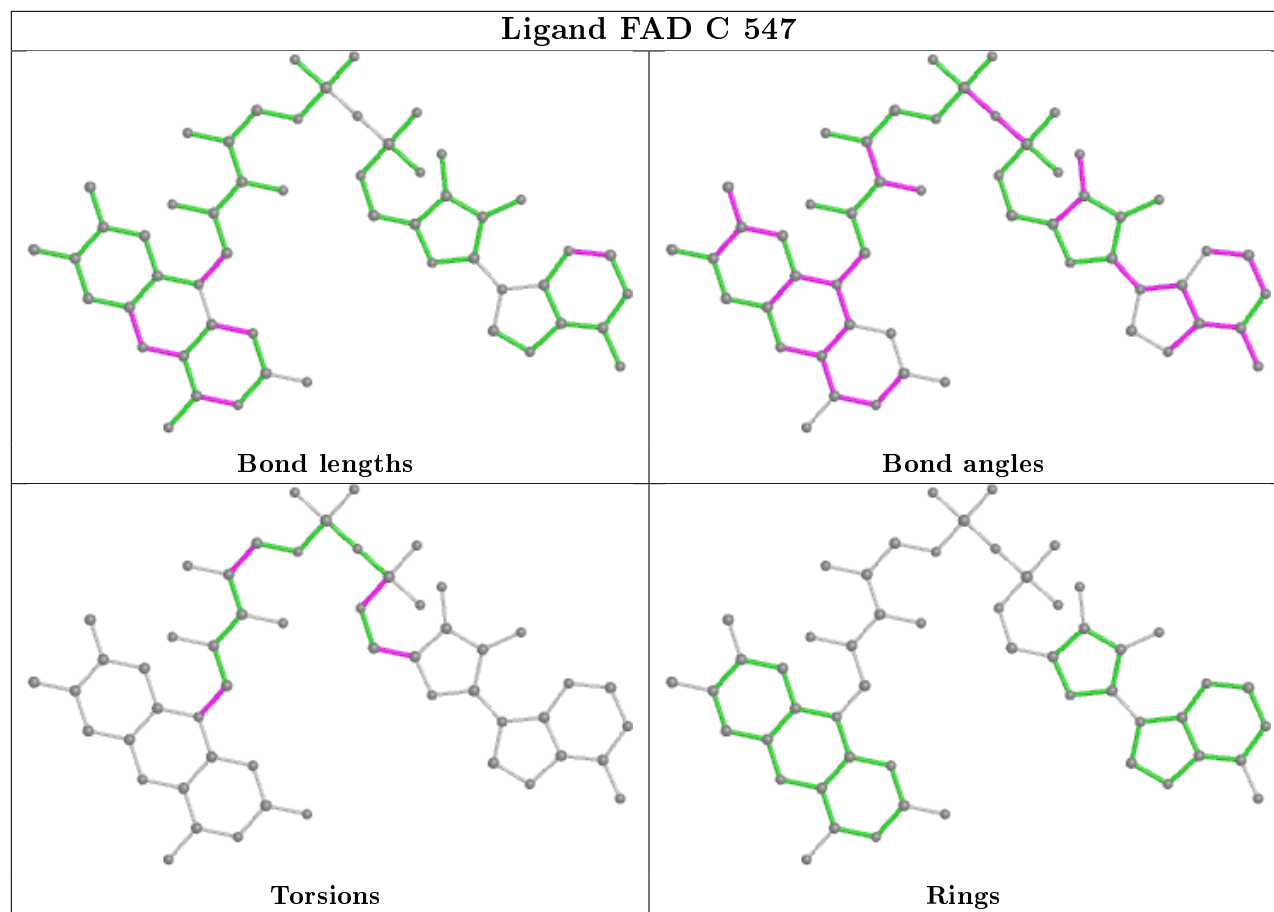
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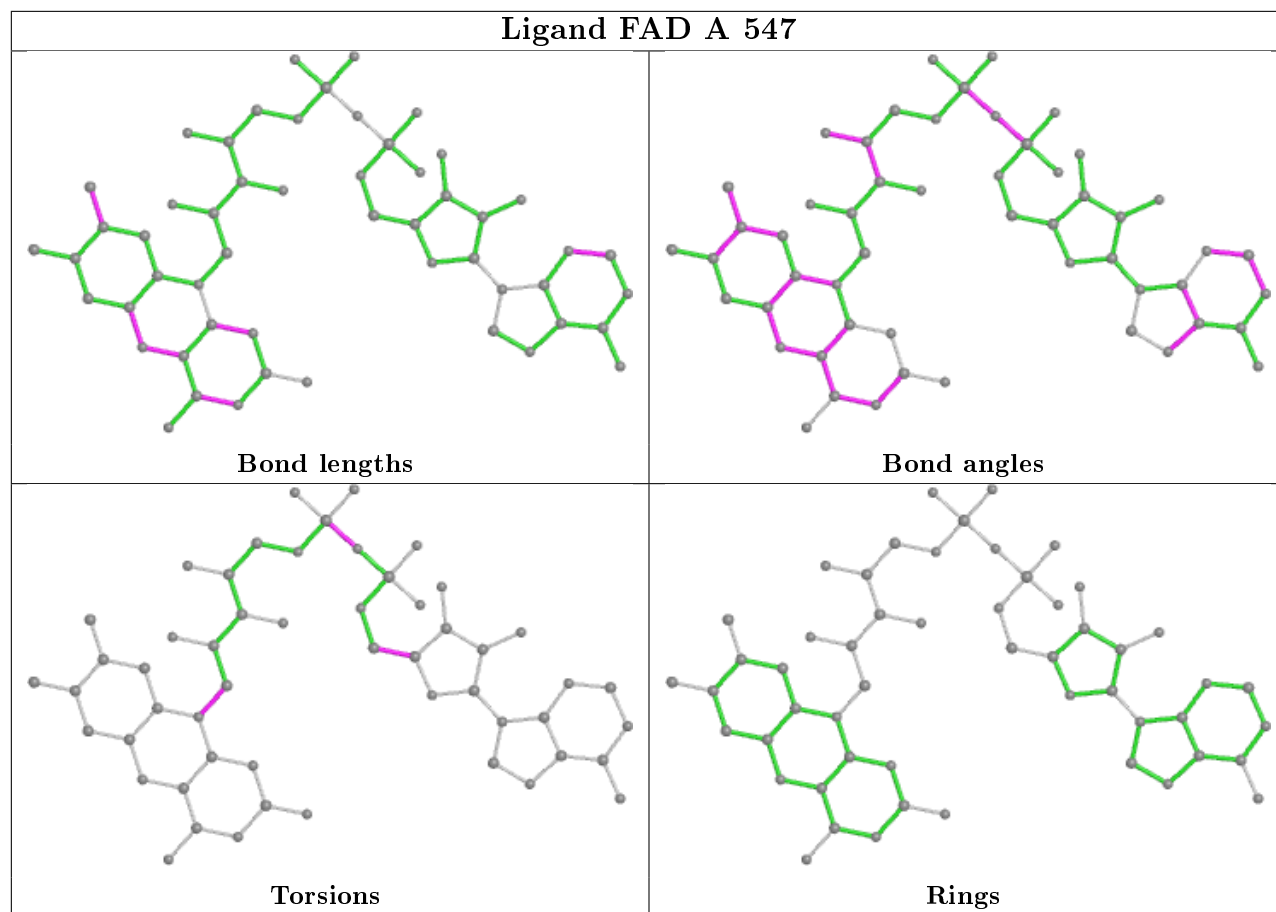
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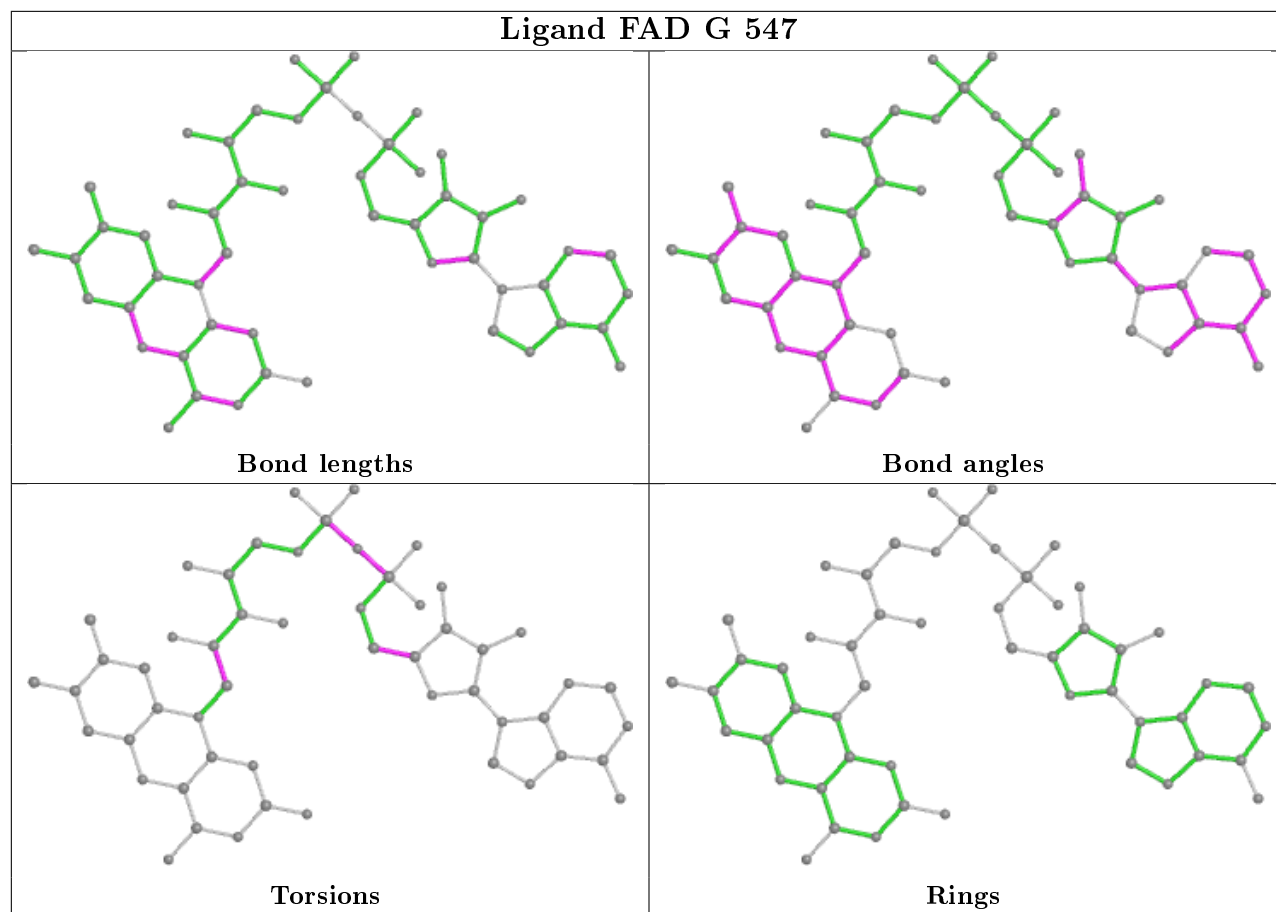
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	547	FAD	6	0
2	G	547	FAD	3	0
2	E	547	FAD	6	0
3	C	601	ACT	1	0
3	H	601	ACT	2	0
2	B	547	FAD	6	0
3	B	601	ACT	1	0
2	F	547	FAD	7	0
2	D	547	FAD	4	0
2	H	547	FAD	7	0
3	A	601	ACT	3	0

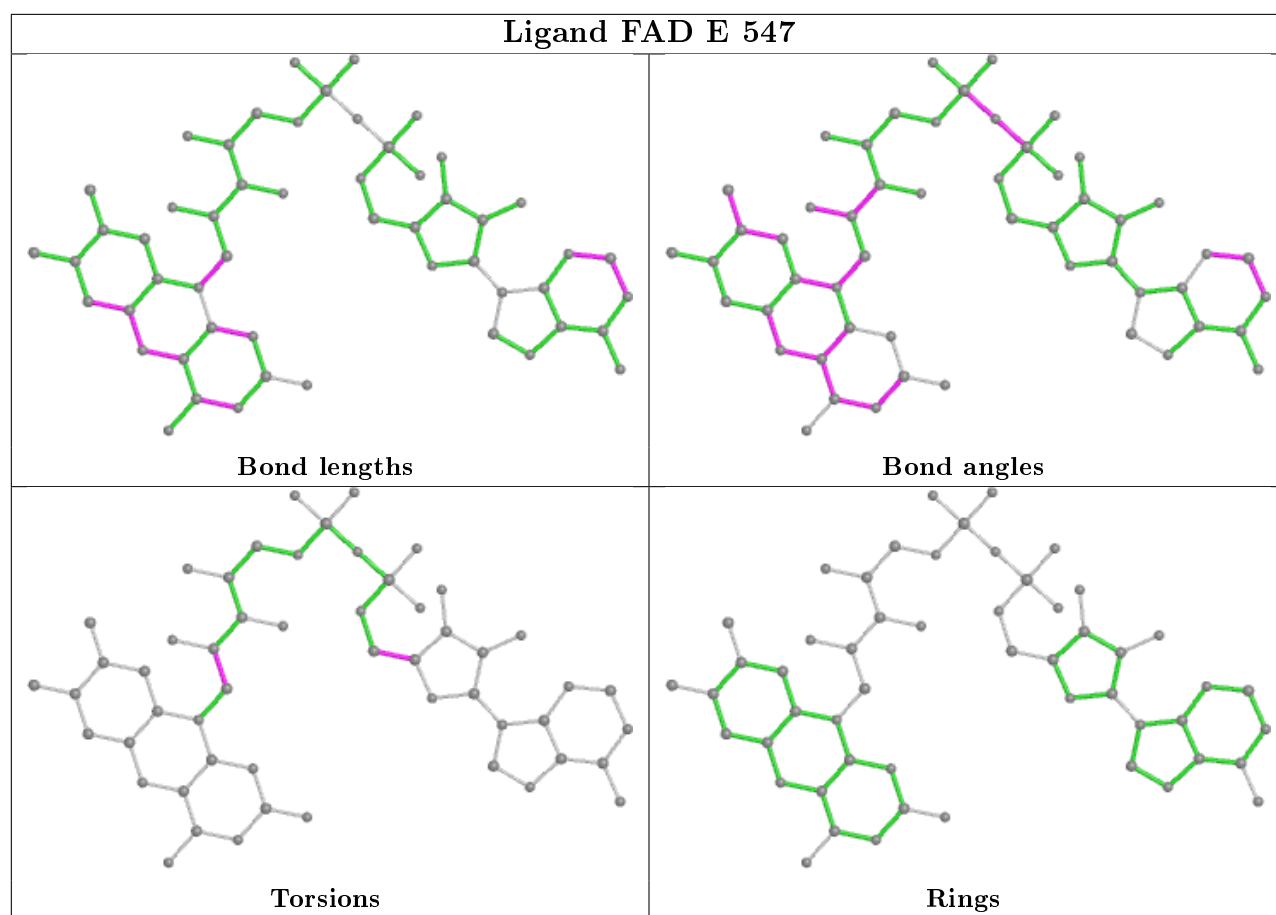
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

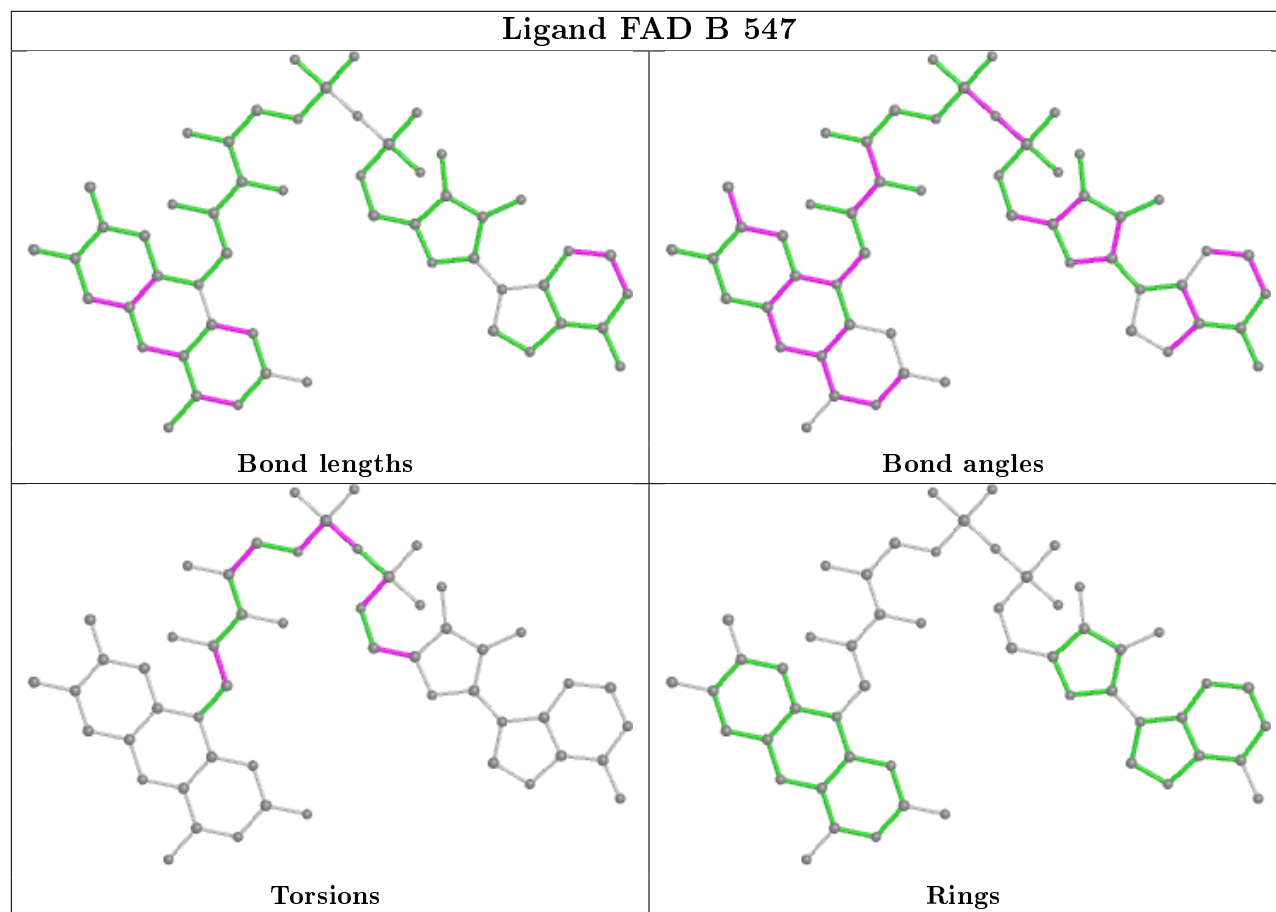


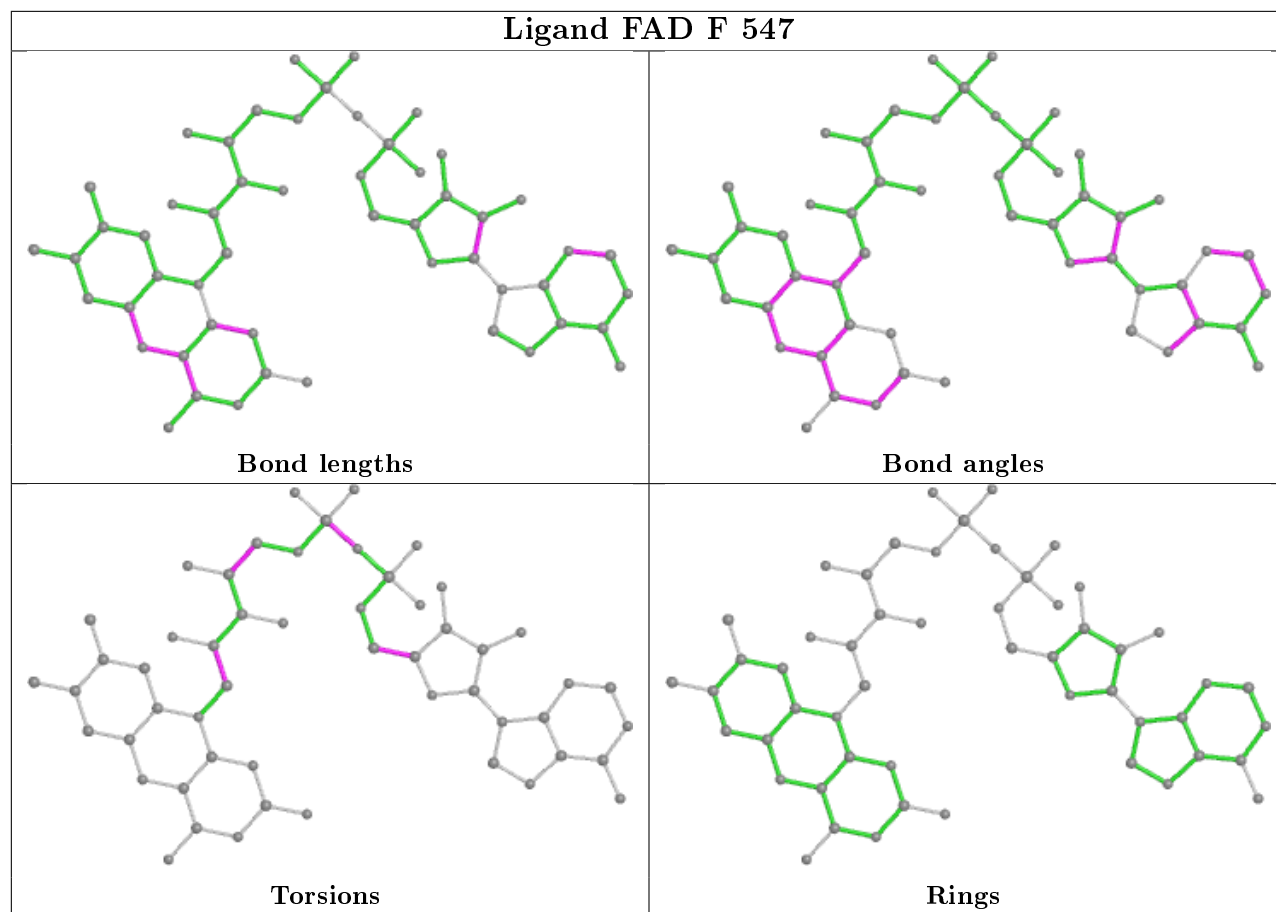


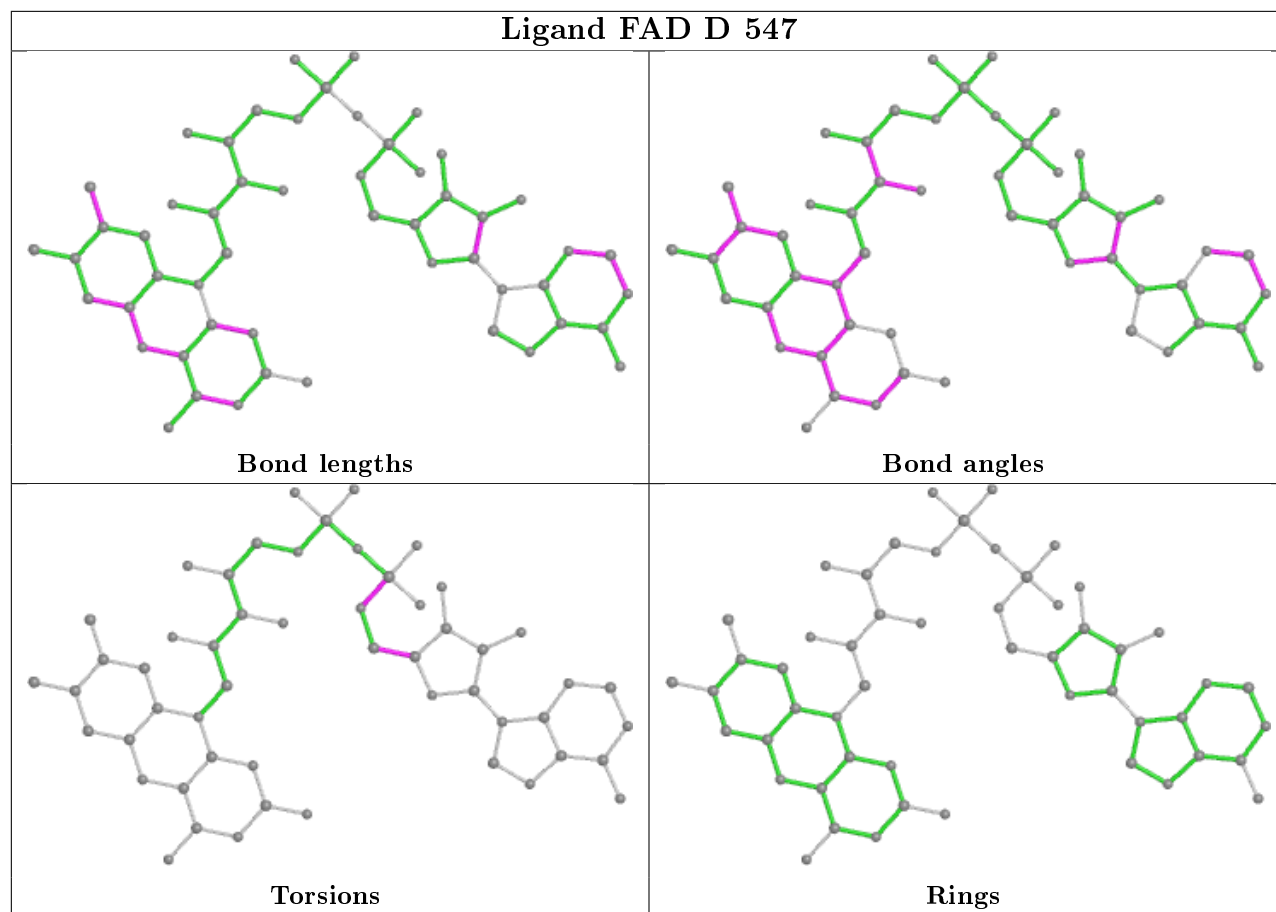


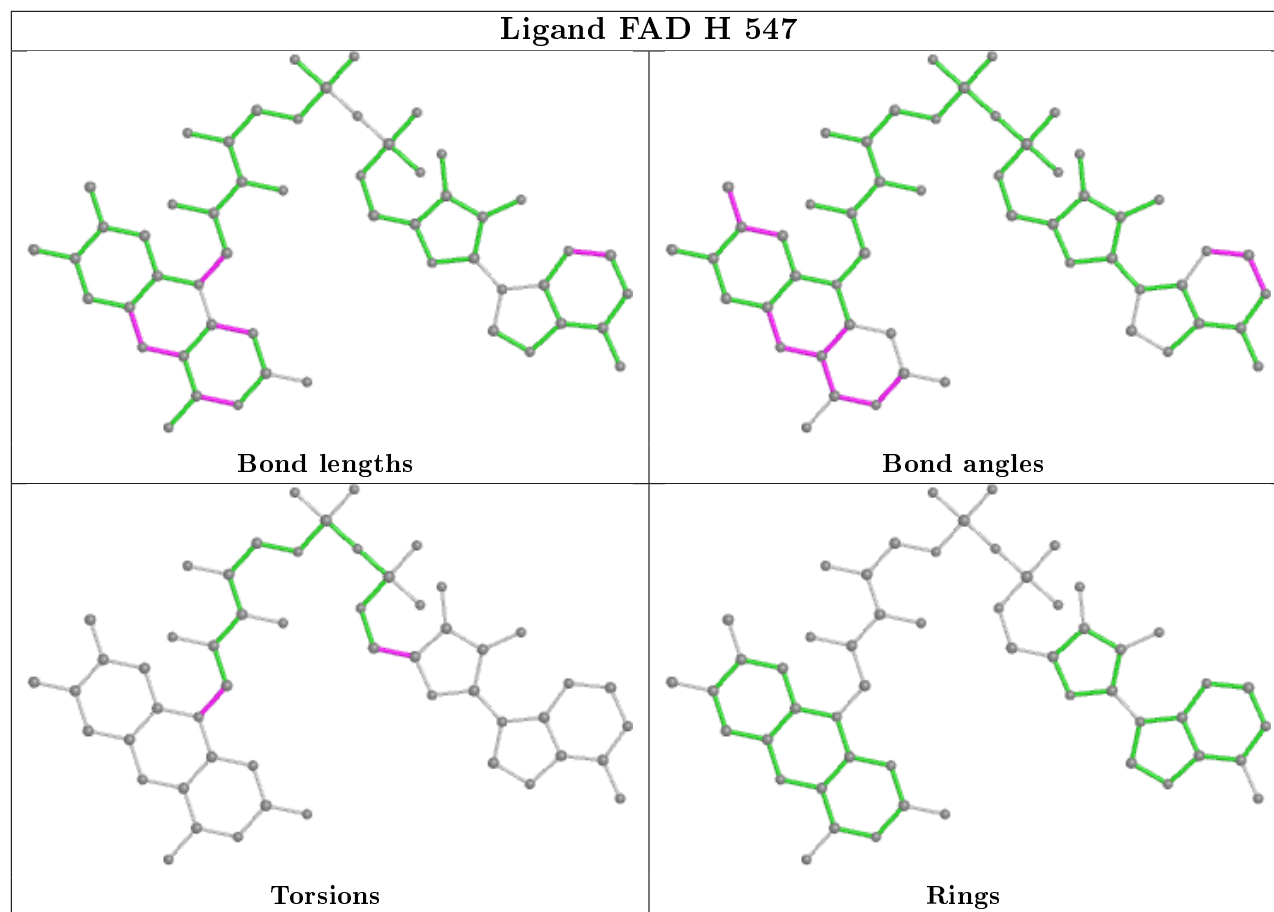












## 5.7 Other polymers [i](#)

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	530/546 (97%)	0.01	10 (1%) 66 68	20, 32, 49, 64	0
1	B	530/546 (97%)	0.05	17 (3%) 47 50	12, 27, 50, 66	0
1	C	528/546 (96%)	-0.10	4 (0%) 86 87	15, 26, 39, 51	0
1	D	530/546 (97%)	-0.02	6 (1%) 80 82	17, 29, 43, 52	0
1	E	530/546 (97%)	0.09	21 (3%) 38 40	14, 32, 54, 67	0
1	F	530/546 (97%)	-0.17	9 (1%) 70 71	7, 21, 42, 56	0
1	G	529/546 (96%)	-0.08	6 (1%) 80 82	11, 25, 40, 49	0
1	H	530/546 (97%)	0.28	27 (5%) 28 29	19, 35, 56, 70	0
All	All	4237/4368 (97%)	0.01	100 (2%) 59 61	7, 29, 48, 70	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	1	MET	6.6
1	G	529	ALA	5.6
1	B	251	SER	5.0
1	H	37	ALA	4.8
1	H	1	MET	4.7
1	A	3	ILE	3.5
1	B	10	SER	3.4
1	B	252	ALA	3.4
1	H	290	ALA	3.3
1	H	500	ALA	3.2
1	A	252	ALA	3.2
1	H	475	ALA	3.2
1	H	5	ASN	3.1
1	A	253	PHE	3.1
1	B	325	ALA	3.1
1	A	410	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	8	ASN	3.1
1	B	268	SER	3.0
1	F	7	GLU	3.0
1	A	1	MET	3.0
1	D	10	SER	3.0
1	C	1	MET	3.0
1	H	10	SER	2.9
1	D	25	GLY	2.8
1	C	240	ASP	2.8
1	B	224	PHE	2.8
1	D	268	SER	2.8
1	E	24	ALA	2.7
1	D	222	GLU	2.7
1	G	1	MET	2.7
1	A	10	SER	2.6
1	H	528	SER	2.6
1	D	529	ALA	2.6
1	E	26	ALA	2.6
1	E	239	ALA	2.6
1	E	410	GLU	2.6
1	H	253	PHE	2.5
1	F	251	SER	2.5
1	G	268	SER	2.5
1	E	498	ALA	2.5
1	B	222	GLU	2.5
1	A	222	GLU	2.5
1	H	498	ALA	2.5
1	E	268	SER	2.5
1	D	20	GLY	2.4
1	G	446	GLU	2.4
1	H	524	ASP	2.4
1	E	500	ALA	2.4
1	B	253	PHE	2.4
1	H	239	ALA	2.4
1	E	20	GLY	2.4
1	H	7	GLU	2.4
1	F	255	HIS	2.4
1	C	475	ALA	2.4
1	H	499	ASP	2.3
1	A	7	GLU	2.3
1	E	4	ASP	2.3
1	H	36	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	501	SER	2.3
1	B	151	ASP	2.3
1	H	267	LEU	2.3
1	A	435	GLU	2.3
1	E	5	ASN	2.3
1	B	498	ALA	2.3
1	H	25	GLY	2.2
1	E	222	GLU	2.2
1	E	7	GLU	2.2
1	E	36	PRO	2.2
1	G	240	ASP	2.2
1	H	219	VAL	2.2
1	A	528	SER	2.2
1	E	497	VAL	2.2
1	H	38	VAL	2.2
1	H	476	VAL	2.2
1	E	1	MET	2.2
1	E	326	GLU	2.2
1	E	526	ILE	2.1
1	H	256	THR	2.1
1	H	269	THR	2.1
1	B	11	ASP	2.1
1	H	497	VAL	2.1
1	H	527	ARG	2.1
1	B	22	GLY	2.1
1	H	270	GLY	2.1
1	B	36	PRO	2.1
1	F	219	VAL	2.1
1	F	475	ALA	2.1
1	B	240	ASP	2.1
1	B	455[A]	ASP	2.1
1	F	268	SER	2.1
1	H	295	GLU	2.1
1	C	7	GLU	2.1
1	B	203	ALA	2.1
1	F	500	ALA	2.1
1	H	29	ALA	2.1
1	E	38	VAL	2.1
1	B	7	GLU	2.1
1	E	529	ALA	2.0
1	G	222	GLU	2.0
1	F	326	GLU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

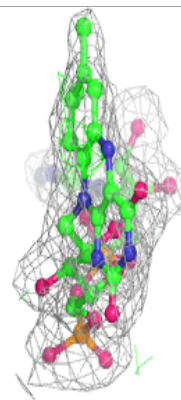
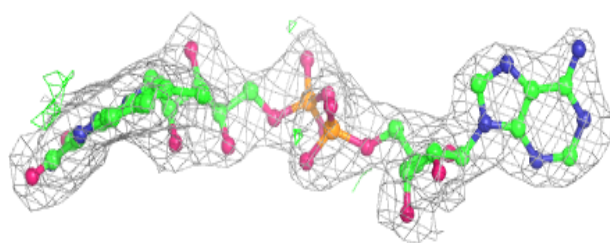
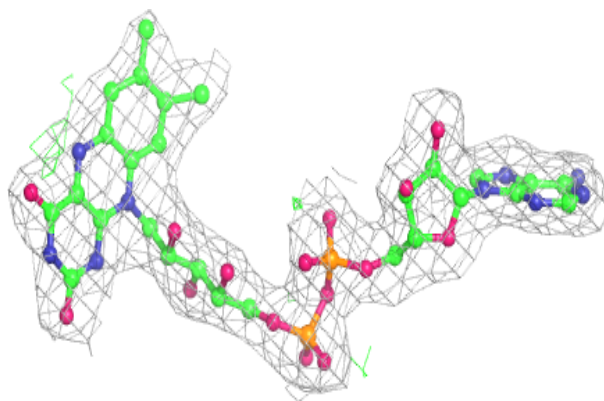
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ACT	H	601	4/4	0.83	1.11	23,24,24,25	4
3	ACT	F	601	4/4	0.85	0.73	3,3,3,3	4
3	ACT	C	601	4/4	0.89	0.92	18,18,18,19	4
3	ACT	D	601	4/4	0.89	0.68	3,3,3,3	4
3	ACT	A	601	4/4	0.90	0.70	18,18,18,18	4
2	FAD	A	547	53/53	0.94	0.17	16,25,28,29	0
3	ACT	B	601	4/4	0.94	0.81	4,4,4,4	4
3	ACT	E	601	4/4	0.94	0.66	8,9,9,9	4
3	ACT	G	601	4/4	0.95	0.99	19,19,20,20	4
2	FAD	D	547	53/53	0.95	0.17	13,21,26,27	0
2	FAD	H	547	53/53	0.95	0.20	16,28,41,41	0
2	FAD	B	547	53/53	0.95	0.21	14,22,29,31	0
2	FAD	G	547	53/53	0.96	0.15	8,15,20,22	0
2	FAD	E	547	53/53	0.96	0.17	17,22,31,33	0
2	FAD	F	547	53/53	0.96	0.18	5,15,19,20	0
2	FAD	C	547	53/53	0.97	0.15	8,15,22,24	0

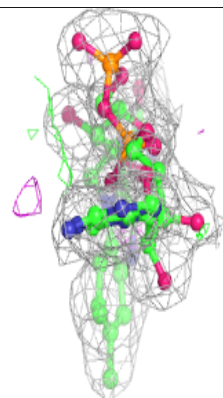
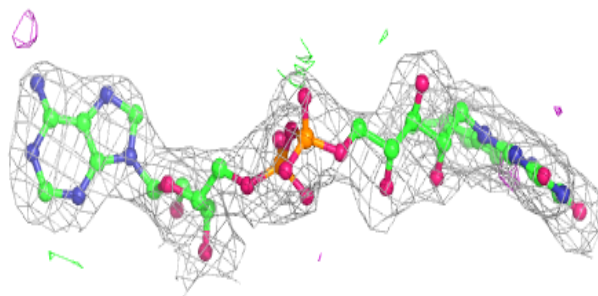
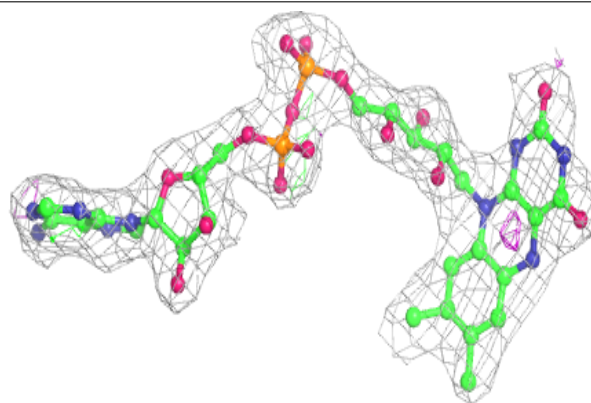
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around FAD A 547:**

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

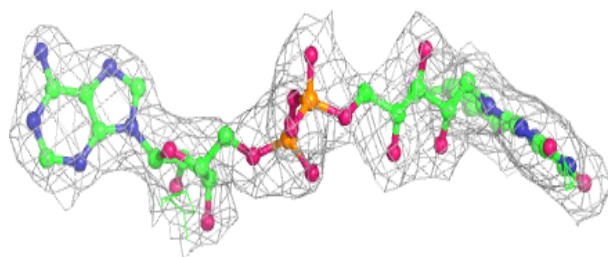
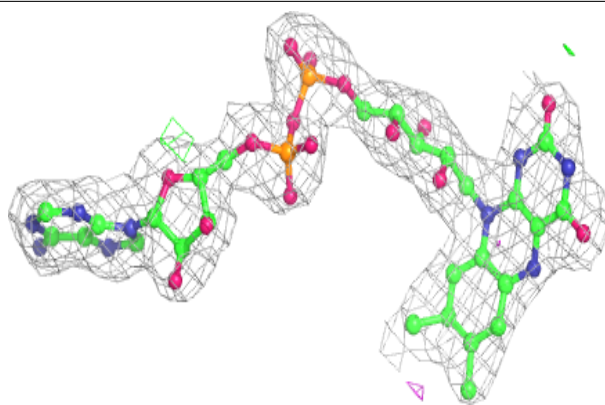
**Electron density around FAD D 547:**

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

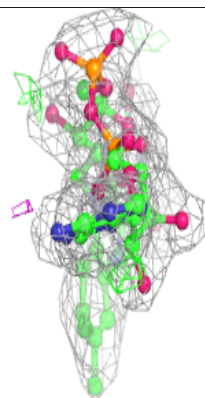
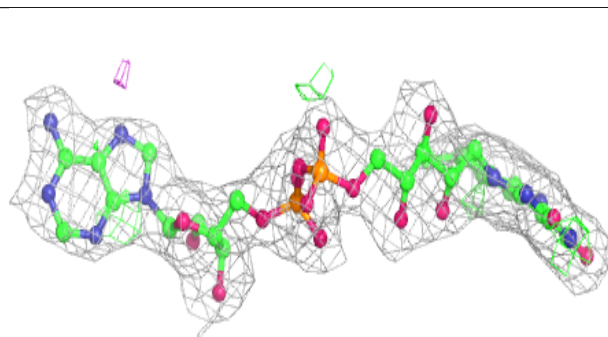
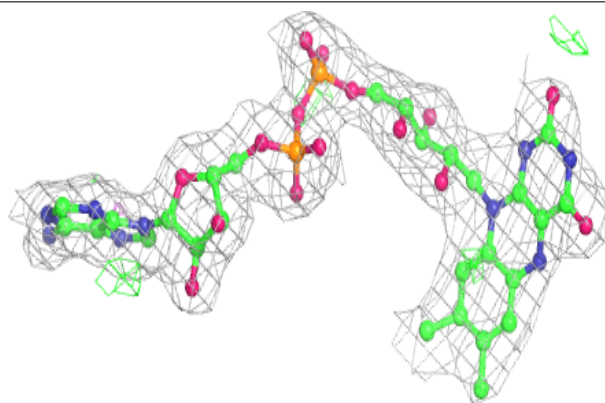


**Electron density around FAD H 547:**

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

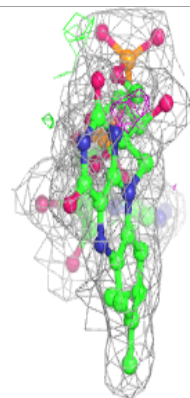
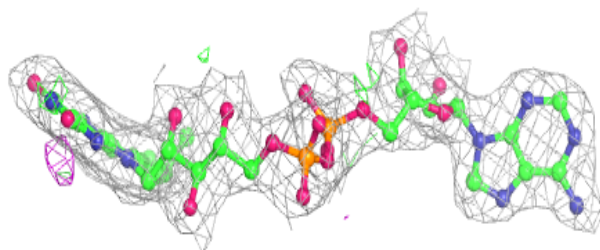
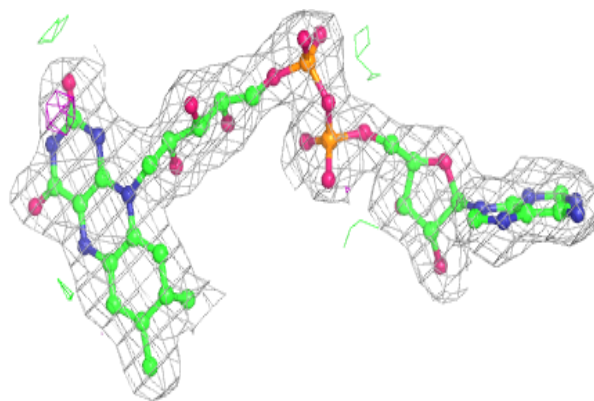
**Electron density around FAD B 547:**

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

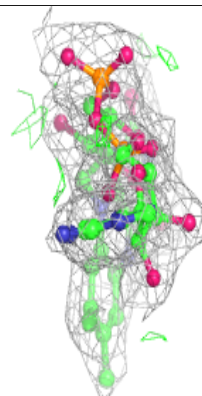
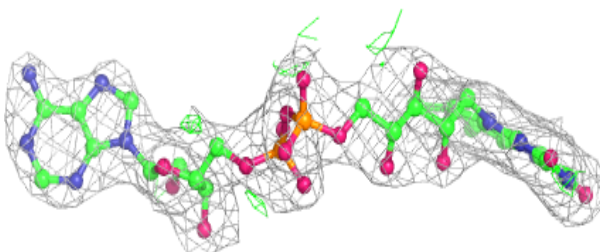
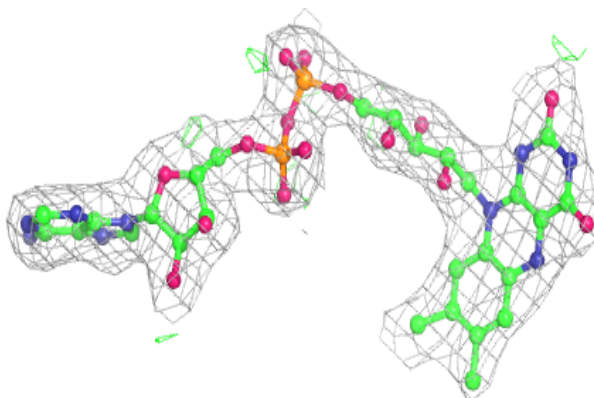


**Electron density around FAD G 547:**

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

**Electron density around FAD E 547:**

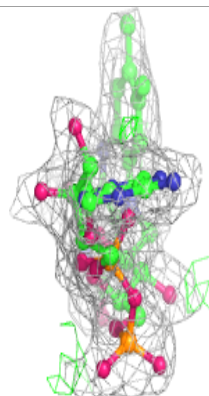
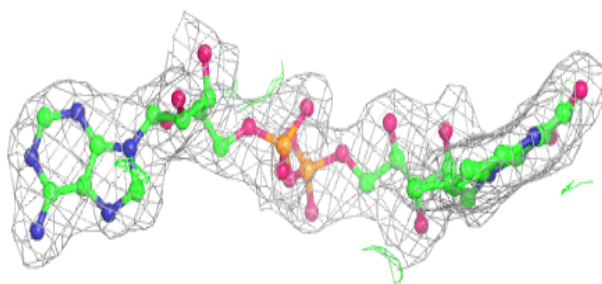
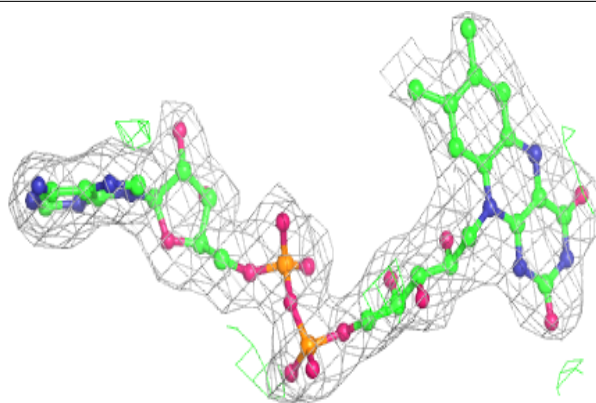
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



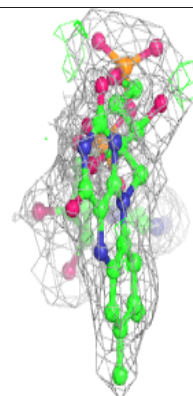
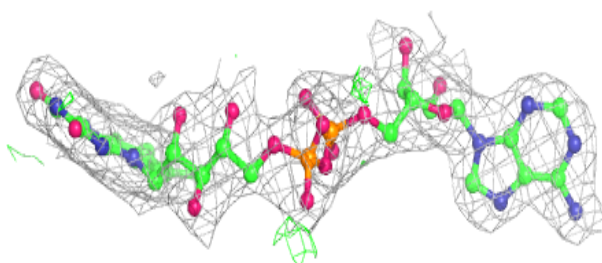
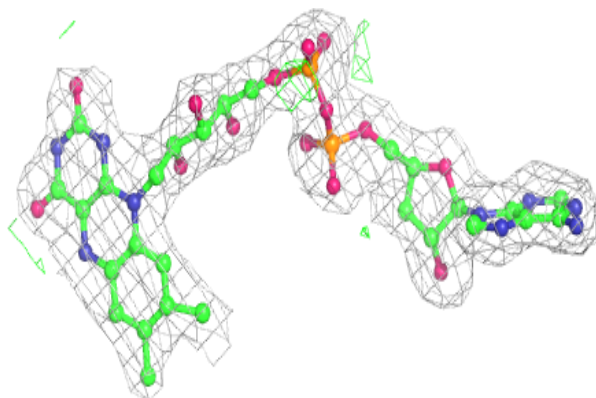


**Electron density around FAD F 547:**

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

**Electron density around FAD C 547:**

$2mF_o-DF_c$  (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.