



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:57 AM GMT

PDB ID : 3K4M
Title : Pyranose 2-oxidase Y456W mutant in complex with 2FG
Authors : Divne, C.; Tan, T.C.
Deposited on : 2009-10-05
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

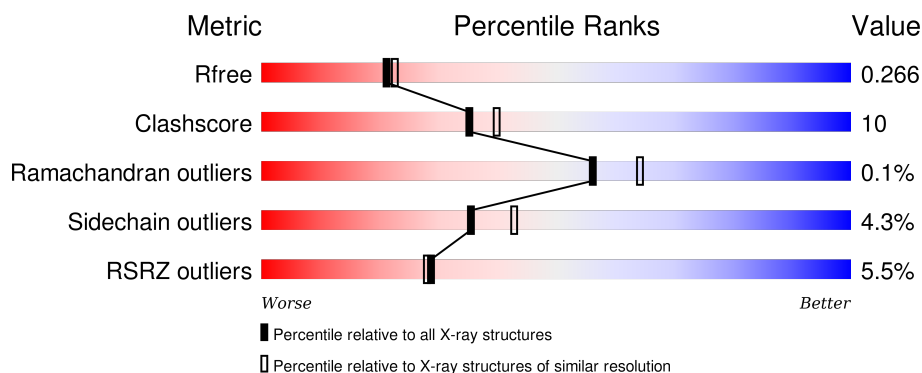
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	623	<div> <div>4%</div> <div>71% 19% 8%</div> </div>
1	B	623	<div> <div>4%</div> <div>75% 16% 7%</div> </div>
1	C	623	<div> <div>7%</div> <div>74% 17% 8%</div> </div>
1	D	623	<div> <div>6%</div> <div>75% 15% 8%</div> </div>
1	E	623	<div> <div>7%</div> <div>73% 18% 8%</div> </div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FAD	A	801	X	-	-	-
2	FAD	B	801	X	-	-	-
2	FAD	C	801	X	-	-	-
2	FAD	E	801	X	-	-	-
2	FAD	F	801	X	-	-	-
2	FAD	H	801	X	-	-	-
3	SHG	A	901	-	-	-	X
3	SHG	B	901	X	-	-	X
3	SHG	C	901	-	-	-	X
3	SHG	D	901	X	-	-	X
3	SHG	E	901	X	-	X	X
3	SHG	F	901	-	-	-	X
3	SHG	G	901	X	-	-	X
3	SHG	H	901	X	-	-	X
4	MES	B	902	-	-	X	X
4	MES	C	624	-	-	X	X
4	MES	C	902	-	-	X	X
4	MES	E	902	-	-	X	X
4	MES	H	624	-	-	X	X
4	MES	H	902	-	-	X	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 38766 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 2-oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	574	Total	C	N	O	S	0	0	0
			4528	2861	776	867	24			
1	B	577	Total	C	N	O	S	0	0	0
			4551	2874	779	873	25			
1	C	574	Total	C	N	O	S	0	0	0
			4527	2859	776	868	24			
1	D	574	Total	C	N	O	S	0	0	0
			4527	2859	776	868	24			
1	E	576	Total	C	N	O	S	0	0	0
			4544	2870	778	871	25			
1	F	573	Total	C	N	O	S	0	0	0
			4520	2855	775	866	24			
1	G	573	Total	C	N	O	S	0	0	0
			4520	2855	775	866	24			
1	H	573	Total	C	N	O	S	0	0	0
			4520	2855	775	866	24			

There are 8 discrepancies between the modelled and reference sequences:

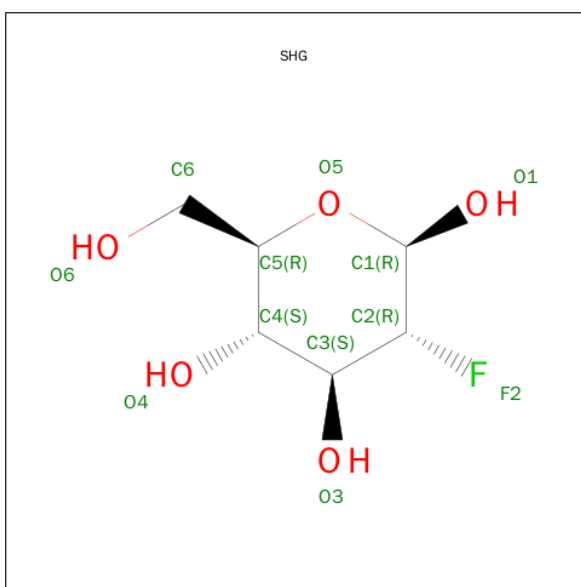
Chain	Residue	Modelled	Actual	Comment	Reference
A	456	TRP	TYR	ENGINEERED	UNP Q7ZA32
B	456	TRP	TYR	ENGINEERED	UNP Q7ZA32
C	456	TRP	TYR	ENGINEERED	UNP Q7ZA32
D	456	TRP	TYR	ENGINEERED	UNP Q7ZA32
E	456	TRP	TYR	ENGINEERED	UNP Q7ZA32
F	456	TRP	TYR	ENGINEERED	UNP Q7ZA32
G	456	TRP	TYR	ENGINEERED	UNP Q7ZA32
H	456	TRP	TYR	ENGINEERED	UNP Q7ZA32

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	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 SUGAR (2-DEOXY-2-FLUORO-BETA-D-GLUCOPYRANOSE) (three-letter code: SHG) (formula: C₆H₁₁FO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	F	O	0	0
			12	6	1	5		
3	B	1	Total	C	F	O	0	0
			12	6	1	5		
3	C	1	Total	C	F	O	0	0
			12	6	1	5		
3	D	1	Total	C	F	O	0	0
			12	6	1	5		
3	E	1	Total	C	F	O	0	0
			12	6	1	5		
3	F	1	Total	C	F	O	0	0
			12	6	1	5		
3	G	1	Total	C	F	O	0	0
			12	6	1	5		
3	H	1	Total	C	F	O	0	0
			12	6	1	5		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	303	Total	O	0	0
			303	303		
5	B	277	Total	O	0	0
			277	277		
5	C	191	Total	O	0	0
			191	191		
5	D	235	Total	O	0	0
			235	235		

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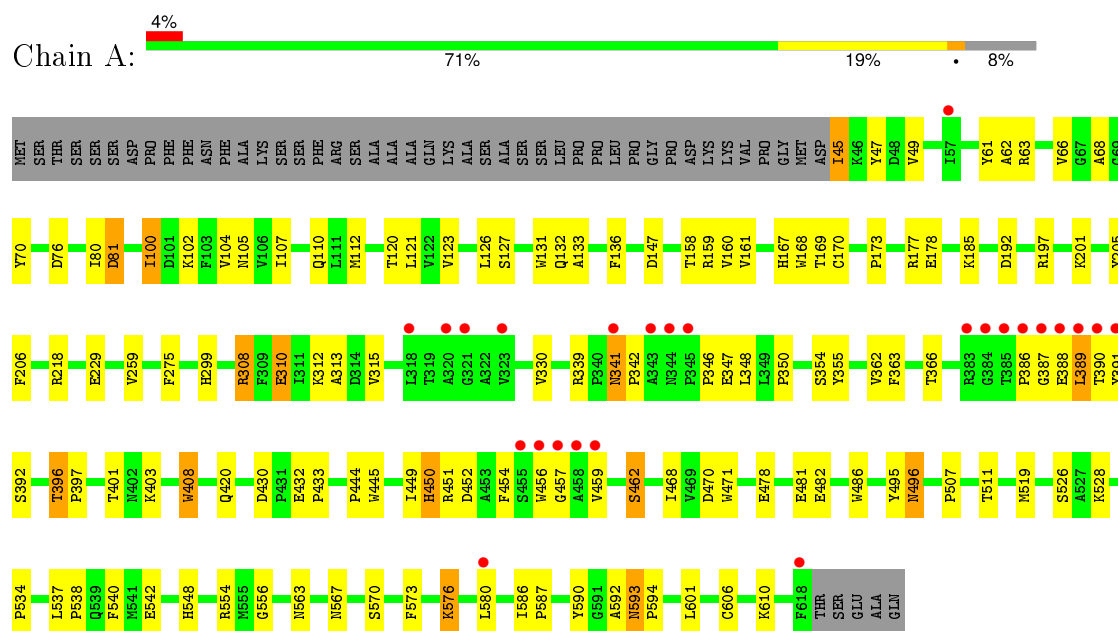
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	204	Total 204	O 204	0	0
5	F	199	Total 199	O 199	0	0
5	G	230	Total 230	O 230	0	0
5	H	274	Total 274	O 274	0	0

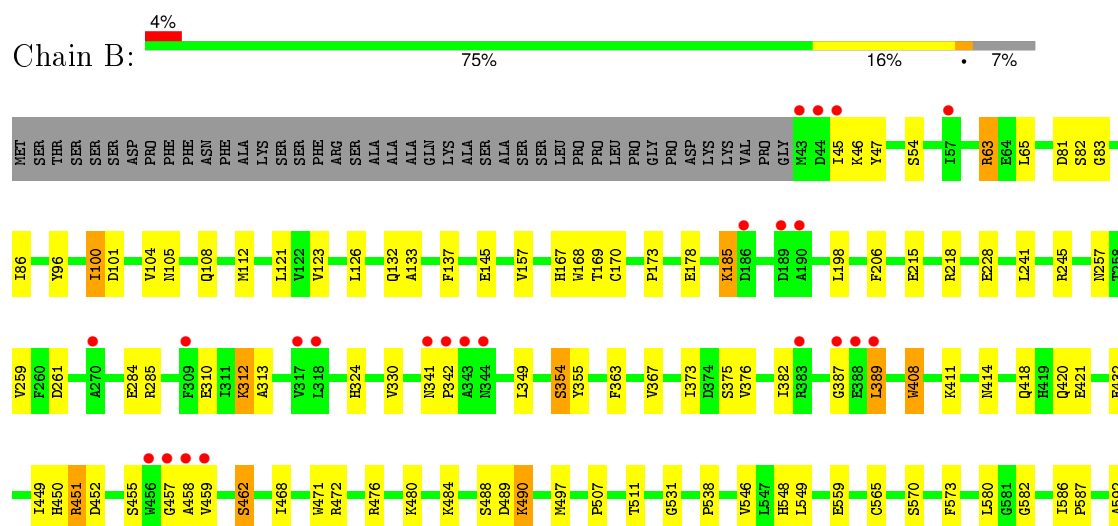
3 Residue-property plots

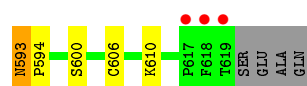
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 2-oxidase

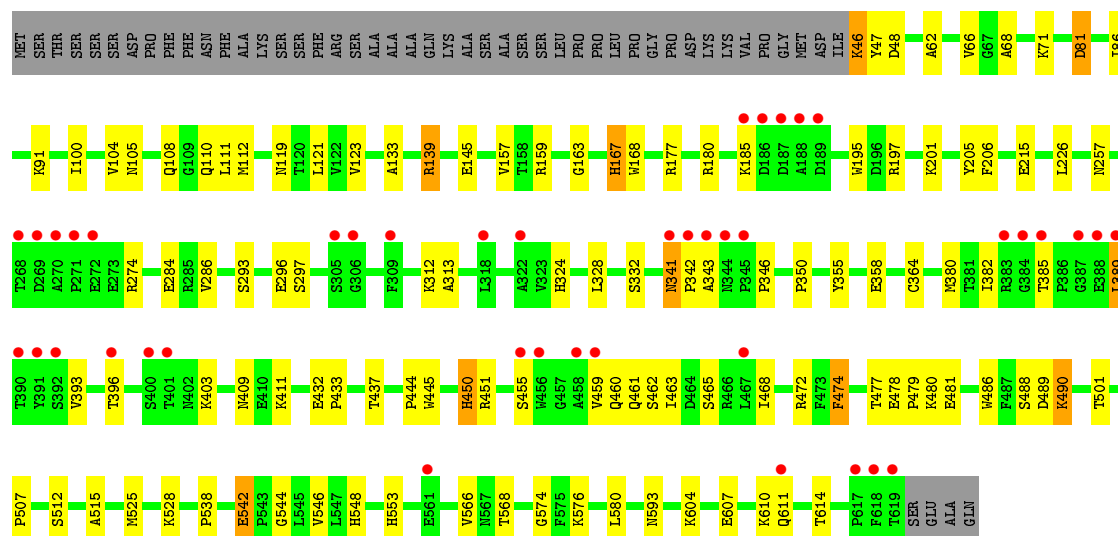
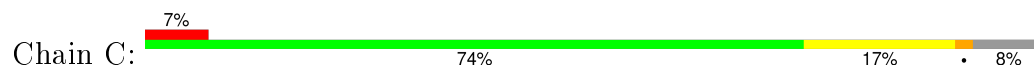


• Molecule 1: Pyranose 2-oxidase

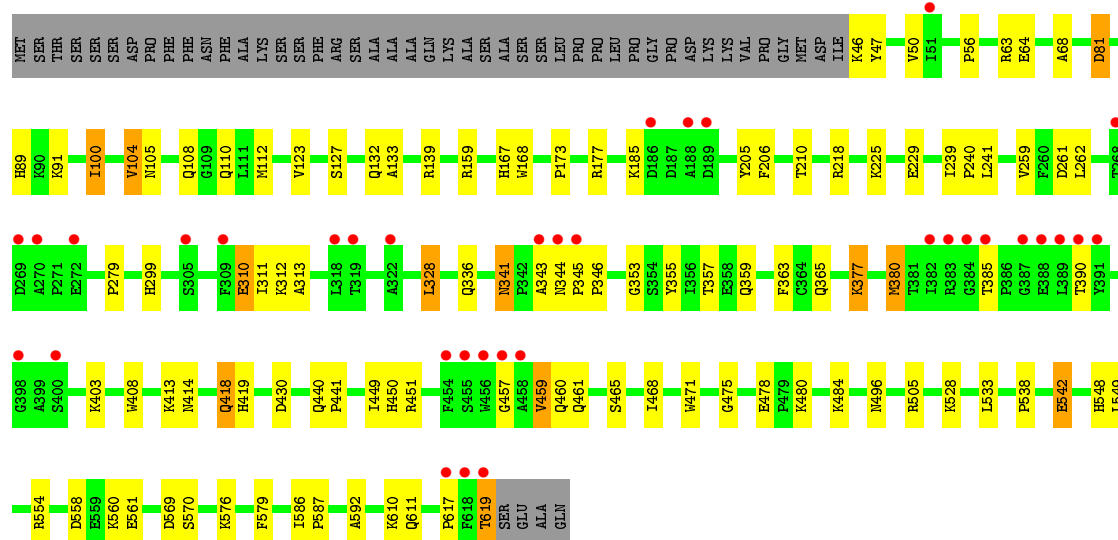
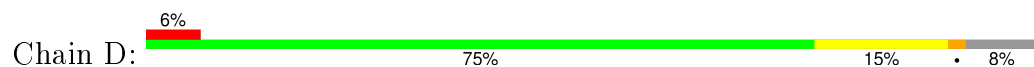




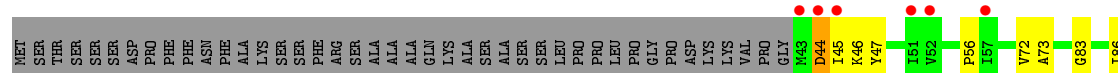
• Molecule 1: Pyranose 2-oxidase

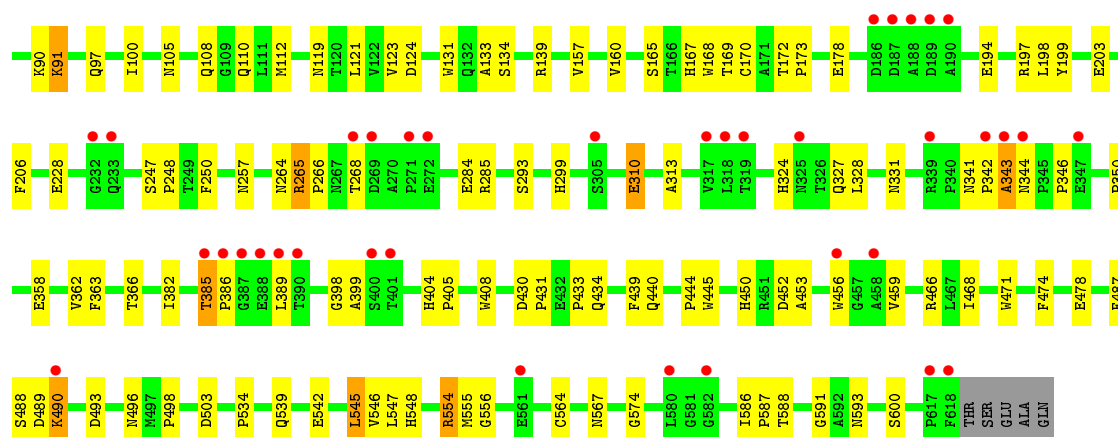


• Molecule 1: Pyranose 2-oxidase

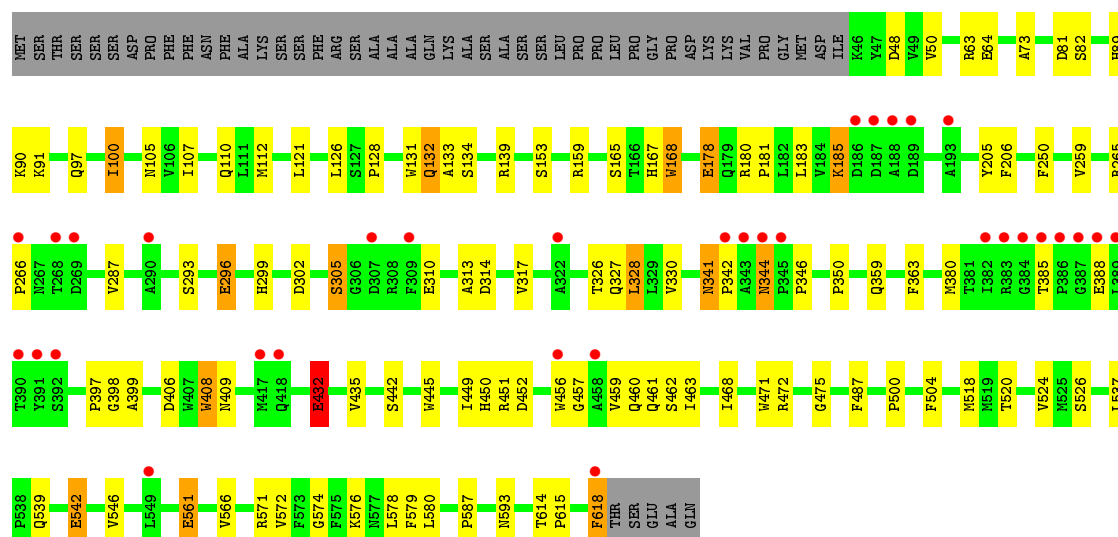
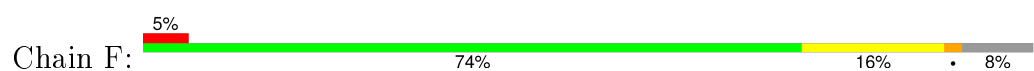


• Molecule 1: Pyranose 2-oxidase

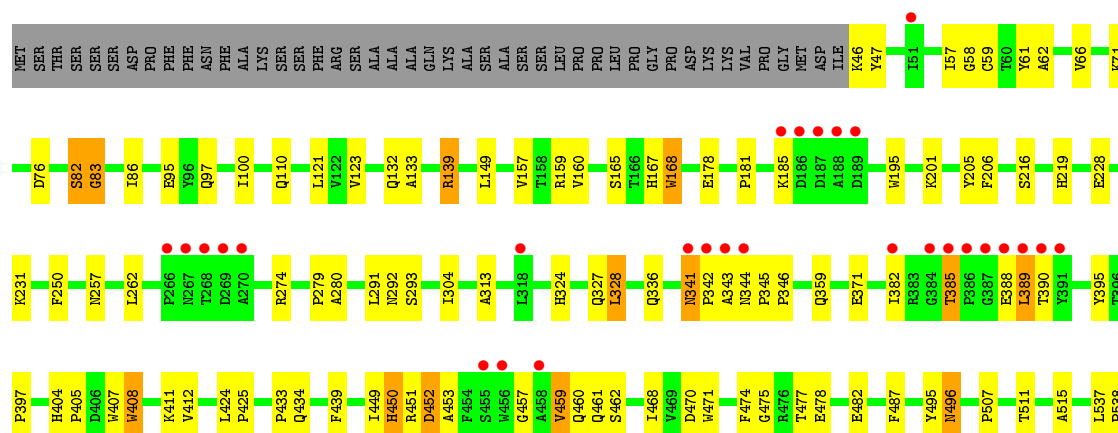


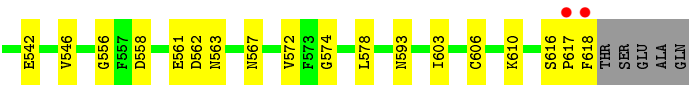


• Molecule 1: Pyranose 2-oxidase

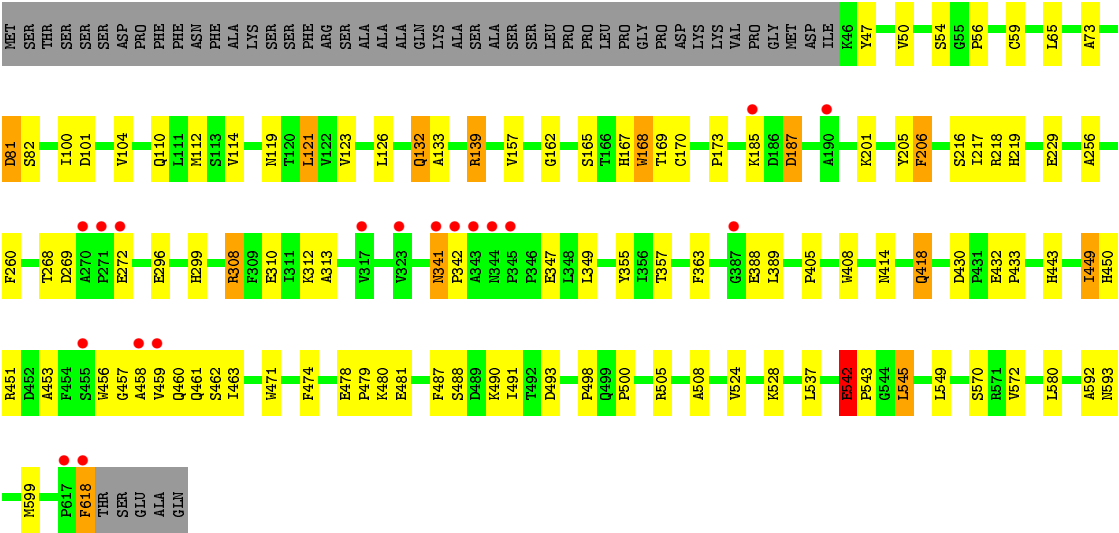
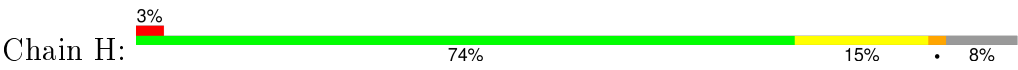


• Molecule 1: Pyranose 2-oxidase





● Molecule 1: Pyranose 2-oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	168.19Å 103.14Å 168.71Å 90.00° 106.47° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 29.98 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.4 (30.00-2.20) 97.4 (29.98-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.207 , 0.266 0.211 , 0.266	Depositor DCC
R_{free} test set	2798 reflections (1.04%)	DCC
Wilson B-factor (Å ²)	21.5	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 47.0	EDS
Estimated twinning fraction	0.022 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 273070 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	38766	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MES, FAD, SHG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.09	11/4645 (0.2%)	0.92	6/6317 (0.1%)
1	B	1.04	4/4668 (0.1%)	0.94	10/6348 (0.2%)
1	C	0.94	3/4644 (0.1%)	0.87	4/6316 (0.1%)
1	D	0.99	4/4644 (0.1%)	0.91	3/6316 (0.0%)
1	E	0.94	5/4661 (0.1%)	0.86	1/6338 (0.0%)
1	F	0.95	6/4637 (0.1%)	0.89	3/6306 (0.0%)
1	G	0.98	2/4637 (0.0%)	0.90	5/6306 (0.1%)
1	H	1.03	4/4637 (0.1%)	0.91	3/6306 (0.0%)
All	All	1.00	39/37173 (0.1%)	0.90	35/50553 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	H	0	1
All	All	0	2

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	432	GLU	CG-CD	8.23	1.64	1.51
1	D	478	GLU	CG-CD	7.61	1.63	1.51
1	E	542	GLU	CG-CD	7.35	1.62	1.51
1	A	481	GLU	CG-CD	7.33	1.62	1.51
1	D	310	GLU	CG-CD	7.32	1.62	1.51
1	D	310	GLU	CB-CG	7.14	1.65	1.52
1	H	508	ALA	CA-CB	7.04	1.67	1.52
1	F	561	GLU	CG-CD	7.00	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	310	GLU	CB-CG	6.98	1.65	1.52
1	F	561	GLU	CB-CG	6.83	1.65	1.52
1	A	482	GLU	CG-CD	6.60	1.61	1.51
1	C	312	LYS	CB-CG	6.50	1.70	1.52
1	G	482	GLU	CG-CD	6.50	1.61	1.51
1	C	542	GLU	CG-CD	6.34	1.61	1.51
1	F	432	GLU	CB-CG	6.17	1.63	1.52
1	E	310	GLU	CG-CD	6.03	1.60	1.51
1	E	478	GLU	CG-CD	6.01	1.60	1.51
1	C	364	CYS	CB-SG	-5.94	1.72	1.81
1	A	573	PHE	CE1-CZ	5.67	1.48	1.37
1	B	228	GLU	CG-CD	5.51	1.60	1.51
1	A	161	VAL	CB-CG1	-5.44	1.41	1.52
1	A	61	TYR	CE2-CZ	-5.39	1.31	1.38
1	A	275	PHE	CD1-CE1	-5.34	1.28	1.39
1	B	421	GLU	CB-CG	5.33	1.62	1.52
1	H	524	VAL	CB-CG1	5.31	1.64	1.52
1	A	178	GLU	CD-OE2	5.27	1.31	1.25
1	B	310	GLU	CB-CG	5.25	1.62	1.52
1	H	474	PHE	CE1-CZ	5.23	1.47	1.37
1	H	542	GLU	CG-CD	5.20	1.59	1.51
1	G	160	VAL	CB-CG1	5.19	1.63	1.52
1	A	310	GLU	CB-CG	5.17	1.61	1.52
1	A	478	GLU	CG-CD	5.17	1.59	1.51
1	A	486	TRP	CB-CG	5.16	1.59	1.50
1	B	108	GLN	CG-CD	5.15	1.62	1.51
1	E	108	GLN	CG-CD	5.15	1.62	1.51
1	F	178	GLU	CB-CG	-5.12	1.42	1.52
1	F	542	GLU	CG-CD	5.05	1.59	1.51
1	D	542	GLU	CG-CD	5.04	1.59	1.51
1	A	330	VAL	CB-CG1	-5.02	1.42	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	139	ARG	NE-CZ-NH2	-9.79	115.41	120.30
1	F	139	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	F	180	ARG	NE-CZ-NH1	-7.73	116.44	120.30
1	H	81	ASP	CB-CG-OD1	-7.07	111.94	118.30
1	G	139	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	G	83	GLY	N-CA-C	-6.60	96.60	113.10
1	G	452	ASP	CB-CG-OD1	-6.56	112.39	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	139	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	B	81	ASP	CB-CG-OD1	-6.12	112.79	118.30
1	B	82	SER	CB-CA-C	-5.84	99.00	110.10
1	D	81	ASP	CB-CG-OD1	-5.83	113.06	118.30
1	H	81	ASP	CB-CG-OD2	5.73	123.46	118.30
1	A	339	ARG	NE-CZ-NH2	5.72	123.16	120.30
1	D	139	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	C	489	ASP	CB-CG-OD1	5.67	123.41	118.30
1	B	63	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	D	104	VAL	CB-CA-C	-5.63	100.70	111.40
1	A	470	ASP	CB-CG-OD1	5.58	123.33	118.30
1	C	197	ARG	NE-CZ-NH2	5.54	123.07	120.30
1	A	81	ASP	CB-CG-OD1	-5.52	113.33	118.30
1	C	472	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	339	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	C	139	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	E	503	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	G	76	ASP	CB-CG-OD2	5.40	123.16	118.30
1	B	81	ASP	CB-CG-OD2	5.33	123.09	118.30
1	B	245	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	B	549	LEU	CA-CB-CG	5.23	127.34	115.30
1	A	147	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	63	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	B	245	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	B	472	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	B	451	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	A	76	ASP	CB-CG-OD1	5.01	122.81	118.30
1	F	472	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	449	ILE	Peptide
1	H	449	ILE	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	4528	0	4376	91	0
1	B	4551	0	4396	82	0
1	C	4527	0	4372	93	0
1	D	4527	0	4372	73	0
1	E	4544	0	4389	105	0
1	F	4520	0	4365	86	0
1	G	4520	0	4365	98	0
1	H	4520	0	4365	97	0
2	A	53	0	28	2	0
2	B	53	0	29	5	0
2	C	53	0	26	5	0
2	D	53	0	27	6	0
2	E	53	0	27	9	0
2	F	53	0	26	1	0
2	G	53	0	27	3	0
2	H	53	0	26	3	0
3	A	12	0	10	2	0
3	B	12	0	10	3	0
3	C	12	0	11	5	0
3	D	12	0	9	4	0
3	E	12	0	10	6	0
3	F	12	0	11	1	0
3	G	12	0	10	3	0
3	H	12	0	10	1	0
4	A	12	0	12	4	0
4	B	12	0	12	7	0
4	C	24	0	24	21	0
4	E	12	0	12	12	0
4	F	12	0	12	1	0
4	H	24	0	24	23	0
5	A	303	0	0	9	0
5	B	277	0	0	10	0
5	C	191	0	0	2	0
5	D	235	0	0	6	0
5	E	204	0	0	4	0
5	F	199	0	0	2	0
5	G	230	0	0	6	0
5	H	274	0	0	12	0
All	All	38766	0	35393	708	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 10.

All (708) 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:167:HIS:HE2	2:B:801:FAD:C8M	1.09	1.59
1:B:167:HIS:NE2	2:B:801:FAD:HM82	1.06	1.38
1:C:133:ALA:CB	4:C:902:MES:H71	1.58	1.32
1:E:490:LYS:NZ	1:E:490:LYS:HB3	1.50	1.16
1:G:82:SER:HB2	1:G:83:GLY:CA	1.70	1.16
1:B:167:HIS:CD2	2:B:801:FAD:HM82	1.84	1.13
1:G:82:SER:C	1:H:81:ASP:HA	1.67	1.13
1:C:133:ALA:HB2	4:C:902:MES:O1S	1.50	1.07
1:C:133:ALA:HB2	4:C:902:MES:H71	1.32	1.07
1:G:82:SER:HB2	1:G:83:GLY:HA3	1.07	1.07
1:E:167:HIS:NE2	2:E:801:FAD:HM81	1.70	1.06
1:G:133:ALA:HB3	4:H:902:MES:H71	1.35	1.06
1:G:82:SER:CB	1:G:83:GLY:HA3	1.88	1.02
1:C:133:ALA:HB3	4:C:902:MES:H71	1.36	1.01
1:G:82:SER:O	1:H:81:ASP:HA	1.60	1.01
1:G:133:ALA:CB	4:H:902:MES:H71	1.92	1.00
1:B:133:ALA:HB2	4:B:902:MES:H71	1.44	0.97
1:A:110:GLN:HE21	1:A:167:HIS:HD1	1.08	0.97
1:G:389:LEU:H	1:G:389:LEU:HD13	1.27	0.96
1:B:167:HIS:HE2	2:B:801:FAD:HM81	1.27	0.95
1:H:308:ARG:CG	1:H:308:ARG:HH11	1.80	0.94
1:E:490:LYS:HZ3	1:E:490:LYS:HB3	1.12	0.94
1:G:201:LYS:HE2	1:G:205:TYR:OH	1.66	0.94
1:B:133:ALA:CB	4:B:902:MES:H71	1.98	0.93
1:C:201:LYS:HE2	1:C:205:TYR:OH	1.70	0.91
1:B:101:ASP:HB2	5:B:2756:HOH:O	1.71	0.90
1:D:468:ILE:HD13	1:D:533:LEU:HD22	1.55	0.88
1:F:302:ASP:OD2	1:F:305:SER:HB3	1.74	0.87
1:D:110:GLN:HE21	1:D:167:HIS:HD1	1.22	0.86
1:H:308:ARG:HG3	1:H:308:ARG:HH11	1.38	0.86
1:H:490:LYS:HB3	5:H:2805:HOH:O	1.76	0.85
1:E:90:LYS:NZ	1:E:110:GLN:OE1	2.10	0.83
1:A:308:ARG:HH11	1:A:308:ARG:HG3	1.43	0.82
1:G:110:GLN:HE21	1:G:167:HIS:HD1	1.28	0.80
2:D:801:FAD:N5	3:D:901:SHG:H3	1.96	0.80
1:G:123:VAL:H	4:H:902:MES:H62	1.45	0.79
1:H:133:ALA:HB3	4:H:624:MES:H71	1.62	0.79
1:D:104:VAL:HG12	1:D:108:GLN:NE2	1.97	0.79
1:B:414:ASN:O	1:B:418:GLN:HG3	1.81	0.79
1:E:131:TRP:HZ3	4:E:902:MES:O3S	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:902:MES:O1S	4:H:902:MES:H32	1.84	0.78
1:F:542:GLU:HG3	5:G:2703:HOH:O	1.82	0.78
1:G:459:VAL:HG22	1:H:123:VAL:HG22	1.66	0.78
1:E:490:LYS:CB	1:E:490:LYS:NZ	2.39	0.78
1:E:341:ASN:HD22	1:E:342:PRO:HD2	1.46	0.78
1:H:545:LEU:O	1:H:545:LEU:HD12	1.82	0.78
1:E:110:GLN:HE21	1:E:167:HIS:HD1	1.33	0.77
1:B:185:LYS:HZ2	1:B:185:LYS:HB3	1.49	0.77
4:C:624:MES:H71	1:D:133:ALA:CB	2.14	0.77
1:G:133:ALA:HB2	4:H:902:MES:O1S	1.85	0.76
1:C:133:ALA:HB3	4:C:902:MES:C7	2.15	0.76
1:G:478:GLU:HG2	1:G:511:THR:OG1	1.84	0.76
1:B:185:LYS:NZ	1:B:185:LYS:CB	2.48	0.76
1:F:457:GLY:H	1:F:460:GLN:HE21	1.33	0.76
1:D:377:LYS:HE2	5:D:1992:HOH:O	1.85	0.76
1:G:342:PRO:O	1:G:345:PRO:HD3	1.84	0.76
1:G:389:LEU:H	1:G:389:LEU:CD1	1.99	0.76
1:A:123:VAL:HG22	1:B:459:VAL:HG12	1.65	0.76
1:E:121:LEU:O	4:E:902:MES:H61	1.86	0.75
1:H:110:GLN:HE21	1:H:167:HIS:HD1	1.35	0.75
1:F:328:LEU:HD12	1:F:328:LEU:O	1.87	0.74
2:H:801:FAD:H8A	5:H:1886:HOH:O	1.85	0.74
1:H:133:ALA:HB2	4:H:624:MES:O1S	1.87	0.74
1:E:459:VAL:HG22	1:F:121:LEU:HD22	1.68	0.74
1:E:167:HIS:CE1	2:E:801:FAD:C8M	2.68	0.74
1:G:459:VAL:HG23	1:H:121:LEU:HD22	1.67	0.74
1:D:341:ASN:HD22	1:D:343:ALA:H	1.36	0.74
1:G:82:SER:O	1:H:81:ASP:CA	2.36	0.74
1:E:385:THR:HG22	1:E:386:PRO:HD2	1.69	0.74
1:G:542:GLU:HG2	5:G:1501:HOH:O	1.87	0.74
1:A:63:ARG:HD2	1:A:259:VAL:O	1.89	0.73
1:B:185:LYS:HB3	1:B:185:LYS:NZ	2.04	0.73
1:E:459:VAL:HG22	1:F:121:LEU:CD2	2.18	0.73
1:A:299:HIS:NE2	1:A:308:ARG:HD3	2.04	0.72
1:F:100:ILE:HG12	1:F:100:ILE:O	1.88	0.71
1:E:490:LYS:HZ2	1:E:490:LYS:HB3	1.50	0.71
1:E:167:HIS:CD2	2:E:801:FAD:C8M	2.69	0.71
1:B:47:TYR:O	1:B:313:ALA:HA	1.92	0.70
1:H:443:HIS:HD2	5:H:2462:HOH:O	1.75	0.70
4:E:902:MES:H52	1:F:462:SER:OG	1.92	0.70
1:C:139:ARG:HD3	4:C:902:MES:H81	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:229:GLU:HG3	1:H:528:LYS:HD3	1.73	0.69
1:C:110:GLN:HE21	1:C:167:HIS:HD1	1.39	0.69
1:F:178:GLU:HG3	5:F:2087:HOH:O	1.91	0.69
1:H:443:HIS:HE1	5:H:1574:HOH:O	1.76	0.69
1:E:545:LEU:HD12	1:E:545:LEU:O	1.92	0.69
4:C:624:MES:H71	1:D:133:ALA:HB3	1.74	0.69
1:F:128:PRO:HG2	1:G:515:ALA:CB	2.22	0.69
1:F:110:GLN:HE21	1:F:167:HIS:HD1	1.41	0.69
1:F:50:VAL:HG12	1:F:73:ALA:HB3	1.75	0.68
4:E:902:MES:C5	1:F:462:SER:OG	2.42	0.68
1:H:505:ARG:NH1	5:H:2159:HOH:O	2.26	0.68
1:A:495:TYR:O	1:A:496:ASN:HB2	1.93	0.67
1:A:110:GLN:NE2	1:A:167:HIS:HD1	1.88	0.67
1:E:293:SER:HA	1:E:574:GLY:O	1.95	0.67
1:B:104:VAL:HG11	1:B:455:SER:HB3	1.77	0.67
1:H:218:ARG:HD2	5:H:1490:HOH:O	1.94	0.66
1:F:131:TRP:CH2	1:F:133:ALA:HB2	2.29	0.66
1:E:167:HIS:NE2	2:E:801:FAD:C8	2.55	0.66
2:H:801:FAD:N5	3:H:901:SHG:H3	2.11	0.66
1:H:133:ALA:CB	4:H:624:MES:H71	2.25	0.66
1:D:299:HIS:HB2	1:D:310:GLU:OE1	1.95	0.66
1:B:126:LEU:HD12	1:B:132:GLN:HG3	1.78	0.66
1:E:139:ARG:HD3	4:E:902:MES:O1S	1.97	0.65
1:C:389:LEU:H	1:C:389:LEU:HD22	1.61	0.65
1:D:279:PRO:HG2	5:D:2891:HOH:O	1.96	0.65
1:H:490:LYS:HD2	5:H:2805:HOH:O	1.95	0.65
1:G:82:SER:O	1:H:82:SER:N	2.29	0.64
1:F:296:GLU:HA	1:F:296:GLU:OE1	1.98	0.64
1:H:490:LYS:HD3	1:H:491:ILE:HD13	1.80	0.64
1:D:341:ASN:ND2	1:D:343:ALA:H	1.95	0.64
1:G:46:LYS:O	1:G:71:LYS:NZ	2.28	0.64
1:F:302:ASP:OD2	1:F:305:SER:CB	2.45	0.64
1:A:121:LEU:HD13	1:B:459:VAL:HG22	1.80	0.64
1:B:341:ASN:HD22	1:B:342:PRO:HD2	1.61	0.64
1:G:449:ILE:HG12	1:G:471:TRP:CZ3	2.32	0.64
1:E:133:ALA:CB	4:E:902:MES:H71	2.27	0.63
1:F:287:VAL:CG2	1:F:299:HIS:CD2	2.82	0.63
2:G:801:FAD:N5	3:G:901:SHG:H3	2.14	0.63
1:B:349:LEU:HD13	1:B:565:CYS:HB3	1.80	0.63
1:D:104:VAL:HG12	1:D:108:GLN:HE21	1.61	0.63
1:A:68:ALA:HB2	1:A:610:LYS:HE2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:47:TYR:CD2	1:H:73:ALA:HB2	2.33	0.62
1:H:405:PRO:HD3	5:H:2123:HOH:O	1.98	0.62
1:D:104:VAL:CG1	1:D:108:GLN:NE2	2.61	0.62
1:H:414:ASN:O	1:H:418:GLN:HB2	1.99	0.62
1:F:63:ARG:HD2	1:F:259:VAL:O	1.99	0.62
1:H:618:PHE:C	1:H:618:PHE:HD1	2.03	0.62
1:H:119:ASN:O	1:H:139:ARG:NH2	2.31	0.62
1:B:133:ALA:HB2	4:B:902:MES:O1S	1.99	0.61
1:C:382:ILE:HG12	1:C:393:VAL:HG22	1.81	0.61
1:E:97:GLN:HG3	1:E:250:PHE:CE2	2.35	0.61
1:F:328:LEU:HD12	1:F:328:LEU:C	2.20	0.61
1:H:355:TYR:CZ	1:H:481:GLU:HB2	2.34	0.61
1:E:452:ASP:O	1:E:453:ALA:C	2.39	0.61
1:G:457:GLY:O	1:G:461:GLN:HG3	2.00	0.61
1:A:576:LYS:NZ	5:A:2827:HOH:O	2.23	0.61
1:A:308:ARG:HH11	1:A:308:ARG:CG	2.14	0.61
1:G:328:LEU:HD12	1:G:328:LEU:O	2.01	0.61
1:C:444:PRO:HD2	1:C:445:TRP:CZ3	2.35	0.61
1:F:82:SER:HB3	1:F:90:LYS:HG2	1.83	0.60
1:H:618:PHE:C	1:H:618:PHE:CD1	2.72	0.60
1:H:478:GLU:HG3	1:H:480:LYS:HE3	1.83	0.60
1:E:548:HIS:NE2	3:E:901:SHG:O3	2.34	0.60
1:C:296:GLU:O	1:C:297:SER:HB3	2.00	0.60
1:H:216:SER:HB3	1:H:219:HIS:HB3	1.82	0.60
1:E:47:TYR:O	1:E:313:ALA:HA	2.01	0.60
1:B:389:LEU:HD12	1:B:389:LEU:H	1.65	0.60
1:H:299:HIS:ND1	1:H:310:GLU:OE1	2.34	0.60
1:F:287:VAL:HG23	1:F:299:HIS:HD2	1.66	0.60
1:A:218:ARG:HD2	5:A:1616:HOH:O	2.02	0.60
1:H:542:GLU:HG2	1:H:545:LEU:HB2	1.83	0.60
1:D:380:MET:HE1	1:D:413:LYS:HB2	1.84	0.60
1:E:342:PRO:O	1:E:344:ASN:N	2.35	0.59
1:F:299:HIS:CE1	1:F:310:GLU:HB2	2.37	0.59
1:F:326:THR:O	1:F:330:VAL:HG23	2.03	0.59
1:C:133:ALA:HB2	4:C:902:MES:C7	2.22	0.59
1:H:299:HIS:NE2	1:H:308:ARG:HD2	2.18	0.59
1:D:110:GLN:NE2	1:D:167:HIS:HD1	1.96	0.59
4:C:624:MES:O3S	1:D:133:ALA:HB2	2.03	0.59
1:H:47:TYR:O	1:H:313:ALA:HA	2.03	0.59
1:F:293:SER:HA	1:F:574:GLY:O	2.03	0.58
1:D:56:PRO:HD2	2:D:801:FAD:O1P	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LEU:HD13	1:A:132:GLN:HG2	1.85	0.58
1:G:133:ALA:CB	4:H:902:MES:C7	2.77	0.58
1:G:449:ILE:HG12	1:G:471:TRP:CE3	2.38	0.58
1:A:606:CYS:O	1:A:610:LYS:HG3	2.04	0.58
1:A:537:LEU:HB3	1:A:538:PRO:HD2	1.84	0.58
1:H:457:GLY:H	1:H:460:GLN:HE21	1.51	0.58
2:E:801:FAD:N5	3:E:901:SHG:H3	2.17	0.58
1:E:299:HIS:HB2	1:E:310:GLU:OE2	2.04	0.58
1:A:132:GLN:OE1	4:A:902:MES:H31	2.03	0.58
1:C:341:ASN:ND2	1:C:343:ALA:H	2.01	0.58
1:C:463:ILE:HA	4:C:624:MES:O1S	2.03	0.58
1:H:487:PHE:CE1	1:H:500:PRO:HB3	2.39	0.58
1:E:167:HIS:CE1	2:E:801:FAD:HM81	2.36	0.58
1:H:272:GLU:HA	1:H:618:PHE:HE2	1.68	0.57
1:F:181:PRO:HG3	1:F:587:PRO:HD2	1.86	0.57
1:E:131:TRP:CZ3	4:E:902:MES:O3S	2.53	0.57
1:D:341:ASN:HD22	1:D:341:ASN:C	2.07	0.57
2:E:801:FAD:C4X	3:E:901:SHG:H3	2.34	0.57
1:A:570:SER:HB3	1:A:580:LEU:O	2.04	0.57
1:E:169:THR:O	1:E:170:CYS:HB2	2.02	0.57
1:H:308:ARG:HG2	1:H:308:ARG:HH11	1.68	0.57
1:B:538:PRO:HG2	1:D:538:PRO:HD2	1.87	0.57
1:F:542:GLU:CB	5:G:2703:HOH:O	2.51	0.57
1:A:457:GLY:HA3	5:A:2242:HOH:O	2.05	0.57
1:D:449:ILE:HG12	1:D:471:TRP:CZ3	2.39	0.57
1:C:451:ARG:HD3	1:C:468:ILE:O	2.05	0.57
1:G:495:TYR:O	1:G:496:ASN:HB2	2.04	0.57
1:G:452:ASP:O	1:G:453:ALA:C	2.43	0.57
1:B:173:PRO:HG2	1:B:592:ALA:HB1	1.86	0.56
1:H:299:HIS:NE2	1:H:308:ARG:CD	2.67	0.56
1:C:380:MET:HE1	1:C:409:ASN:HA	1.87	0.56
1:C:546:VAL:HA	3:C:901:SHG:H6A	1.88	0.56
1:C:177:ARG:HB2	5:C:2187:HOH:O	2.05	0.56
1:E:548:HIS:CE1	3:E:901:SHG:O3	2.58	0.56
1:H:490:LYS:HD3	1:H:491:ILE:CD1	2.34	0.56
4:C:624:MES:H71	1:D:133:ALA:HB2	1.83	0.56
1:B:452:ASP:HA	5:B:2597:HOH:O	2.04	0.56
1:F:296:GLU:OE1	1:F:296:GLU:CA	2.54	0.56
1:F:50:VAL:HG13	1:F:313:ALA:HB2	1.88	0.56
1:B:355:TYR:HA	1:B:480:LYS:O	2.06	0.56
1:D:357:THR:O	1:D:549:LEU:HD12	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:97:GLN:HG3	1:G:250:PHE:CE2	2.40	0.56
1:C:512:SER:O	1:C:515:ALA:HB3	2.05	0.56
1:H:463:ILE:HA	4:H:902:MES:O3S	2.05	0.56
1:D:341:ASN:HD21	1:D:343:ALA:HB3	1.71	0.56
1:E:100:ILE:HD11	5:E:2751:HOH:O	2.05	0.55
1:F:456:TRP:HH2	1:F:468:ILE:HG21	1.69	0.55
1:F:97:GLN:HG3	1:F:250:PHE:CD2	2.41	0.55
1:B:354:SER:OG	1:B:484:LYS:NZ	2.39	0.55
1:F:566:VAL:CG1	1:F:580:LEU:HD12	2.36	0.55
1:A:408:TRP:C	1:A:408:TRP:CD1	2.80	0.55
1:E:493:ASP:C	1:E:493:ASP:OD1	2.45	0.55
1:C:462:SER:O	4:C:624:MES:H81	2.05	0.55
1:G:408:TRP:O	1:G:412:VAL:HG23	2.06	0.55
1:G:157:VAL:HG21	1:G:324:HIS:HE1	1.72	0.55
1:H:308:ARG:CG	1:H:308:ARG:NH1	2.52	0.55
4:C:902:MES:O3S	4:C:902:MES:H31	2.07	0.55
1:F:287:VAL:HG23	1:F:299:HIS:CD2	2.40	0.55
1:E:160:VAL:HG11	5:E:2035:HOH:O	2.06	0.55
1:A:131:TRP:CH2	1:A:133:ALA:HB2	2.41	0.55
1:E:554:ARG:O	1:E:564:CYS:HB2	2.07	0.55
1:H:201:LYS:HE2	1:H:205:TYR:OH	2.07	0.55
1:A:495:TYR:O	1:A:496:ASN:CB	2.55	0.54
1:B:157:VAL:HG21	1:B:324:HIS:HE1	1.72	0.54
1:G:123:VAL:H	4:H:902:MES:C6	2.19	0.54
1:H:104:VAL:HG23	1:H:453:ALA:HB1	1.87	0.54
1:A:126:LEU:CD1	1:A:132:GLN:CG	2.86	0.54
1:H:341:ASN:C	1:H:341:ASN:HD22	2.10	0.54
1:C:437:THR:HG23	1:C:437:THR:O	2.06	0.54
1:E:265:ARG:HA	1:E:266:PRO:C	2.28	0.54
1:D:414:ASN:O	1:D:418:GLN:HB2	2.08	0.54
1:E:328:LEU:HD23	1:E:328:LEU:C	2.28	0.54
1:H:457:GLY:H	1:H:460:GLN:NE2	2.04	0.54
1:B:489:ASP:OD1	1:B:490:LYS:HD2	2.08	0.54
4:H:902:MES:C3	4:H:902:MES:O1S	2.53	0.54
1:H:341:ASN:ND2	1:H:341:ASN:C	2.56	0.54
1:D:47:TYR:O	1:D:313:ALA:HA	2.07	0.54
1:B:363:PHE:HA	1:B:471:TRP:O	2.08	0.54
1:H:173:PRO:HG2	1:H:592:ALA:HB1	1.90	0.54
1:H:462:SER:O	4:H:902:MES:O3S	2.26	0.53
1:F:542:GLU:HB2	5:G:2703:HOH:O	2.08	0.53
1:D:457:GLY:H	1:D:460:GLN:HE21	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:ASP:CB	5:B:2756:HOH:O	2.42	0.53
1:G:462:SER:O	4:H:624:MES:H81	2.08	0.53
1:A:132:GLN:OE1	4:A:902:MES:C3	2.56	0.53
1:C:474:PHE:CD1	1:C:474:PHE:N	2.77	0.53
1:E:341:ASN:HD22	1:E:342:PRO:CD	2.16	0.53
1:A:123:VAL:CG2	1:B:459:VAL:HG12	2.38	0.53
1:E:328:LEU:HD23	1:E:328:LEU:O	2.08	0.53
1:E:157:VAL:HG21	1:E:324:HIS:HE1	1.73	0.53
1:G:606:CYS:O	1:G:610:LYS:HG3	2.09	0.53
1:C:159:ARG:HA	2:C:801:FAD:O2B	2.09	0.53
1:A:177:ARG:NH2	1:A:192:ASP:OD2	2.42	0.53
1:E:440:GLN:HA	1:E:440:GLN:OE1	2.09	0.53
1:E:119:ASN:HD21	1:E:121:LEU:HD12	1.72	0.53
1:A:100:ILE:HD13	1:A:100:ILE:O	2.09	0.53
1:A:548:HIS:NE2	3:A:901:SHG:O3	2.39	0.53
1:A:456:TRP:HH2	1:A:468:ILE:HG21	1.73	0.53
1:G:82:SER:C	1:H:81:ASP:CA	2.60	0.53
1:D:505:ARG:HD3	5:D:2440:HOH:O	2.09	0.53
1:B:408:TRP:CD1	1:B:408:TRP:C	2.81	0.53
1:E:91:LYS:O	1:E:91:LYS:HG3	2.08	0.53
1:H:463:ILE:HD13	4:H:902:MES:O3S	2.09	0.52
1:A:387:GLY:N	1:A:420:GLN:OE1	2.30	0.52
1:B:137:PHE:HE1	4:B:902:MES:O1S	1.93	0.52
1:D:218:ARG:HD2	5:D:2005:HOH:O	2.08	0.52
1:H:296:GLU:O	1:H:312:LYS:HD2	2.10	0.52
1:E:342:PRO:C	1:E:344:ASN:N	2.61	0.52
1:G:385:THR:O	1:G:388:GLU:OE2	2.27	0.52
1:A:432:GLU:CD	1:A:432:GLU:H	2.11	0.52
1:F:341:ASN:HD22	1:F:341:ASN:C	2.12	0.52
1:E:548:HIS:CE1	3:E:901:SHG:HO3	2.27	0.52
1:F:542:GLU:CG	5:G:2703:HOH:O	2.49	0.52
1:F:471:TRP:CH2	1:F:526:SER:HA	2.44	0.52
1:A:386:PRO:HG3	1:A:391:TYR:CZ	2.44	0.52
1:A:62:ALA:O	1:A:66:VAL:HG23	2.10	0.52
1:D:418:GLN:HB3	1:D:419:HIS:CD2	2.44	0.52
1:D:50:VAL:HG13	1:D:313:ALA:HB2	1.90	0.52
1:A:534:PRO:HA	5:A:2515:HOH:O	2.10	0.52
1:E:459:VAL:CG2	1:F:121:LEU:HD22	2.39	0.52
1:F:572:VAL:HG21	1:F:578:LEU:HD23	1.92	0.52
1:E:97:GLN:HG3	1:E:250:PHE:CD2	2.45	0.52
1:E:366:THR:O	1:E:468:ILE:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:284:GLU:O	1:E:331:ASN:ND2	2.33	0.51
1:F:398:GLY:O	1:F:399:ALA:C	2.48	0.51
1:G:291:LEU:O	1:G:292:ASN:HB2	2.10	0.51
1:B:559:GLU:HB2	1:B:573:PHE:CD2	2.46	0.51
1:F:159:ARG:HA	2:F:801:FAD:O2B	2.11	0.51
1:E:247:SER:HB2	1:E:248:PRO:HD2	1.92	0.51
1:C:284:GLU:C	1:C:328:LEU:CD1	2.79	0.51
1:E:341:ASN:ND2	1:E:342:PRO:HD2	2.22	0.51
1:G:388:GLU:OE1	1:G:390:THR:OG1	2.28	0.51
1:G:462:SER:OG	4:H:624:MES:H51	2.10	0.51
1:C:548:HIS:NE2	3:C:901:SHG:O3	2.36	0.51
1:A:45:ILE:HG23	5:A:2861:HOH:O	2.10	0.51
4:F:902:MES:H22	1:G:149:LEU:HD22	1.92	0.51
1:B:449:ILE:HG12	1:B:471:TRP:CE3	2.46	0.51
1:F:546:VAL:HA	3:F:901:SHG:H6A	1.92	0.51
1:F:97:GLN:HG3	1:F:250:PHE:CE2	2.47	0.50
1:G:371:GLU:HG3	5:G:1610:HOH:O	2.11	0.50
1:D:81:ASP:CG	1:D:81:ASP:O	2.47	0.50
1:D:104:VAL:CG1	1:D:108:GLN:HE21	2.22	0.50
1:A:158:THR:HG22	1:A:160:VAL:HG22	1.92	0.50
1:B:476:ARG:HG3	1:B:476:ARG:O	2.11	0.50
1:C:463:ILE:HD13	4:C:624:MES:C8	2.41	0.50
1:G:341:ASN:HD21	1:G:343:ALA:HB3	1.75	0.50
1:G:359:GLN:HB3	1:G:475:GLY:O	2.12	0.50
1:B:548:HIS:CE1	3:B:901:SHG:HO3	2.27	0.50
1:H:308:ARG:NH1	1:H:308:ARG:HG3	2.17	0.50
1:C:133:ALA:CB	4:C:902:MES:C7	2.54	0.50
1:A:462:SER:O	4:B:902:MES:H81	2.11	0.50
1:C:68:ALA:HB2	1:C:610:LYS:HE2	1.93	0.50
1:E:534:PRO:HD3	1:F:126:LEU:HD23	1.94	0.50
1:E:439:PHE:CE2	1:E:444:PRO:C	2.84	0.50
1:F:614:THR:HG22	1:F:615:PRO:O	2.12	0.50
1:G:433:PRO:C	1:G:434:GLN:HG2	2.32	0.50
1:D:451:ARG:HH22	1:D:465:SER:HB2	1.76	0.50
1:C:380:MET:HE1	1:C:409:ASN:CA	2.42	0.50
1:E:404:HIS:HB3	1:E:405:PRO:CD	2.42	0.50
1:C:465:SER:HA	1:C:468:ILE:HD12	1.93	0.50
1:H:341:ASN:HD22	1:H:342:PRO:HD2	1.77	0.50
1:G:133:ALA:HB3	4:H:902:MES:C7	2.25	0.50
4:E:902:MES:O2S	1:F:463:ILE:HA	2.12	0.50
1:A:132:GLN:NE2	4:A:902:MES:O3S	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:LEU:HD23	5:B:1658:HOH:O	2.12	0.50
1:C:284:GLU:O	1:C:328:LEU:CD1	2.59	0.49
1:B:548:HIS:NE2	3:B:901:SHG:O3	2.39	0.49
1:F:359:GLN:HG2	1:F:475:GLY:O	2.12	0.49
1:B:185:LYS:HB2	1:B:185:LYS:NZ	2.26	0.49
1:F:128:PRO:HG2	1:G:515:ALA:HB3	1.92	0.49
1:C:48:ASP:HB2	1:C:71:LYS:O	2.13	0.49
1:C:47:TYR:O	1:C:313:ALA:HA	2.12	0.49
1:H:543:PRO:HA	5:H:1880:HOH:O	2.11	0.49
1:C:607:GLU:O	1:C:611:GLN:NE2	2.46	0.49
1:A:47:TYR:O	1:A:313:ALA:HA	2.12	0.49
1:A:49:VAL:HG22	1:A:315:VAL:HB	1.95	0.49
1:E:342:PRO:O	1:E:343:ALA:C	2.49	0.49
1:H:545:LEU:C	1:H:545:LEU:HD12	2.27	0.49
1:A:104:VAL:HG21	1:A:454:PHE:C	2.33	0.49
1:G:178:GLU:OE1	1:G:439:PHE:HE1	1.96	0.49
1:H:451:ARG:NH2	1:H:456:TRP:HZ2	2.11	0.49
1:B:457:GLY:O	1:B:458:ALA:C	2.51	0.49
1:E:198:LEU:HB3	1:E:600:SER:HB3	1.95	0.49
1:F:504:PHE:C	1:F:504:PHE:CD1	2.86	0.49
1:C:450:HIS:N	1:C:450:HIS:CD2	2.81	0.49
1:H:56:PRO:HD2	2:H:801:FAD:O1P	2.13	0.49
1:G:328:LEU:C	1:G:328:LEU:HD12	2.30	0.49
1:D:353:GLY:O	1:D:484:LYS:HA	2.13	0.49
1:B:145:GLU:HG3	1:B:488:SER:HB2	1.94	0.49
1:C:157:VAL:HG21	1:C:324:HIS:HE1	1.78	0.49
1:A:159:ARG:HA	2:A:801:FAD:O2B	2.13	0.49
1:H:47:TYR:CE2	1:H:73:ALA:HB2	2.47	0.49
1:A:593:ASN:HB3	2:A:801:FAD:C2	2.43	0.48
1:H:357:THR:O	1:H:549:LEU:HD12	2.13	0.48
1:B:382:ILE:HD13	5:B:2612:HOH:O	2.12	0.48
1:A:107:ILE:HG12	1:A:167:HIS:HB2	1.95	0.48
1:E:299:HIS:HD1	1:E:310:GLU:CD	2.16	0.48
1:B:198:LEU:HB3	1:B:600:SER:HB3	1.95	0.48
1:B:387:GLY:N	1:B:420:GLN:OE1	2.44	0.48
1:F:451:ARG:HD3	1:F:468:ILE:O	2.14	0.48
1:A:362:VAL:HG11	1:A:519:MET:HB2	1.95	0.48
1:E:83:GLY:N	1:F:81:ASP:HA	2.28	0.48
1:E:382:ILE:N	1:E:382:ILE:HD12	2.29	0.48
1:C:104:VAL:O	1:C:108:GLN:HG3	2.12	0.48
1:C:167:HIS:C	1:C:167:HIS:CD2	2.87	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:GLU:HG3	1:C:488:SER:HB2	1.95	0.48
1:G:293:SER:HA	1:G:574:GLY:O	2.12	0.48
1:H:81:ASP:OD1	1:H:81:ASP:N	2.46	0.48
1:B:101:ASP:CA	5:B:2756:HOH:O	2.60	0.48
1:F:566:VAL:HA	1:F:571:ARG:O	2.14	0.48
1:A:173:PRO:HG2	1:A:592:ALA:HB1	1.94	0.48
1:A:471:TRP:CH2	1:A:526:SER:HA	2.48	0.48
1:G:71:LYS:HB2	1:G:274:ARG:CZ	2.44	0.48
1:G:47:TYR:O	1:G:313:ALA:HA	2.14	0.48
1:B:432:GLU:HB2	1:B:451:ARG:HB2	1.95	0.48
1:C:568:THR:O	1:C:604:LYS:HD3	2.14	0.48
1:F:363:PHE:HA	1:F:471:TRP:O	2.14	0.47
1:F:126:LEU:HD12	1:F:132:GLN:HG3	1.95	0.47
1:E:56:PRO:HD3	1:E:165:SER:HB3	1.96	0.47
1:A:299:HIS:HB2	1:A:310:GLU:OE1	2.14	0.47
1:H:126:LEU:HD12	1:H:132:GLN:HG3	1.95	0.47
1:G:165:SER:HA	1:G:168:TRP:CD1	2.49	0.47
1:B:86:ILE:O	1:B:257:ASN:HB2	2.14	0.47
1:C:286:VAL:O	1:C:286:VAL:HG23	2.13	0.47
1:C:432:GLU:HB2	1:C:433:PRO:HD2	1.96	0.47
1:G:395:TYR:O	1:G:397:PRO:HD3	2.14	0.47
1:H:101:ASP:OD2	1:H:456:TRP:NE1	2.45	0.47
1:G:388:GLU:HG2	1:G:390:THR:H	1.79	0.47
1:G:132:GLN:HG3	4:H:902:MES:H22	1.97	0.47
1:C:462:SER:OG	4:C:624:MES:H51	2.13	0.47
1:F:408:TRP:CD1	1:F:408:TRP:C	2.88	0.47
1:B:96:TYR:O	1:B:100:ILE:HA	2.15	0.47
1:A:80:ILE:O	1:B:83:GLY:HA2	2.14	0.47
1:C:548:HIS:CE1	3:C:901:SHG:O3	2.68	0.47
1:E:404:HIS:ND1	5:E:2502:HOH:O	2.36	0.47
1:B:451:ARG:HD3	1:B:468:ILE:O	2.13	0.47
1:B:606:CYS:O	1:B:610:LYS:HG3	2.15	0.47
1:F:445:TRP:CE3	1:F:518:MET:HB2	2.49	0.47
1:B:570:SER:HB3	1:B:580:LEU:O	2.14	0.47
1:A:299:HIS:ND1	1:A:310:GLU:OE1	2.45	0.47
1:A:123:VAL:HG22	1:B:459:VAL:CG1	2.40	0.47
1:C:341:ASN:HD22	1:C:342:PRO:N	2.12	0.47
1:A:456:TRP:CH2	1:A:468:ILE:HG21	2.49	0.47
1:E:488:SER:O	1:E:498:PRO:HB3	2.15	0.47
1:A:389:LEU:H	1:A:389:LEU:HD23	1.80	0.47
1:D:225:LYS:O	1:D:229:GLU:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:ALA:O	1:C:66:VAL:HB	2.15	0.47
1:G:139:ARG:HD3	4:H:902:MES:H82	1.97	0.47
1:D:341:ASN:ND2	1:D:343:ALA:HB3	2.29	0.47
1:H:451:ARG:HH21	1:H:456:TRP:HZ2	1.61	0.47
1:D:355:TYR:HA	1:D:480:LYS:O	2.15	0.47
1:F:385:THR:O	1:F:388:GLU:HG2	2.15	0.47
1:G:433:PRO:O	1:G:450:HIS:HA	2.14	0.47
1:A:601:LEU:HD23	1:A:601:LEU:HA	1.78	0.47
1:F:537:LEU:HD11	5:F:1685:HOH:O	2.15	0.46
1:C:46:LYS:N	5:C:1772:HOH:O	2.48	0.46
1:A:366:THR:O	1:A:468:ILE:HA	2.16	0.46
1:D:218:ARG:HG3	1:D:430:ASP:OD2	2.16	0.46
1:C:215:GLU:O	1:C:411:LYS:NZ	2.47	0.46
1:D:336:GLN:NE2	1:D:344:ASN:O	2.48	0.46
1:H:218:ARG:HG3	1:H:430:ASP:OD2	2.15	0.46
1:C:346:PRO:CG	1:C:350:PRO:HA	2.45	0.46
1:B:218:ARG:HD2	5:B:1233:HOH:O	2.14	0.46
1:E:404:HIS:HB3	1:E:405:PRO:HD2	1.98	0.46
1:F:64:GLU:OE2	1:F:205:TYR:OH	2.23	0.46
1:H:50:VAL:HG12	1:H:73:ALA:HB3	1.98	0.46
1:G:97:GLN:HG3	1:G:250:PHE:CD2	2.51	0.46
1:H:169:THR:O	1:H:170:CYS:HB2	2.15	0.46
1:F:89:HIS:CE1	1:F:91:LYS:HB2	2.51	0.46
1:E:119:ASN:ND2	1:E:121:LEU:HD12	2.31	0.46
1:E:133:ALA:HB2	4:E:902:MES:H71	1.96	0.46
1:E:489:ASP:OD1	1:E:490:LYS:HG2	2.15	0.46
1:G:71:LYS:HB2	1:G:274:ARG:NH1	2.31	0.46
1:A:538:PRO:HG2	1:C:538:PRO:HG2	1.98	0.46
1:A:444:PRO:HD2	1:A:445:TRP:CZ3	2.50	0.46
1:G:83:GLY:N	1:H:81:ASP:HA	2.27	0.46
1:E:123:VAL:H	4:E:902:MES:H62	1.81	0.46
1:A:433:PRO:O	1:A:450:HIS:HA	2.16	0.46
1:E:105:ASN:O	1:F:105:ASN:HB3	2.16	0.46
1:C:341:ASN:C	1:C:341:ASN:HD22	2.19	0.46
1:F:566:VAL:HG11	1:F:580:LEU:HD12	1.97	0.46
1:C:71:LYS:HB2	1:C:274:ARG:NH1	2.31	0.46
1:E:44:ASP:OD2	1:E:46:LYS:N	2.34	0.46
1:G:617:PRO:O	1:G:618:PHE:C	2.54	0.46
1:H:54:SER:O	1:H:162:GLY:HA2	2.15	0.46
1:C:286:VAL:O	1:C:332:SER:HB3	2.17	0.45
1:G:327:GLN:HB2	1:G:487:PHE:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:GLU:O	1:B:411:LYS:NZ	2.48	0.45
1:E:556:GLY:O	1:E:567:ASN:HA	2.16	0.45
1:H:488:SER:O	1:H:498:PRO:HB3	2.17	0.45
1:G:59:CYS:SG	1:G:262:LEU:HD21	2.57	0.45
2:B:801:FAD:H8A	5:B:2284:HOH:O	2.17	0.45
1:G:133:ALA:HB2	4:H:902:MES:C8	2.47	0.45
1:C:459:VAL:O	1:C:462:SER:HB3	2.17	0.45
1:A:126:LEU:HD13	1:A:132:GLN:CG	2.46	0.45
1:G:562:ASP:O	1:G:563:ASN:C	2.54	0.45
1:A:308:ARG:CG	1:A:308:ARG:NH1	2.77	0.45
1:A:451:ARG:NE	5:A:2395:HOH:O	2.48	0.45
1:C:81:ASP:O	1:C:81:ASP:OD1	2.35	0.45
1:C:123:VAL:HG22	1:D:459:VAL:HG22	1.98	0.45
1:C:566:VAL:CG1	1:C:580:LEU:HD12	2.46	0.45
1:E:346:PRO:HG2	1:E:350:PRO:HA	1.98	0.45
1:D:359:GLN:OE1	1:D:548:HIS:ND1	2.34	0.45
1:D:440:GLN:HB3	1:D:441:PRO:CD	2.46	0.45
1:C:478:GLU:HA	1:C:479:PRO:HD2	1.88	0.45
1:C:163:GLY:CA	2:C:801:FAD:O3B	2.64	0.45
1:G:572:VAL:HG21	1:G:578:LEU:CD2	2.47	0.45
1:B:169:THR:O	1:B:169:THR:HG22	2.16	0.45
1:C:477:THR:HG23	1:C:507:PRO:HD2	1.97	0.45
1:D:173:PRO:HG2	1:D:592:ALA:HB1	1.99	0.45
1:C:111:LEU:HD23	1:C:111:LEU:HA	1.70	0.45
1:H:570:SER:HB3	1:H:580:LEU:O	2.17	0.45
1:A:403:LYS:HG2	5:A:2260:HOH:O	2.16	0.45
1:A:132:GLN:HA	1:A:132:GLN:NE2	2.31	0.45
1:E:327:GLN:HB2	1:E:487:PHE:CE1	2.52	0.45
1:F:435:VAL:HB	1:F:449:ILE:HB	1.99	0.45
1:F:165:SER:HA	1:F:168:TRP:CD1	2.52	0.45
1:B:507:PRO:HD2	1:B:511:THR:HG21	1.98	0.45
1:E:398:GLY:O	1:E:399:ALA:C	2.51	0.45
1:B:375:SER:HA	5:B:2924:HOH:O	2.16	0.45
1:G:459:VAL:O	1:G:462:SER:CB	2.65	0.44
4:C:624:MES:C6	1:D:123:VAL:H	2.30	0.44
1:C:548:HIS:CE1	3:C:901:SHG:HO3	2.30	0.44
1:H:217:ILE:HG23	1:H:408:TRP:CZ2	2.52	0.44
5:A:1428:HOH:O	1:D:542:GLU:HG3	2.16	0.44
1:G:404:HIS:HB3	1:G:405:PRO:HD2	1.98	0.44
1:E:546:VAL:HA	3:E:901:SHG:H6A	1.99	0.44
1:E:86:ILE:O	1:E:257:ASN:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:ILE:O	1:D:241:LEU:HG	2.18	0.44
2:C:801:FAD:N5	3:C:901:SHG:H3	2.31	0.44
1:F:456:TRP:CH2	1:F:468:ILE:HG21	2.52	0.44
1:G:408:TRP:C	1:G:408:TRP:CD1	2.90	0.44
1:A:471:TRP:CZ2	1:A:526:SER:HA	2.52	0.44
1:B:46:LYS:HD3	1:B:312:LYS:HB3	1.99	0.44
1:C:553:HIS:O	1:C:553:HIS:ND1	2.48	0.44
1:B:330:VAL:HG12	1:B:330:VAL:O	2.18	0.44
1:H:218:ARG:NH2	1:H:430:ASP:O	2.48	0.44
1:A:218:ARG:HG3	1:A:430:ASP:OD2	2.16	0.44
1:H:487:PHE:HE1	1:H:500:PRO:HB3	1.83	0.44
1:B:284:GLU:O	1:B:285:ARG:HG3	2.17	0.44
1:A:201:LYS:HE2	1:A:205:TYR:OH	2.17	0.44
1:E:490:LYS:CB	1:E:490:LYS:HZ3	2.02	0.44
1:F:572:VAL:HG21	1:F:578:LEU:CD2	2.48	0.44
1:E:444:PRO:HD2	1:E:445:TRP:CZ3	2.53	0.44
1:A:105:ASN:HB3	1:B:105:ASN:O	2.18	0.44
1:D:63:ARG:HD2	1:D:259:VAL:O	2.17	0.44
1:B:261:ASP:OD1	1:B:261:ASP:C	2.56	0.44
1:H:312:LYS:CE	5:H:1367:HOH:O	2.66	0.44
1:A:389:LEU:N	1:A:389:LEU:HD23	2.32	0.44
1:E:474:PHE:HB2	1:E:591:GLY:O	2.17	0.44
1:G:62:ALA:O	1:G:66:VAL:HB	2.18	0.44
1:B:133:ALA:HB3	4:B:902:MES:C3	2.48	0.44
1:B:170:CYS:O	1:B:241:LEU:HA	2.18	0.44
1:E:199:TYR:O	1:E:203:GLU:HG3	2.16	0.44
1:E:342:PRO:C	1:E:344:ASN:H	2.20	0.44
1:E:47:TYR:CE2	1:E:73:ALA:HB2	2.53	0.44
1:G:279:PRO:O	1:G:280:ALA:HB3	2.18	0.44
1:B:373:ILE:O	1:B:376:VAL:HB	2.17	0.44
1:B:63:ARG:HD2	1:B:259:VAL:O	2.18	0.44
1:G:478:GLU:HG2	1:G:511:THR:HG1	1.82	0.44
1:G:342:PRO:O	1:G:345:PRO:CD	2.62	0.44
1:F:107:ILE:HG12	1:F:167:HIS:HB2	1.99	0.44
1:G:616:SER:HB2	1:G:617:PRO:CD	2.47	0.44
1:D:569:ASP:O	1:D:570:SER:HB2	2.18	0.44
1:G:216:SER:HB3	1:G:219:HIS:HB3	2.00	0.44
1:A:396:THR:HA	1:A:397:PRO:HD3	1.77	0.44
1:D:328:LEU:HD12	1:D:328:LEU:O	2.18	0.44
1:H:219:HIS:HB2	1:H:433:PRO:HA	2.00	0.43
1:B:548:HIS:CE1	3:B:901:SHG:O3	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:VAL:HG13	1:C:105:ASN:N	2.33	0.43
1:A:567:ASN:HB2	5:A:1676:HOH:O	2.18	0.43
1:G:407:TRP:O	1:G:411:LYS:HG3	2.18	0.43
1:G:459:VAL:CG1	1:G:460:GLN:N	2.81	0.43
1:H:478:GLU:HA	1:H:479:PRO:HD3	1.81	0.43
1:A:341:ASN:HA	1:A:342:PRO:HD2	1.72	0.43
1:D:457:GLY:O	1:D:461:GLN:HG3	2.17	0.43
1:D:64:GLU:OE2	1:D:205:TYR:OH	2.30	0.43
1:C:180:ARG:HD2	1:C:195:TRP:CD2	2.53	0.43
1:A:590:TYR:CE2	1:A:594:PRO:HB3	2.53	0.43
1:D:210:THR:HG22	1:D:240:PRO:HA	2.00	0.43
1:D:68:ALA:HB2	1:D:610:LYS:HE2	2.01	0.43
1:H:363:PHE:HA	1:H:471:TRP:O	2.18	0.43
1:E:133:ALA:HB3	4:E:902:MES:H71	1.99	0.43
1:G:159:ARG:HA	2:G:801:FAD:O2B	2.18	0.43
1:H:432:GLU:HB2	1:H:433:PRO:HD2	2.00	0.43
1:A:386:PRO:HG3	1:A:391:TYR:CE1	2.54	0.43
1:C:432:GLU:CB	1:C:433:PRO:HD2	2.48	0.43
1:D:311:ILE:HG22	1:D:312:LYS:N	2.33	0.43
1:G:558:ASP:OD2	1:G:561:GLU:HB2	2.17	0.43
1:F:327:GLN:HB2	1:F:487:PHE:CE1	2.53	0.43
1:H:114:VAL:HB	5:H:1484:HOH:O	2.18	0.43
2:D:801:FAD:C5X	3:D:901:SHG:H3	2.47	0.43
1:F:131:TRP:HH2	1:F:133:ALA:HB2	1.78	0.43
1:C:71:LYS:HB2	1:C:274:ARG:CZ	2.48	0.43
1:E:389:LEU:HA	1:E:389:LEU:HD23	1.68	0.43
1:H:123:VAL:H	4:H:624:MES:C6	2.30	0.43
1:B:100:ILE:HG12	1:B:100:ILE:O	2.18	0.43
1:G:451:ARG:HD3	1:G:468:ILE:O	2.18	0.43
1:E:124:ASP:N	1:E:124:ASP:OD1	2.51	0.43
1:D:229:GLU:HB3	1:D:528:LYS:HD3	2.01	0.43
1:G:121:LEU:HD12	1:H:458:ALA:O	2.19	0.43
1:A:507:PRO:HD2	1:A:511:THR:HG21	2.01	0.43
1:E:194:GLU:CD	1:E:197:ARG:HH21	2.22	0.43
1:D:558:ASP:HB3	1:D:561:GLU:HB2	2.00	0.43
1:E:167:HIS:CD2	2:E:801:FAD:C8	3.01	0.43
2:D:801:FAD:C4X	3:D:901:SHG:H3	2.49	0.43
1:C:284:GLU:O	1:C:328:LEU:HD12	2.19	0.43
1:G:537:LEU:HB3	1:G:538:PRO:HD2	2.01	0.43
1:C:86:ILE:O	1:C:257:ASN:HB2	2.19	0.43
1:E:47:TYR:CD2	1:E:73:ALA:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:902:MES:H61	1:B:462:SER:OG	2.19	0.42
1:C:163:GLY:HA2	2:C:801:FAD:O3B	2.20	0.42
1:E:456:TRP:HH2	1:E:468:ILE:HG21	1.84	0.42
1:H:449:ILE:HG12	1:H:471:TRP:CE3	2.54	0.42
1:F:317:VAL:HG22	1:F:579:PHE:HB2	2.00	0.42
1:C:293:SER:HA	1:C:574:GLY:O	2.19	0.42
1:G:57:ILE:O	1:G:58:GLY:C	2.56	0.42
1:H:187:ASP:OD1	1:H:187:ASP:C	2.58	0.42
1:H:299:HIS:NE2	1:H:308:ARG:HD3	2.34	0.42
1:F:287:VAL:HG21	1:F:299:HIS:NE2	2.35	0.42
1:F:341:ASN:HA	1:F:342:PRO:HD2	1.79	0.42
1:D:89:HIS:CE1	1:D:91:LYS:HE2	2.54	0.42
1:A:197:ARG:HH11	1:A:197:ARG:HG2	1.84	0.42
1:B:593:ASN:HA	1:B:594:PRO:HD3	1.80	0.42
1:H:355:TYR:CE2	1:H:481:GLU:HB2	2.55	0.42
1:F:539:GLN:HB3	1:H:537:LEU:HD13	2.02	0.42
1:F:397:PRO:HB3	1:F:406:ASP:OD2	2.20	0.42
1:C:119:ASN:O	1:C:139:ARG:NH2	2.46	0.42
1:C:133:ALA:HB3	4:C:902:MES:H32	2.00	0.42
1:F:459:VAL:CG1	1:F:460:GLN:N	2.83	0.42
1:G:61:TYR:HA	1:G:606:CYS:SG	2.60	0.42
1:A:363:PHE:HA	1:A:471:TRP:O	2.19	0.42
1:D:345:PRO:HA	1:D:346:PRO:HD3	1.78	0.42
1:A:347:GLU:HB3	1:A:348:LEU:HG	2.02	0.42
1:F:346:PRO:HG2	1:F:350:PRO:HA	2.01	0.42
1:G:495:TYR:O	1:G:496:ASN:CB	2.65	0.42
1:C:346:PRO:HG3	1:C:350:PRO:HA	2.02	0.42
1:G:181:PRO:HG2	1:G:195:TRP:HZ2	1.85	0.42
1:C:185:LYS:H	1:C:185:LYS:HG2	1.66	0.42
1:D:177:ARG:HG3	5:D:2704:HOH:O	2.19	0.42
1:E:133:ALA:HB2	4:E:902:MES:C8	2.50	0.42
1:D:336:GLN:HB2	1:D:346:PRO:HG3	2.01	0.42
1:G:336:GLN:HB2	1:G:346:PRO:HG3	2.02	0.42
1:G:477:THR:HG23	1:G:507:PRO:HD2	2.02	0.42
1:H:349:LEU:HD11	1:H:572:VAL:HG13	2.01	0.42
1:G:86:ILE:O	1:G:257:ASN:ND2	2.51	0.42
1:D:100:ILE:HD13	1:D:100:ILE:C	2.40	0.42
1:C:486:TRP:CZ2	1:C:501:THR:HG21	2.55	0.42
1:B:341:ASN:HA	1:B:342:PRO:HD2	1.73	0.42
1:A:540:PHE:CE2	1:D:127:SER:HB2	2.54	0.42
1:E:586:ILE:HA	1:E:587:PRO:HD3	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:SER:HB3	1:B:531:GLY:HA3	2.02	0.42
1:E:474:PHE:CD1	1:E:474:PHE:N	2.88	0.42
1:H:165:SER:HA	1:H:168:TRP:CD1	2.55	0.42
1:H:133:ALA:CB	4:H:624:MES:O1S	2.64	0.41
1:C:460:GLN:C	1:C:462:SER:N	2.73	0.41
1:G:546:VAL:HA	3:G:901:SHG:H6A	2.01	0.41
1:E:487:PHE:HB3	1:E:498:PRO:HB2	2.00	0.41
1:C:525:MET:O	1:C:528:LYS:HB2	2.20	0.41
1:H:493:ASP:C	1:H:493:ASP:OD1	2.58	0.41
1:F:432:GLU:H	1:F:432:GLU:HG2	1.54	0.41
1:C:451:ARG:HH22	1:C:465:SER:HB2	1.85	0.41
1:C:284:GLU:C	1:C:328:LEU:HD11	2.40	0.41
1:G:424:LEU:HA	1:G:425:PRO:HD3	1.85	0.41
1:D:579:PHE:CD1	1:D:579:PHE:N	2.88	0.41
1:G:82:SER:O	1:H:81:ASP:C	2.58	0.41
1:C:463:ILE:HD13	4:C:624:MES:H81	2.03	0.41
1:C:105:ASN:HB3	1:D:105:ASN:O	2.20	0.41
1:A:120:THR:HA	1:A:136:PHE:CD1	2.55	0.41
1:D:365:GLN:OE1	1:D:533:LEU:HD23	2.20	0.41
1:A:299:HIS:NE2	1:A:308:ARG:CD	2.80	0.41
1:D:359:GLN:HG2	1:D:475:GLY:O	2.20	0.41
1:B:157:VAL:HG21	1:B:324:HIS:CE1	2.55	0.41
1:D:81:ASP:N	1:D:81:ASP:OD1	2.53	0.41
1:F:183:LEU:HD23	1:F:183:LEU:HA	1.88	0.41
1:E:167:HIS:CD2	1:E:167:HIS:C	2.93	0.41
1:E:264:ASN:C	1:E:265:ARG:HG3	2.40	0.41
1:D:440:GLN:HB3	1:D:441:PRO:HD2	2.03	0.41
1:H:59:CYS:HB3	1:H:260:PHE:HB3	2.02	0.41
1:F:618:PHE:C	1:F:618:PHE:CD1	2.93	0.41
1:E:362:VAL:HA	1:E:539:GLN:O	2.19	0.41
1:D:548:HIS:NE2	3:D:901:SHG:O3	2.41	0.41
1:G:616:SER:HB2	1:G:617:PRO:HD2	2.03	0.41
1:F:185:LYS:HE2	1:F:185:LYS:HB3	1.92	0.41
1:D:261:ASP:O	1:D:262:LEU:HB2	2.20	0.41
1:F:153:SER:OG	1:F:542:GLU:HG2	2.21	0.41
1:C:463:ILE:HD13	4:C:624:MES:H82	2.02	0.41
1:A:556:GLY:O	1:A:567:ASN:HA	2.20	0.41
1:F:265:ARG:HA	1:F:266:PRO:C	2.41	0.41
1:C:358:GLU:HG2	1:C:544:GLY:HA2	2.03	0.41
1:E:547:LEU:CD1	2:E:801:FAD:HM83	2.51	0.41
1:B:121:LEU:CD2	1:C:121:LEU:CD2	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:466:ARG:HG2	5:E:2798:HOH:O	2.21	0.41
1:F:48:ASP:O	1:F:314:ASP:HB2	2.21	0.41
1:E:358:GLU:HA	1:E:358:GLU:OE1	2.21	0.41
1:B:586:ILE:HA	1:B:587:PRO:HD3	1.77	0.41
1:A:229:GLU:HG3	1:A:528:LYS:HD3	2.03	0.41
1:B:123:VAL:H	4:B:902:MES:C6	2.33	0.41
1:G:201:LYS:HB3	1:G:603:ILE:HD13	2.02	0.41
1:E:119:ASN:O	1:E:139:ARG:NH2	2.48	0.41
2:G:801:FAD:C4X	3:G:901:SHG:H3	2.51	0.41
1:C:104:VAL:HG21	1:C:455:SER:HB3	2.02	0.41
1:E:44:ASP:C	1:E:44:ASP:OD2	2.59	0.41
1:A:354:SER:O	1:A:355:TYR:HB2	2.21	0.41
1:F:380:MET:CE	1:F:409:ASN:HB3	2.51	0.41
1:G:556:GLY:O	1:G:567:ASN:HA	2.21	0.41
1:C:490:LYS:HE3	1:C:490:LYS:HA	2.03	0.41
1:A:586:ILE:HA	1:A:587:PRO:HD3	1.89	0.41
1:D:159:ARG:HA	2:D:801:FAD:O2B	2.21	0.41
1:E:72:VAL:HG12	1:E:73:ALA:N	2.36	0.41
1:G:450:HIS:O	1:G:470:ASP:HB2	2.21	0.41
1:B:284:GLU:HA	1:B:497:MET:CE	2.51	0.41
1:F:487:PHE:CE1	1:F:500:PRO:HB3	2.56	0.41
1:B:546:VAL:HG22	1:B:546:VAL:O	2.19	0.41
1:C:355:TYR:HA	1:C:480:LYS:O	2.21	0.41
1:F:520:THR:O	1:F:524:VAL:HG23	2.21	0.41
1:H:206:PHE:CE2	1:H:599:MET:CE	3.05	0.41
2:D:801:FAD:H8A	5:D:1671:HOH:O	2.21	0.40
1:A:346:PRO:HG2	1:A:350:PRO:HA	2.02	0.40
1:G:474:PHE:N	1:G:474:PHE:CD1	2.89	0.40
1:A:538:PRO:HG2	1:C:538:PRO:CG	2.52	0.40
1:D:363:PHE:HA	1:D:471:TRP:O	2.21	0.40
2:C:801:FAD:HM71	2:C:801:FAD:HM83	1.90	0.40
1:E:433:PRO:C	1:E:434:GLN:HG2	2.41	0.40
1:C:226:LEU:HA	1:C:226:LEU:HD23	1.92	0.40
1:A:70:TYR:OH	1:A:610:LYS:HA	2.22	0.40
1:H:537:LEU:HD11	5:H:1450:HOH:O	2.22	0.40
1:D:617:PRO:O	1:D:619:THR:HG22	2.21	0.40
1:B:582:GLY:HA3	5:B:1045:HOH:O	2.21	0.40
1:E:172:THR:N	1:E:173:PRO:HD3	2.37	0.40
1:E:363:PHE:HA	1:E:471:TRP:O	2.22	0.40
1:A:126:LEU:CD2	1:B:367:VAL:HG21	2.51	0.40
1:C:437:THR:CG2	1:C:437:THR:O	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:THR:O	1:A:170:CYS:HB2	2.21	0.40
1:A:554:ARG:HD3	1:A:563:ASN:O	2.20	0.40
1:H:65:LEU:HD23	1:H:65:LEU:HA	1.84	0.40
4:H:902:MES:C3	4:H:902:MES:S	3.09	0.40
1:C:341:ASN:HD22	1:C:342:PRO:CD	2.35	0.40
1:A:548:HIS:CE1	3:A:901:SHG:O3	2.74	0.40
1:F:471:TRP:CZ2	1:F:526:SER:HA	2.57	0.40
1:E:555:MET:CG	1:E:556:GLY:N	2.84	0.40
1:H:59:CYS:SG	1:H:256:ALA:HB1	2.62	0.40
1:D:586:ILE:HA	1:D:587:PRO:HD3	1.94	0.40
1:E:430:ASP:HA	1:E:431:PRO:HD3	1.96	0.40
1:B:65:LEU:HD23	1:B:65:LEU:HA	1.82	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	572/623 (92%)	548 (96%)	24 (4%)	0	100	100
1	B	575/623 (92%)	544 (95%)	31 (5%)	0	100	100
1	C	572/623 (92%)	545 (95%)	26 (4%)	1 (0%)	52	59
1	D	572/623 (92%)	548 (96%)	24 (4%)	0	100	100
1	E	574/623 (92%)	547 (95%)	26 (4%)	1 (0%)	52	59
1	F	571/623 (92%)	539 (94%)	31 (5%)	1 (0%)	52	59
1	G	571/623 (92%)	545 (95%)	26 (5%)	0	100	100
1	H	571/623 (92%)	555 (97%)	15 (3%)	1 (0%)	52	59
All	All	4578/4984 (92%)	4371 (96%)	203 (4%)	4 (0%)	56	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	343	ALA
1	H	187	ASP
1	C	81	ASP
1	F	344	ASN

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	502/542 (93%)	476 (95%)	26 (5%)	29	33
1	B	505/542 (93%)	489 (97%)	16 (3%)	46	57
1	C	502/542 (93%)	481 (96%)	21 (4%)	36	44
1	D	502/542 (93%)	478 (95%)	24 (5%)	31	37
1	E	504/542 (93%)	483 (96%)	21 (4%)	36	44
1	F	501/542 (92%)	479 (96%)	22 (4%)	35	42
1	G	501/542 (92%)	481 (96%)	20 (4%)	38	47
1	H	501/542 (92%)	478 (95%)	23 (5%)	33	40
All	All	4018/4336 (93%)	3845 (96%)	173 (4%)	35	43

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ILE
1	A	81	ASP
1	A	100	ILE
1	A	102	LYS
1	A	112	MET
1	A	168	TRP
1	A	185	LYS
1	A	206	PHE
1	A	308	ARG
1	A	312	LYS
1	A	341	ASN
1	A	388	GLU

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Mol	Chain	Res	Type
1	A	389	LEU
1	A	390	THR
1	A	392	SER
1	A	396	THR
1	A	401	THR
1	A	408	TRP
1	A	450	HIS
1	A	452	ASP
1	A	459	VAL
1	A	462	SER
1	A	496	ASN
1	A	542	GLU
1	A	576	LYS
1	A	593	ASN
1	B	45	ILE
1	B	54	SER
1	B	100	ILE
1	B	112	MET
1	B	168	TRP
1	B	178	GLU
1	B	185	LYS
1	B	206	PHE
1	B	312	LYS
1	B	354	SER
1	B	389	LEU
1	B	408	TRP
1	B	450	HIS
1	B	462	SER
1	B	490	LYS
1	B	593	ASN
1	C	46	LYS
1	C	91	LYS
1	C	100	ILE
1	C	112	MET
1	C	167	HIS
1	C	168	TRP
1	C	206	PHE
1	C	341	ASN
1	C	385	THR
1	C	389	LEU
1	C	396	THR
1	C	403	LYS

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Mol	Chain	Res	Type
1	C	450	HIS
1	C	461	GLN
1	C	474	PHE
1	C	481	GLU
1	C	490	LYS
1	C	542	GLU
1	C	576	LYS
1	C	593	ASN
1	C	614	THR
1	D	46	LYS
1	D	100	ILE
1	D	112	MET
1	D	132	GLN
1	D	168	TRP
1	D	185	LYS
1	D	206	PHE
1	D	328	LEU
1	D	341	ASN
1	D	377	LYS
1	D	380	MET
1	D	385	THR
1	D	390	THR
1	D	403	LYS
1	D	408	TRP
1	D	418	GLN
1	D	450	HIS
1	D	459	VAL
1	D	496	ASN
1	D	554	ARG
1	D	560	LYS
1	D	576	LYS
1	D	611	GLN
1	D	619	THR
1	E	44	ASP
1	E	45	ILE
1	E	91	LYS
1	E	112	MET
1	E	134	SER
1	E	168	TRP
1	E	178	GLU
1	E	206	PHE
1	E	228	GLU

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Mol	Chain	Res	Type
1	E	265	ARG
1	E	268	THR
1	E	285	ARG
1	E	385	THR
1	E	408	TRP
1	E	450	HIS
1	E	490	LYS
1	E	496	ASN
1	E	545	LEU
1	E	554	ARG
1	E	588	THR
1	E	593	ASN
1	F	100	ILE
1	F	112	MET
1	F	132	GLN
1	F	134	SER
1	F	168	TRP
1	F	185	LYS
1	F	206	PHE
1	F	296	GLU
1	F	305	SER
1	F	328	LEU
1	F	341	ASN
1	F	344	ASN
1	F	408	TRP
1	F	432	GLU
1	F	442	SER
1	F	450	HIS
1	F	452	ASP
1	F	461	GLN
1	F	561	GLU
1	F	576	LYS
1	F	593	ASN
1	F	618	PHE
1	G	82	SER
1	G	95	GLU
1	G	100	ILE
1	G	168	TRP
1	G	185	LYS
1	G	206	PHE
1	G	228	GLU
1	G	231	LYS

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Mol	Chain	Res	Type
1	G	304	ILE
1	G	328	LEU
1	G	341	ASN
1	G	344	ASN
1	G	382	ILE
1	G	385	THR
1	G	389	LEU
1	G	408	TRP
1	G	450	HIS
1	G	459	VAL
1	G	496	ASN
1	G	593	ASN
1	H	100	ILE
1	H	112	MET
1	H	121	LEU
1	H	132	GLN
1	H	157	VAL
1	H	168	TRP
1	H	185	LYS
1	H	206	PHE
1	H	268	THR
1	H	269	ASP
1	H	308	ARG
1	H	341	ASN
1	H	347	GLU
1	H	388	GLU
1	H	389	LEU
1	H	418	GLN
1	H	450	HIS
1	H	459	VAL
1	H	461	GLN
1	H	542	GLU
1	H	545	LEU
1	H	593	ASN
1	H	618	PHE

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	263	GLN
1	A	460	GLN
1	B	132	GLN

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Mol	Chain	Res	Type
1	B	263	GLN
1	B	341	ASN
1	B	460	GLN
1	B	461	GLN
1	C	341	ASN
1	C	344	ASN
1	C	404	HIS
1	C	611	GLN
1	D	108	GLN
1	D	257	ASN
1	D	263	GLN
1	D	336	GLN
1	D	341	ASN
1	D	419	HIS
1	D	460	GLN
1	E	105	ASN
1	E	108	GLN
1	E	341	ASN
1	E	443	HIS
1	E	460	GLN
1	F	105	ASN
1	F	108	GLN
1	F	263	GLN
1	F	299	HIS
1	F	331	ASN
1	F	341	ASN
1	F	460	GLN
1	F	461	GLN
1	G	263	GLN
1	G	341	ASN
1	G	344	ASN
1	G	460	GLN
1	G	461	GLN
1	H	105	ASN
1	H	263	GLN
1	H	341	ASN
1	H	443	HIS
1	H	460	GLN
1	H	612	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

24 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	A	801	1	48,58,58	1.46	8 (16%)	54,89,89	4.14	19 (35%)
3	SHG	A	901	-	11,12,12	0.69	0	15,17,17	3.06	9 (60%)
4	MES	A	902	-	11,12,12	0.74	0	14,16,16	6.18	8 (57%)
2	FAD	B	801	1	48,58,58	1.54	8 (16%)	54,89,89	3.33	22 (40%)
3	SHG	B	901	-	11,12,12	1.28	0	15,17,17	3.85	7 (46%)
4	MES	B	902	-	11,12,12	0.72	0	14,16,16	7.96	9 (64%)
4	MES	C	624	-	11,12,12	0.82	0	14,16,16	8.42	7 (50%)
2	FAD	C	801	1	48,58,58	1.44	8 (16%)	54,89,89	4.31	19 (35%)
3	SHG	C	901	-	11,12,12	0.67	0	15,17,17	2.56	5 (33%)
4	MES	C	902	-	11,12,12	0.92	0	14,16,16	6.56	8 (57%)
2	FAD	D	801	1	48,58,58	1.20	4 (8%)	54,89,89	5.16	21 (38%)
3	SHG	D	901	-	11,12,12	0.77	0	15,17,17	4.63	6 (40%)
2	FAD	E	801	1	48,58,58	1.19	5 (10%)	54,89,89	4.44	20 (37%)
3	SHG	E	901	-	11,12,12	1.09	1 (9%)	15,17,17	5.37	7 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MES	E	902	-	11,12,12	0.95	1 (9%)	14,16,16	9.35	8 (57%)
2	FAD	F	801	1	48,58,58	1.37	8 (16%)	54,89,89	3.85	22 (40%)
3	SHG	F	901	-	11,12,12	0.76	0	15,17,17	3.20	8 (53%)
4	MES	F	902	-	11,12,12	1.00	0	14,16,16	5.68	9 (64%)
2	FAD	G	801	1	48,58,58	1.37	6 (12%)	54,89,89	3.55	20 (37%)
3	SHG	G	901	-	11,12,12	1.21	1 (9%)	15,17,17	4.81	8 (53%)
4	MES	H	624	-	11,12,12	0.82	0	14,16,16	10.46	8 (57%)
2	FAD	H	801	1	48,58,58	1.33	6 (12%)	54,89,89	5.33	22 (40%)
3	SHG	H	901	-	11,12,12	0.83	0	15,17,17	4.13	8 (53%)
4	MES	H	902	-	11,12,12	0.91	0	14,16,16	7.58	7 (50%)

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	A	801	1	1/1/9/9	0/30/50/50	0/6/6/6
3	SHG	A	901	-	-	0/2/22/22	0/1/1/1
4	MES	A	902	-	-	0/6/14/14	0/1/1/1
2	FAD	B	801	1	1/1/9/9	0/30/50/50	0/6/6/6
3	SHG	B	901	-	1/1/5/5	0/2/22/22	0/1/1/1
4	MES	B	902	-	-	0/6/14/14	0/1/1/1
4	MES	C	624	-	-	0/6/14/14	0/1/1/1
2	FAD	C	801	1	2/2/9/9	0/30/50/50	0/6/6/6
3	SHG	C	901	-	-	0/2/22/22	0/1/1/1
4	MES	C	902	-	-	0/6/14/14	0/1/1/1
2	FAD	D	801	1	-	0/30/50/50	0/6/6/6
3	SHG	D	901	-	1/1/5/5	0/2/22/22	0/1/1/1
2	FAD	E	801	1	1/1/9/9	0/30/50/50	0/6/6/6
3	SHG	E	901	-	1/1/5/5	0/2/22/22	0/1/1/1
4	MES	E	902	-	-	0/6/14/14	0/1/1/1
2	FAD	F	801	1	2/2/9/9	0/30/50/50	0/6/6/6
3	SHG	F	901	-	-	0/2/22/22	0/1/1/1
4	MES	F	902	-	-	0/6/14/14	0/1/1/1
2	FAD	G	801	1	-	0/30/50/50	0/6/6/6
3	SHG	G	901	-	1/1/5/5	0/2/22/22	0/1/1/1
4	MES	H	624	-	-	0/6/14/14	0/1/1/1
2	FAD	H	801	1	2/2/9/9	0/30/50/50	0/6/6/6
3	SHG	H	901	-	1/1/5/5	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MES	H	902	-	-	0/6/14/14	0/1/1/1

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	801	FAD	O3B-C3B	-2.79	1.36	1.43
2	A	801	FAD	C4A-N3A	-2.76	1.31	1.35
2	F	801	FAD	C2B-C3B	-2.65	1.46	1.53
2	A	801	FAD	O2'-C2'	-2.61	1.37	1.43
2	G	801	FAD	O4B-C4B	-2.53	1.39	1.45
2	F	801	FAD	C9A-C5X	-2.46	1.37	1.42
2	B	801	FAD	C10-N10	-2.44	1.36	1.39
2	A	801	FAD	O2B-C2B	-2.44	1.37	1.43
2	H	801	FAD	C10-N10	-2.42	1.36	1.39
2	C	801	FAD	O4B-C4B	-2.38	1.39	1.45
2	F	801	FAD	O4B-C4B	-2.24	1.39	1.45
2	A	801	FAD	O3'-C3'	-2.21	1.37	1.43
2	H	801	FAD	O3B-C3B	-2.17	1.37	1.43
2	D	801	FAD	C9A-C5X	-2.16	1.38	1.42
2	H	801	FAD	PA-O1A	-2.16	1.43	1.51
2	E	801	FAD	O3'-C3'	-2.12	1.37	1.43
2	B	801	FAD	O2B-C2B	-2.06	1.38	1.43
2	D	801	FAD	C4X-C10	-2.06	1.37	1.41
2	C	801	FAD	C9A-N10	2.09	1.41	1.38
2	E	801	FAD	O4B-C1B	2.10	1.43	1.41
2	C	801	FAD	C10-N1	2.12	1.39	1.35
2	B	801	FAD	C6-C5X	2.13	1.45	1.41
2	G	801	FAD	C9A-N10	2.16	1.41	1.38
2	A	801	FAD	O4B-C1B	2.16	1.43	1.41
2	F	801	FAD	C4-N3	2.17	1.37	1.33
2	C	801	FAD	C9-C8	2.18	1.43	1.37
2	A	801	FAD	C4-N3	2.32	1.37	1.33
2	E	801	FAD	C2A-N3A	2.35	1.36	1.32
2	G	801	FAD	C6-C5X	2.39	1.45	1.41
2	B	801	FAD	O4B-C1B	2.45	1.44	1.41
2	G	801	FAD	C4-N3	2.50	1.37	1.33
2	H	801	FAD	C4-N3	2.50	1.37	1.33
4	E	902	MES	O3S-S	2.56	1.53	1.46
3	E	901	SHG	C2-C3	2.64	1.54	1.52
2	H	801	FAD	C2A-N3A	2.73	1.37	1.32
2	D	801	FAD	C2A-N3A	2.82	1.37	1.32
2	C	801	FAD	C2A-N1A	2.83	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	801	FAD	C2A-N3A	2.85	1.37	1.32
2	F	801	FAD	C2A-N1A	2.90	1.39	1.33
2	B	801	FAD	C4-N3	2.90	1.38	1.33
2	E	801	FAD	C1'-N10	2.94	1.51	1.48
2	F	801	FAD	C4-C4X	2.97	1.47	1.41
2	C	801	FAD	C4-N3	2.98	1.38	1.33
2	A	801	FAD	C1'-N10	3.16	1.51	1.48
2	D	801	FAD	C4-C4X	3.36	1.48	1.41
2	B	801	FAD	C2A-N3A	3.40	1.38	1.32
3	G	901	SHG	C2-C3	3.47	1.55	1.52
2	C	801	FAD	C2A-N3A	3.60	1.38	1.32
2	E	801	FAD	C4-C4X	3.71	1.48	1.41
2	H	801	FAD	C4-C4X	3.75	1.48	1.41
2	G	801	FAD	C2A-N3A	3.87	1.39	1.32
2	G	801	FAD	C4-C4X	3.95	1.49	1.41
2	B	801	FAD	C4-C4X	3.99	1.49	1.41
2	B	801	FAD	C1'-N10	4.10	1.52	1.48
2	A	801	FAD	C4-C4X	4.24	1.49	1.41
2	C	801	FAD	C4-C4X	4.72	1.50	1.41

All (287) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	624	MES	O1S-S-C8	-35.26	76.82	106.91
4	E	902	MES	O1S-S-C8	-27.04	83.83	106.91
4	B	902	MES	O1S-S-C8	-24.53	85.98	106.91
2	H	801	FAD	C4-C4X-C10	-23.51	104.89	119.94
4	C	624	MES	O2S-S-C8	-23.49	86.86	106.91
4	H	902	MES	O1S-S-C8	-23.11	87.18	106.91
4	E	902	MES	O2S-S-C8	-19.89	89.94	106.91
4	C	624	MES	O1S-S-C8	-18.60	91.03	106.91
4	C	902	MES	O2S-S-C8	-18.40	91.20	106.91
2	D	801	FAD	C4X-C4-N3	-16.82	100.59	123.59
2	H	801	FAD	C4-N3-C2	-15.69	101.68	115.25
4	A	902	MES	O2S-S-C8	-14.75	94.32	106.91
2	F	801	FAD	C4-C4X-C10	-14.42	110.71	119.94
4	A	902	MES	O1S-S-C8	-14.35	94.66	106.91
4	F	902	MES	O2S-S-C8	-14.08	94.89	106.91
4	H	902	MES	O2S-S-C8	-13.46	95.42	106.91
2	C	801	FAD	C4X-C4-N3	-13.42	105.25	123.59
4	H	624	MES	O2S-S-C8	-13.18	95.66	106.91
4	B	902	MES	O2S-S-C8	-12.80	95.98	106.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	801	FAD	N3A-C2A-N1A	-12.68	119.18	128.89
2	A	801	FAD	C4X-C4-N3	-12.47	106.54	123.59
2	H	801	FAD	N3A-C2A-N1A	-12.19	119.56	128.89
2	B	801	FAD	N3A-C2A-N1A	-11.92	119.77	128.89
2	A	801	FAD	N3A-C2A-N1A	-11.46	120.12	128.89
4	F	902	MES	O1S-S-C8	-11.36	97.21	106.91
2	E	801	FAD	N3A-C2A-N1A	-11.31	120.24	128.89
2	C	801	FAD	N3A-C2A-N1A	-11.19	120.32	128.89
4	C	902	MES	O1S-S-C8	-10.97	97.54	106.91
2	E	801	FAD	C4X-C4-N3	-10.73	108.92	123.59
2	F	801	FAD	N3A-C2A-N1A	-9.74	121.44	128.89
2	D	801	FAD	N3A-C2A-N1A	-9.74	121.44	128.89
2	G	801	FAD	C4-C4X-C10	-7.98	114.84	119.94
2	B	801	FAD	C4B-O4B-C1B	-7.84	101.11	109.72
2	F	801	FAD	C4X-C4-N3	-7.41	113.45	123.59
2	H	801	FAD	C4B-O4B-C1B	-7.36	101.63	109.72
2	E	801	FAD	C4B-O4B-C1B	-7.14	101.88	109.72
2	B	801	FAD	C4-C4X-C10	-7.09	115.41	119.94
2	E	801	FAD	C4-C4X-C10	-6.89	115.53	119.94
2	A	801	FAD	C4-C4X-C10	-6.74	115.63	119.94
2	F	801	FAD	C4B-O4B-C1B	-6.32	102.77	109.72
2	B	801	FAD	C4X-C4-N3	-5.80	115.65	123.59
2	C	801	FAD	C4-C4X-C10	-5.37	116.50	119.94
2	D	801	FAD	C4B-O4B-C1B	-5.27	103.92	109.72
2	A	801	FAD	C4B-O4B-C1B	-5.06	104.16	109.72
2	G	801	FAD	C4X-C4-N3	-5.00	116.75	123.59
2	F	801	FAD	C4X-C10-N10	-4.66	117.78	120.52
2	F	801	FAD	C1B-N9A-C4A	-4.35	120.37	126.94
2	G	801	FAD	C9A-C5X-N5	-3.96	116.50	122.36
2	G	801	FAD	C4B-O4B-C1B	-3.73	105.61	109.72
2	C	801	FAD	C4X-C10-N10	-3.67	118.36	120.52
4	B	902	MES	C6-C5-N4	-3.67	104.57	110.12
2	A	801	FAD	O3'-C3'-C4'	-3.59	99.71	108.75
2	E	801	FAD	C1B-N9A-C4A	-3.45	121.73	126.94
2	F	801	FAD	C9A-C5X-N5	-3.31	117.45	122.36
4	H	624	MES	C6-C5-N4	-3.30	105.13	110.12
2	B	801	FAD	C9A-C5X-N5	-3.29	117.49	122.36
2	H	801	FAD	C1B-N9A-C4A	-3.23	122.07	126.94
2	G	801	FAD	C4X-C10-N10	-3.13	118.67	120.52
3	F	901	SHG	O6-C6-C5	-3.02	101.37	111.33
2	D	801	FAD	C1B-N9A-C4A	-2.91	122.56	126.94
2	A	801	FAD	C9A-C5X-N5	-2.90	118.06	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	FAD	C4-C4X-N5	-2.83	115.28	118.72
3	G	901	SHG	O6-C6-C5	-2.82	102.01	111.33
2	H	801	FAD	C9A-C5X-N5	-2.82	118.19	122.36
2	B	801	FAD	C1B-N9A-C4A	-2.75	122.79	126.94
2	F	801	FAD	C8M-C8-C9	-2.72	112.88	120.28
4	C	902	MES	O1-C6-C5	-2.70	105.65	111.84
4	B	902	MES	O1-C6-C5	-2.62	105.83	111.84
3	H	901	SHG	O4-C4-C3	-2.58	104.54	110.34
2	B	801	FAD	P-O3P-PA	-2.56	125.55	132.73
2	C	801	FAD	C9A-C5X-N5	-2.55	118.58	122.36
4	E	902	MES	O1-C6-C5	-2.55	106.00	111.84
2	C	801	FAD	C4B-O4B-C1B	-2.41	107.07	109.72
2	E	801	FAD	P-O3P-PA	-2.37	126.08	132.73
2	H	801	FAD	C4A-C5A-N7A	-2.35	107.32	109.48
2	H	801	FAD	O2'-C2'-C1'	-2.34	104.21	109.94
2	G	801	FAD	O3'-C3'-C4'	-2.31	102.92	108.75
3	A	901	SHG	O6-C6-C5	-2.29	103.78	111.33
3	E	901	SHG	O4-C4-C5	-2.28	103.21	109.24
2	F	801	FAD	C4-C4X-N5	-2.27	115.97	118.72
2	D	801	FAD	O5'-P-O1P	-2.24	100.92	109.62
3	B	901	SHG	O4-C4-C3	-2.23	105.32	110.34
2	D	801	FAD	C4A-C5A-N7A	-2.17	107.48	109.48
2	D	801	FAD	O4'-C4'-C5'	-2.16	105.48	110.19
2	B	801	FAD	O5'-P-O1P	-2.12	101.39	109.62
2	E	801	FAD	C9-C8-C7	-2.07	116.09	120.04
2	B	801	FAD	O5B-C5B-C4B	2.01	116.52	109.12
2	C	801	FAD	O2A-PA-O1A	2.01	123.41	112.53
2	E	801	FAD	C5X-C9A-N10	2.02	119.15	117.62
2	D	801	FAD	O2A-PA-O1A	2.04	123.56	112.53
2	H	801	FAD	C2A-N1A-C6A	2.04	122.41	118.77
2	F	801	FAD	O2A-PA-O3P	2.06	114.45	105.09
3	G	901	SHG	O5-C5-C6	2.07	111.59	106.36
2	G	801	FAD	O2A-PA-O1A	2.09	123.87	112.53
2	B	801	FAD	O3B-C3B-C2B	2.15	118.82	111.83
4	B	902	MES	O3S-S-O2S	2.17	116.67	111.61
3	C	901	SHG	F2-C2-C3	2.18	110.07	108.52
4	F	902	MES	C2-C3-N4	2.19	113.45	110.12
4	A	902	MES	C7-N4-C5	2.22	116.95	111.27
4	F	902	MES	C6-C5-N4	2.22	113.50	110.12
3	C	901	SHG	O5-C1-C2	2.22	118.19	110.46
4	H	624	MES	O3S-S-O2S	2.23	116.80	111.61
4	C	902	MES	C7-N4-C5	2.23	116.98	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	FAD	O4'-C4'-C3'	2.23	114.63	109.02
2	A	801	FAD	O2A-PA-O3P	2.25	115.31	105.09
2	D	801	FAD	C5B-C4B-C3B	2.26	124.17	115.21
2	C	801	FAD	O4B-C4B-C3B	2.26	109.70	105.15
2	G	801	FAD	O2A-PA-O3P	2.27	115.41	105.09
2	A	801	FAD	C5B-C4B-C3B	2.39	124.68	115.21
4	C	902	MES	C2-C3-N4	2.39	113.74	110.12
2	F	801	FAD	C4X-N5-C5X	2.41	119.53	116.76
2	D	801	FAD	C1'-N10-C9A	2.44	121.61	118.86
2	A	801	FAD	O4B-C1B-N9A	2.45	113.23	108.10
2	B	801	FAD	O2A-PA-O3P	2.48	116.35	105.09
2	A	801	FAD	C4X-N5-C5X	2.50	119.64	116.76
3	F	901	SHG	O4-C4-C5	2.50	115.86	109.24
2	F	801	FAD	C5B-C4B-C3B	2.53	125.24	115.21
4	H	902	MES	C7-N4-C5	2.55	117.80	111.27
2	H	801	FAD	O4B-C4B-C3B	2.56	110.30	105.15
2	H	801	FAD	O3'-C3'-C2'	2.57	115.22	108.75
2	E	801	FAD	O4B-C4B-C3B	2.63	110.44	105.15
2	B	801	FAD	O3B-C3B-C4B	2.63	118.94	111.05
2	B	801	FAD	O3P-P-O5'	2.66	110.00	102.94
4	A	902	MES	C6-C5-N4	2.66	114.16	110.12
4	E	902	MES	C7-N4-C3	2.69	118.16	111.27
2	A	801	FAD	O4B-C4B-C3B	2.71	110.61	105.15
4	F	902	MES	C7-N4-C3	2.73	118.27	111.27
4	A	902	MES	C7-N4-C3	2.75	118.33	111.27
4	C	624	MES	O3S-S-O1S	2.77	118.06	111.61
2	H	801	FAD	O4B-C4B-C5B	2.79	119.29	109.32
4	C	624	MES	C7-N4-C5	2.80	118.45	111.27
2	E	801	FAD	C5B-C4B-C3B	2.84	126.47	115.21
2	H	801	FAD	C5B-C4B-C3B	2.85	126.50	115.21
4	H	624	MES	C7-N4-C5	2.87	118.63	111.27
2	C	801	FAD	O4B-C4B-C5B	2.88	119.64	109.32
2	B	801	FAD	C4X-N5-C5X	2.89	120.08	116.76
4	C	902	MES	C7-N4-C3	2.90	118.70	111.27
4	E	902	MES	O3S-S-O2S	2.92	118.40	111.61
2	F	801	FAD	O3B-C3B-C4B	2.93	119.84	111.05
4	B	902	MES	C7-N4-C5	2.94	118.80	111.27
2	A	801	FAD	C1'-N10-C9A	2.96	122.18	118.86
3	F	901	SHG	F2-C2-C1	2.96	112.77	108.59
3	G	901	SHG	C3-C4-C5	2.99	115.40	110.20
2	A	801	FAD	O2B-C2B-C3B	3.00	121.60	111.83
2	C	801	FAD	C5B-C4B-C3B	3.03	127.22	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	FAD	O2B-C2B-C3B	3.03	121.70	111.83
2	G	801	FAD	C5B-C4B-C3B	3.05	127.30	115.21
2	E	801	FAD	O2P-P-O1P	3.07	129.16	112.53
2	D	801	FAD	O4B-C1B-N9A	3.12	114.63	108.10
2	D	801	FAD	O4B-C4B-C3B	3.17	111.54	105.15
2	E	801	FAD	C4-C4X-N5	3.18	122.58	118.72
4	E	902	MES	C7-N4-C5	3.20	119.48	111.27
2	F	801	FAD	C5X-C9A-N10	3.22	120.06	117.62
4	H	624	MES	C7-N4-C3	3.22	119.53	111.27
2	F	801	FAD	C1'-N10-C9A	3.23	122.48	118.86
3	A	901	SHG	F2-C2-C3	3.23	110.82	108.52
2	H	801	FAD	O3B-C3B-C2B	3.28	122.49	111.83
2	G	801	FAD	O3P-P-O5'	3.32	111.74	102.94
3	D	901	SHG	C3-C4-C5	3.32	115.99	110.20
3	H	901	SHG	O4-C4-C5	3.33	118.07	109.24
3	A	901	SHG	O5-C1-C2	3.34	122.08	110.46
4	H	902	MES	O3S-S-O1S	3.40	119.51	111.61
3	B	901	SHG	O3-C3-C2	3.40	115.11	109.05
2	D	801	FAD	O4B-C4B-C5B	3.40	121.48	109.32
4	A	902	MES	O3S-S-O1S	3.41	119.55	111.61
2	E	801	FAD	O4B-C4B-C5B	3.42	121.56	109.32
3	F	901	SHG	O5-C5-C6	3.43	115.03	106.36
2	F	801	FAD	C6-C5X-N5	3.44	123.39	118.96
2	B	801	FAD	C5B-C4B-C3B	3.44	128.85	115.21
3	H	901	SHG	C3-C4-C5	3.49	116.28	110.20
2	E	801	FAD	C1'-N10-C9A	3.49	122.78	118.86
2	G	801	FAD	C4-C4X-N5	3.49	122.95	118.72
4	C	624	MES	C7-N4-C3	3.55	120.38	111.27
4	B	902	MES	C7-N4-C3	3.57	120.41	111.27
2	B	801	FAD	C1'-N10-C9A	3.57	122.87	118.86
3	A	901	SHG	O5-C5-C4	3.58	116.39	109.68
3	A	901	SHG	F2-C2-C1	3.62	113.70	108.59
3	A	901	SHG	O4-C4-C5	3.63	118.85	109.24
2	G	801	FAD	O4B-C1B-N9A	3.63	115.71	108.10
2	C	801	FAD	O3B-C3B-C4B	3.64	121.96	111.05
3	B	901	SHG	C3-C4-C5	3.64	116.54	110.20
2	A	801	FAD	C6-C5X-N5	3.64	123.64	118.96
2	B	801	FAD	O4B-C4B-C5B	3.66	122.43	109.32
4	F	902	MES	C7-N4-C5	3.67	120.68	111.27
2	A	801	FAD	O3B-C3B-C4B	3.68	122.08	111.05
2	B	801	FAD	O2B-C2B-C3B	3.72	123.92	111.83
2	F	801	FAD	O3B-C3B-C2B	3.76	124.06	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	FAD	O4B-C4B-C5B	3.76	122.78	109.32
2	G	801	FAD	O2B-C2B-C3B	3.77	124.10	111.83
2	G	801	FAD	O4B-C4B-C5B	3.79	122.89	109.32
2	C	801	FAD	O3B-C3B-C2B	3.96	124.70	111.83
2	C	801	FAD	C4-C4X-N5	3.98	123.54	118.72
3	C	901	SHG	C3-C4-C5	4.02	117.20	110.20
2	G	801	FAD	C5X-C9A-N10	4.07	120.72	117.62
3	G	901	SHG	O3-C3-C2	4.10	116.37	109.05
3	A	901	SHG	C3-C4-C5	4.15	117.43	110.20
2	F	801	FAD	O4B-C4B-C5B	4.17	124.23	109.32
3	C	901	SHG	O5-C5-C4	4.17	117.52	109.68
2	D	801	FAD	C4X-N5-C5X	4.21	121.61	116.76
2	A	801	FAD	C4-C4X-N5	4.21	123.83	118.72
2	C	801	FAD	O2B-C2B-C3B	4.21	125.53	111.83
4	E	902	MES	O3S-S-O1S	4.25	121.49	111.61
2	F	801	FAD	O2B-C2B-C3B	4.30	125.82	111.83
2	H	801	FAD	C4X-N5-C5X	4.33	121.74	116.76
4	H	902	MES	O3S-S-O2S	4.38	121.80	111.61
3	E	901	SHG	F2-C2-C1	4.38	114.78	108.59
3	H	901	SHG	C1-O5-C5	4.40	121.60	113.47
4	H	902	MES	C7-N4-C3	4.42	122.61	111.27
2	E	801	FAD	O4B-C1B-N9A	4.46	117.44	108.10
2	G	801	FAD	O3B-C3B-C4B	4.52	124.60	111.05
4	F	902	MES	O3S-S-O1S	4.54	122.18	111.61
2	B	801	FAD	C4-N3-C2	4.57	119.20	115.25
2	E	801	FAD	C4X-N5-C5X	4.60	122.06	116.76
3	A	901	SHG	C1-O5-C5	4.63	122.03	113.47
3	D	901	SHG	C1-O5-C5	4.63	122.03	113.47
2	E	801	FAD	O2B-C2B-C3B	4.64	126.91	111.83
3	F	901	SHG	O5-C5-C4	4.69	118.49	109.68
2	B	801	FAD	O4B-C1B-N9A	4.71	117.95	108.10
3	H	901	SHG	O3-C3-C2	4.75	117.53	109.05
4	A	902	MES	O3S-S-O2S	4.78	122.72	111.61
3	F	901	SHG	O3-C3-C2	4.80	117.61	109.05
3	D	901	SHG	O3-C3-C2	4.80	117.62	109.05
2	H	801	FAD	O4B-C1B-N9A	4.84	118.23	108.10
3	D	901	SHG	F2-C2-C1	4.87	115.46	108.59
2	H	801	FAD	C1'-N10-C9A	4.92	124.39	118.86
4	H	902	MES	C5-N4-C3	4.93	119.57	108.90
3	F	901	SHG	F2-C2-C3	4.95	112.04	108.52
2	H	801	FAD	O2B-C2B-C3B	4.97	128.00	111.83
3	A	901	SHG	O3-C3-C2	5.18	118.30	109.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	624	MES	O3S-S-O2S	5.25	123.84	111.61
3	E	901	SHG	C1-O5-C5	5.48	123.62	113.47
4	B	902	MES	C5-N4-C3	5.49	120.79	108.90
4	F	902	MES	C5-N4-C3	5.52	120.86	108.90
3	G	901	SHG	C1-O5-C5	5.61	123.84	113.47
2	H	801	FAD	O3B-C3B-C4B	5.64	127.97	111.05
4	C	624	MES	C5-N4-C3	5.67	121.17	108.90
2	D	801	FAD	O3B-C3B-C4B	5.80	128.44	111.05
2	C	801	FAD	O4B-C1B-N9A	5.84	120.33	108.10
4	F	902	MES	O3S-S-O2S	5.94	125.42	111.61
4	H	624	MES	C5-N4-C3	5.94	121.76	108.90
2	E	801	FAD	O3B-C3B-C4B	5.94	128.88	111.05
3	E	901	SHG	O5-C5-C4	5.99	120.92	109.68
3	H	901	SHG	O5-C5-C4	6.06	121.06	109.68
3	B	901	SHG	F2-C2-C3	6.08	112.83	108.52
2	C	801	FAD	C1'-N10-C9A	6.12	125.74	118.86
2	B	801	FAD	C4-C4X-N5	6.13	126.16	118.72
3	E	901	SHG	O3-C3-C2	6.15	120.02	109.05
3	B	901	SHG	O5-C5-C4	6.16	121.25	109.68
3	E	901	SHG	C3-C4-C5	6.17	120.94	110.20
4	E	902	MES	C5-N4-C3	6.18	122.29	108.90
2	F	801	FAD	O4B-C1B-N9A	6.20	121.07	108.10
3	C	901	SHG	C1-O5-C5	6.41	125.32	113.47
4	B	902	MES	O3S-S-O1S	6.44	126.59	111.61
4	H	624	MES	O3S-S-O1S	6.46	126.65	111.61
3	F	901	SHG	C1-O5-C5	6.48	125.45	113.47
3	G	901	SHG	O5-C5-C4	6.60	122.07	109.68
2	C	801	FAD	C4X-N5-C5X	6.81	124.60	116.76
2	G	801	FAD	C4X-N5-C5X	6.87	124.66	116.76
3	G	901	SHG	F2-C2-C1	7.05	118.53	108.59
4	C	902	MES	C5-N4-C3	7.12	124.31	108.90
3	B	901	SHG	C1-O5-C5	7.28	126.94	113.47
4	A	902	MES	C5-N4-C3	7.29	124.69	108.90
4	C	902	MES	O3S-S-O2S	7.31	128.63	111.61
3	B	901	SHG	F2-C2-C1	7.42	119.06	108.59
3	D	901	SHG	O5-C5-C4	7.64	124.02	109.68
3	H	901	SHG	F2-C2-C3	7.85	114.09	108.52
2	E	801	FAD	C2B-C1B-N9A	7.99	126.51	114.29
2	F	801	FAD	C2B-C1B-N9A	8.02	126.55	114.29
2	G	801	FAD	C2B-C1B-N9A	8.37	127.07	114.29
3	H	901	SHG	F2-C2-C1	8.79	120.99	108.59
2	B	801	FAD	C2B-C1B-N9A	9.15	128.27	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	801	FAD	C4X-C4-N3	9.16	136.11	123.59
2	D	801	FAD	C4-C4X-C10	9.17	125.81	119.94
2	H	801	FAD	C2B-C1B-N9A	9.40	128.66	114.29
2	F	801	FAD	C4-N3-C2	9.66	123.60	115.25
2	C	801	FAD	C2B-C1B-N9A	10.29	130.01	114.29
2	A	801	FAD	C2B-C1B-N9A	10.55	130.41	114.29
2	G	801	FAD	C4-N3-C2	10.62	124.43	115.25
2	D	801	FAD	C2B-C1B-N9A	11.30	131.56	114.29
2	H	801	FAD	C4-C4X-N5	11.82	133.06	118.72
3	D	901	SHG	F2-C2-C3	13.07	117.79	108.52
3	G	901	SHG	F2-C2-C3	13.37	118.00	108.52
3	E	901	SHG	F2-C2-C3	16.04	119.90	108.52
2	C	801	FAD	C4-N3-C2	16.76	129.74	115.25
2	A	801	FAD	C4-N3-C2	17.08	130.01	115.25
2	E	801	FAD	C4-N3-C2	21.09	133.48	115.25
2	D	801	FAD	C4-N3-C2	25.44	137.24	115.25

All (14) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	H	801	FAD	C2B
2	H	801	FAD	C1B
3	H	901	SHG	C2
3	E	901	SHG	C2
2	B	801	FAD	C4B
3	G	901	SHG	C2
3	D	901	SHG	C2
2	F	801	FAD	C4B
2	F	801	FAD	C1B
2	E	801	FAD	C4B
3	B	901	SHG	C2
2	C	801	FAD	C2B
2	C	801	FAD	C1B
2	A	801	FAD	C4B

There are no torsion outliers.

There are no ring outliers.

24 monomers are involved in 118 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	FAD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	SHG	2	0
4	A	902	MES	4	0
2	B	801	FAD	5	0
3	B	901	SHG	3	0
4	B	902	MES	7	0
4	C	624	MES	11	0
2	C	801	FAD	5	0
3	C	901	SHG	5	0
4	C	902	MES	10	0
2	D	801	FAD	6	0
3	D	901	SHG	4	0
2	E	801	FAD	9	0
3	E	901	SHG	6	0
4	E	902	MES	12	0
2	F	801	FAD	1	0
3	F	901	SHG	1	0
4	F	902	MES	1	0
2	G	801	FAD	3	0
3	G	901	SHG	3	0
4	H	624	MES	7	0
2	H	801	FAD	3	0
3	H	901	SHG	1	0
4	H	902	MES	16	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	574/623 (92%)	-0.01	25 (4%)	38	37	11, 18, 31, 52	0
1	B	577/623 (92%)	-0.00	26 (4%)	37	36	11, 19, 33, 45	0
1	C	574/623 (92%)	0.16	42 (7%)	18	17	13, 23, 39, 53	0
1	D	574/623 (92%)	0.06	35 (6%)	25	24	12, 21, 34, 48	0
1	E	576/623 (92%)	0.20	43 (7%)	17	17	15, 24, 40, 54	0
1	F	573/623 (91%)	0.16	33 (5%)	26	26	13, 23, 36, 49	0
1	G	573/623 (91%)	0.09	30 (5%)	31	30	14, 21, 36, 52	0
1	H	573/623 (91%)	-0.02	18 (3%)	52	51	12, 19, 32, 46	0
All	All	4594/4984 (92%)	0.08	252 (5%)	29	28	11, 21, 36, 54	0

All (252) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	619	THR	8.1
1	C	619	THR	6.9
1	C	389	LEU	6.6
1	C	343	ALA	5.9
1	B	619	THR	5.6
1	G	343	ALA	5.5
1	C	618	PHE	5.4
1	E	389	LEU	5.3
1	D	389	LEU	5.2
1	F	385	THR	5.2
1	H	270	ALA	5.1
1	E	45	ILE	5.0
1	C	458	ALA	5.0
1	A	343	ALA	4.9
1	F	343	ALA	4.9
1	F	458	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	390	THR	4.9
1	E	385	THR	4.8
1	B	389	LEU	4.8
1	A	388	GLU	4.7
1	G	389	LEU	4.6
1	E	343	ALA	4.6
1	D	385	THR	4.5
1	F	390	THR	4.5
1	C	456	TRP	4.5
1	D	388	GLU	4.5
1	A	389	LEU	4.4
1	A	385	THR	4.4
1	C	387	GLY	4.4
1	C	617	PRO	4.4
1	E	43	MET	4.4
1	E	388	GLU	4.3
1	G	385	THR	4.3
1	C	390	THR	4.3
1	G	456	TRP	4.2
1	F	386	PRO	4.2
1	E	458	ALA	4.1
1	C	384	GLY	4.1
1	E	44	ASP	4.1
1	G	387	GLY	4.1
1	G	388	GLU	4.0
1	F	388	GLU	4.0
1	B	343	ALA	3.9
1	B	458	ALA	3.9
1	E	190	ALA	3.9
1	H	618	PHE	3.9
1	B	456	TRP	3.9
1	F	389	LEU	3.9
1	C	385	THR	3.8
1	F	391	TYR	3.8
1	C	305	SER	3.7
1	E	318	LEU	3.7
1	C	345	PRO	3.7
1	G	458	ALA	3.7
1	E	617	PRO	3.7
1	C	383	ARG	3.7
1	F	268	THR	3.7
1	B	387	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	268	THR	3.6
1	D	618	PHE	3.6
1	E	342	PRO	3.5
1	E	387	GLY	3.5
1	B	459	VAL	3.5
1	E	186	ASP	3.5
1	D	455	SER	3.5
1	E	268	THR	3.4
1	H	344	ASN	3.4
1	D	188	ALA	3.4
1	C	392	SER	3.3
1	H	343	ALA	3.3
1	C	561	GLU	3.3
1	E	490	LYS	3.3
1	A	456	TRP	3.3
1	G	344	ASN	3.3
1	E	390	THR	3.2
1	G	268	THR	3.2
1	H	455	SER	3.2
1	C	344	ASN	3.2
1	A	458	ALA	3.2
1	G	188	ALA	3.2
1	C	459	VAL	3.2
1	F	344	ASN	3.2
1	E	344	ASN	3.2
1	F	307	ASP	3.1
1	D	390	THR	3.1
1	F	456	TRP	3.1
1	G	618	PHE	3.1
1	C	396	THR	3.1
1	B	388	GLU	3.1
1	A	459	VAL	3.1
1	B	341	ASN	3.0
1	C	309	PHE	3.0
1	C	306	GLY	3.0
1	A	344	ASN	3.0
1	C	270	ALA	3.0
1	A	384	GLY	3.0
1	G	341	ASN	3.0
1	D	269	ASP	3.0
1	E	232	GLY	3.0
1	B	318	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	272	GLU	2.9
1	A	618	PHE	2.9
1	G	189	ASP	2.9
1	A	387	GLY	2.9
1	B	344	ASN	2.9
1	C	271	PRO	2.8
1	F	387	GLY	2.8
1	F	417	MET	2.8
1	D	383	ARG	2.8
1	E	400	SER	2.8
1	C	388	GLU	2.8
1	C	268	THR	2.8
1	E	271	PRO	2.8
1	F	266	PRO	2.8
1	D	391	TYR	2.8
1	D	344	ASN	2.8
1	A	318	LEU	2.8
1	E	347	GLU	2.8
1	B	342	PRO	2.8
1	C	269	ASP	2.8
1	A	455	SER	2.7
1	E	233	GLN	2.7
1	E	269	ASP	2.7
1	G	384	GLY	2.7
1	C	341	ASN	2.7
1	F	384	GLY	2.7
1	E	618	PHE	2.7
1	G	386	PRO	2.7
1	A	391	TYR	2.7
1	G	391	TYR	2.7
1	E	580	LEU	2.7
1	E	272	GLU	2.7
1	C	342	PRO	2.7
1	D	309	PHE	2.6
1	C	272	GLU	2.6
1	H	185	LYS	2.6
1	G	269	ASP	2.6
1	H	617	PRO	2.6
1	F	188	ALA	2.6
1	E	319	THR	2.6
1	H	345	PRO	2.6
1	E	188	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	323	VAL	2.6
1	C	401	THR	2.6
1	B	57	ILE	2.6
1	E	57	ILE	2.6
1	D	456	TRP	2.6
1	E	386	PRO	2.6
1	B	190	ALA	2.6
1	F	189	ASP	2.5
1	H	271	PRO	2.5
1	F	269	ASP	2.5
1	F	418	GLN	2.5
1	A	383	ARG	2.5
1	E	561	GLU	2.5
1	F	383	ARG	2.5
1	B	618	PHE	2.5
1	G	455	SER	2.5
1	H	387	GLY	2.5
1	H	342	PRO	2.5
1	D	270	ALA	2.5
1	B	44	ASP	2.5
1	G	186	ASP	2.5
1	F	187	ASP	2.4
1	D	387	GLY	2.4
1	D	322	ALA	2.4
1	D	318	LEU	2.4
1	A	345	PRO	2.4
1	H	458	ALA	2.4
1	F	392	SER	2.4
1	G	270	ALA	2.4
1	C	322	ALA	2.4
1	F	193	ALA	2.4
1	C	611	GLN	2.3
1	G	390	THR	2.3
1	C	187	ASP	2.3
1	E	187	ASP	2.3
1	A	457	GLY	2.3
1	C	189	ASP	2.3
1	C	391	TYR	2.3
1	D	319	THR	2.3
1	D	343	ALA	2.3
1	H	341	ASN	2.3
1	B	617	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	309	PHE	2.3
1	E	305	SER	2.3
1	A	386	PRO	2.3
1	H	272	GLU	2.3
1	A	323	VAL	2.3
1	F	382	ILE	2.3
1	E	189	ASP	2.3
1	H	317	VAL	2.2
1	B	189	ASP	2.2
1	D	458	ALA	2.2
1	E	51	ILE	2.2
1	C	400	SER	2.2
1	E	317	VAL	2.2
1	B	43	MET	2.2
1	C	467	LEU	2.2
1	D	186	ASP	2.2
1	C	188	ALA	2.2
1	A	341	ASN	2.2
1	C	318	LEU	2.2
1	D	384	GLY	2.2
1	C	455	SER	2.2
1	G	382	ILE	2.2
1	B	186	ASP	2.2
1	B	457	GLY	2.2
1	E	582	GLY	2.2
1	F	186	ASP	2.2
1	B	309	PHE	2.2
1	G	185	LYS	2.2
1	G	266	PRO	2.2
1	D	305	SER	2.2
1	D	454	PHE	2.1
1	F	322	ALA	2.1
1	A	580	LEU	2.1
1	B	383	ARG	2.1
1	E	339	ARG	2.1
1	B	270	ALA	2.1
1	E	325	ASN	2.1
1	G	51	ILE	2.1
1	G	342	PRO	2.1
1	D	400	SER	2.1
1	E	456	TRP	2.1
1	F	549	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	290	ALA	2.1
1	H	190	ALA	2.1
1	D	398	GLY	2.1
1	G	267	ASN	2.1
1	D	617	PRO	2.1
1	G	617	PRO	2.1
1	F	618	PHE	2.1
1	A	321	GLY	2.1
1	D	189	ASP	2.1
1	F	345	PRO	2.1
1	C	185	LYS	2.1
1	H	459	VAL	2.1
1	D	457	GLY	2.0
1	C	186	ASP	2.0
1	G	187	ASP	2.0
1	F	342	PRO	2.0
1	B	317	VAL	2.0
1	G	318	LEU	2.0
1	D	345	PRO	2.0
1	A	57	ILE	2.0
1	B	45	ILE	2.0
1	D	51	ILE	2.0
1	D	382	ILE	2.0
1	E	52	VAL	2.0
1	E	401	THR	2.0
1	A	320	ALA	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	MES	C	902	12/12	0.76	0.32	8.08	65,68,69,72	0
4	MES	C	624	12/12	0.68	0.39	7.05	99,101,101,101	0
4	MES	E	902	12/12	0.83	0.30	6.68	76,78,79,81	0
4	MES	H	902	12/12	0.73	0.31	5.71	70,77,78,78	0
4	MES	B	902	12/12	0.85	0.25	5.64	70,73,76,78	0
3	SHG	C	901	12/12	0.96	0.21	4.81	37,39,46,46	0
3	SHG	H	901	12/12	0.96	0.23	4.68	39,41,45,49	0
3	SHG	D	901	12/12	0.95	0.20	3.98	38,40,42,44	0
3	SHG	E	901	12/12	0.93	0.20	3.21	43,46,48,50	0
3	SHG	B	901	12/12	0.96	0.20	2.93	34,37,42,42	0
3	SHG	A	901	12/12	0.94	0.22	2.83	32,35,40,43	0
3	SHG	G	901	12/12	0.93	0.20	2.55	41,44,48,49	0
3	SHG	F	901	12/12	0.95	0.21	2.33	28,31,35,40	0
4	MES	H	624	12/12	0.88	0.21	2.32	68,71,73,73	0
4	MES	A	902	12/12	0.94	0.19	1.95	44,48,53,53	0
2	FAD	C	801	53/53	0.97	0.18	1.32	20,30,35,41	0
2	FAD	H	801	53/53	0.97	0.20	1.29	17,25,31,32	0
2	FAD	B	801	53/53	0.96	0.20	1.14	16,26,31,33	0
2	FAD	G	801	53/53	0.96	0.20	1.10	16,24,28,30	0
2	FAD	D	801	53/53	0.97	0.18	0.87	16,25,29,34	0
2	FAD	F	801	53/53	0.97	0.19	0.83	13,27,36,41	0
2	FAD	A	801	53/53	0.97	0.19	0.63	16,21,26,27	0
2	FAD	E	801	53/53	0.96	0.17	0.36	21,28,34,36	0
4	MES	F	902	12/12	0.96	0.13	0.32	38,40,41,43	0

6.5 Other polymers ⓘ

There are no such residues in this entry.