



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:40 AM GMT

PDB ID : 3BG7  
Title : Pyranose 2-oxidase from Trametes multicolor, L537G mutant  
Authors : Norberg, P.; Tan, T.C.; Divne, C.  
Deposited on : 2007-11-26  
Resolution : 2.10 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (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

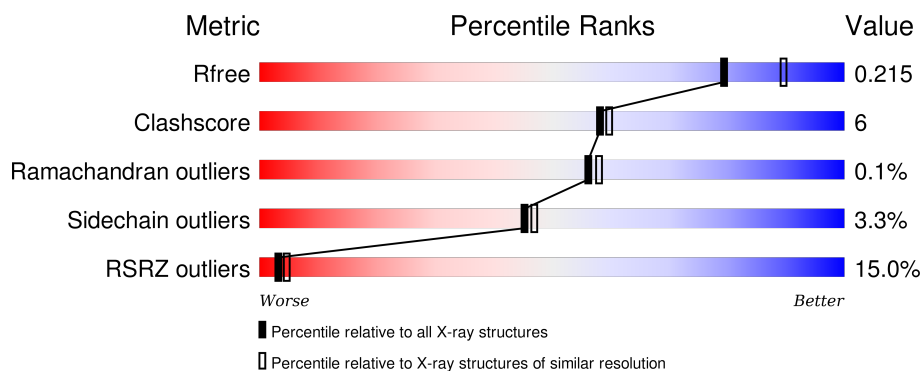
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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. 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>12%</div> <div>81%</div> <div>11%</div> <div>7%</div> </div>
1	B	623	<div> <div>11%</div> <div>80%</div> <div>11%</div> <div>7%</div> </div>
1	C	623	<div> <div>15%</div> <div>81%</div> <div>10%</div> <div>7%</div> </div>
1	D	623	<div> <div>14%</div> <div>82%</div> <div>9%</div> <div>7%</div> </div>
1	E	623	<div> <div>16%</div> <div>83%</div> <div>9%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	623	<div><div></div><div>17%</div><div>83%</div><div>8%7%</div></div>
1	G	623	<div><div></div><div>14%</div><div>83%</div><div>8%7%</div></div>
1	H	623	<div><div></div><div>12%</div><div>80%</div><div>11%7%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 38641 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

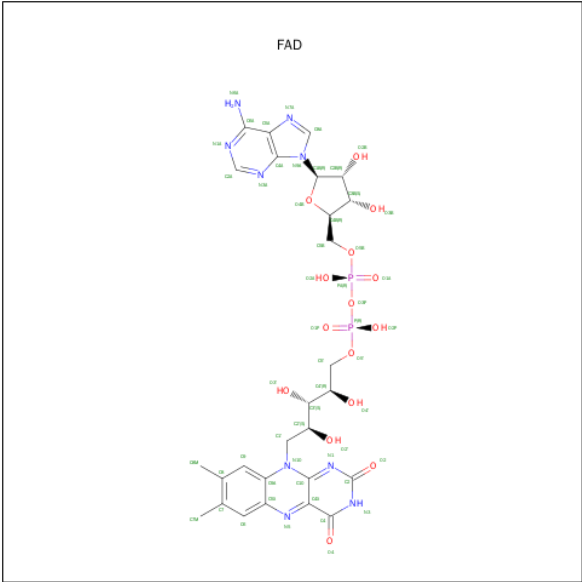
- Molecule 1 is a protein called Pyranose oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	577	Total	C	N	O	S	0	0	0
			4545	2868	778	874	25			
1	B	577	Total	C	N	O	S	0	0	0
			4545	2868	778	874	25			
1	C	577	Total	C	N	O	S	0	0	0
			4545	2868	778	874	25			
1	D	577	Total	C	N	O	S	0	0	0
			4545	2868	778	874	25			
1	E	577	Total	C	N	O	S	0	0	0
			4545	2868	778	874	25			
1	F	577	Total	C	N	O	S	0	0	0
			4545	2868	778	874	25			
1	G	577	Total	C	N	O	S	0	0	0
			4545	2868	778	874	25			
1	H	577	Total	C	N	O	S	0	0	0
			4545	2868	778	874	25			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	537	GLY	LEU	ENGINEERED	UNP Q7ZA32
B	537	GLY	LEU	ENGINEERED	UNP Q7ZA32
C	537	GLY	LEU	ENGINEERED	UNP Q7ZA32
D	537	GLY	LEU	ENGINEERED	UNP Q7ZA32
E	537	GLY	LEU	ENGINEERED	UNP Q7ZA32
F	537	GLY	LEU	ENGINEERED	UNP Q7ZA32
G	537	GLY	LEU	ENGINEERED	UNP Q7ZA32
H	537	GLY	LEU	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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	257	Total	O	0	0
			257	257		
3	B	279	Total	O	0	0
			279	279		
3	C	209	Total	O	0	0
			209	209		
3	D	231	Total	O	0	0
			231	231		

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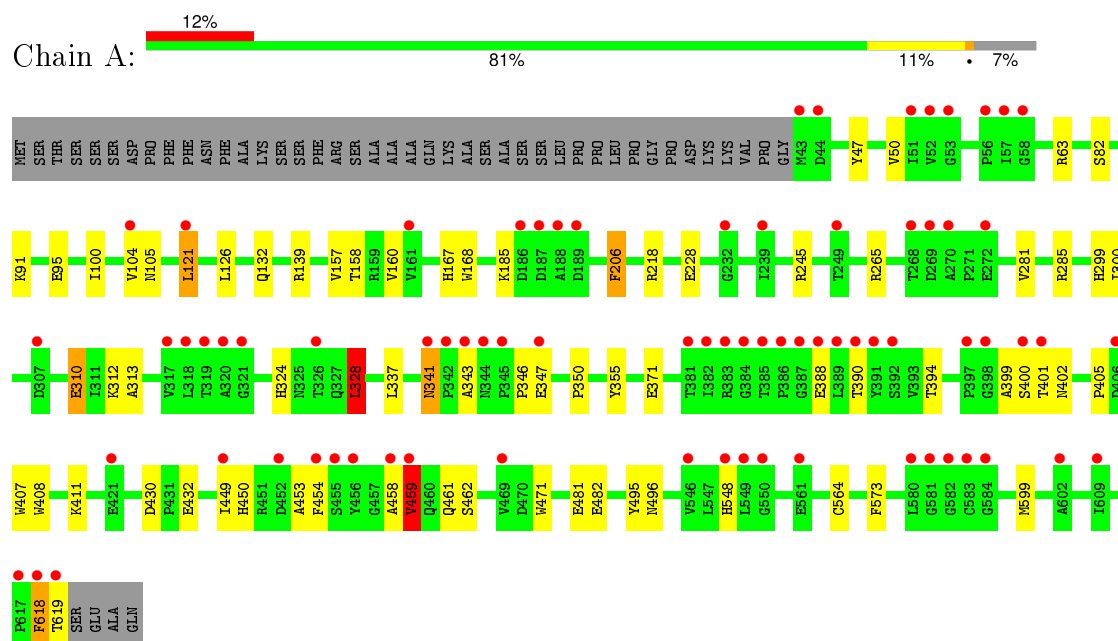
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	197	Total 197	O 197	0	0
3	F	197	Total 197	O 197	0	0
3	G	231	Total 231	O 231	0	0
3	H	256	Total 256	O 256	0	0

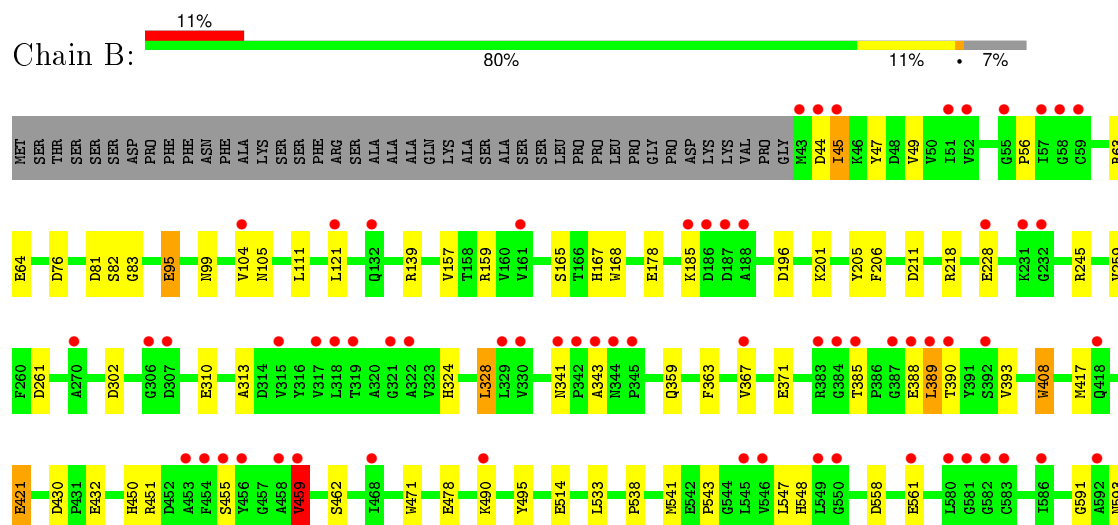
### 3 Residue-property plots

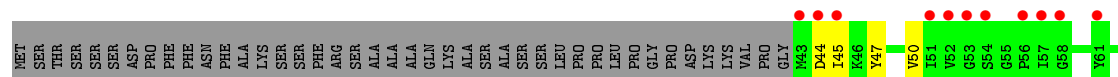
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

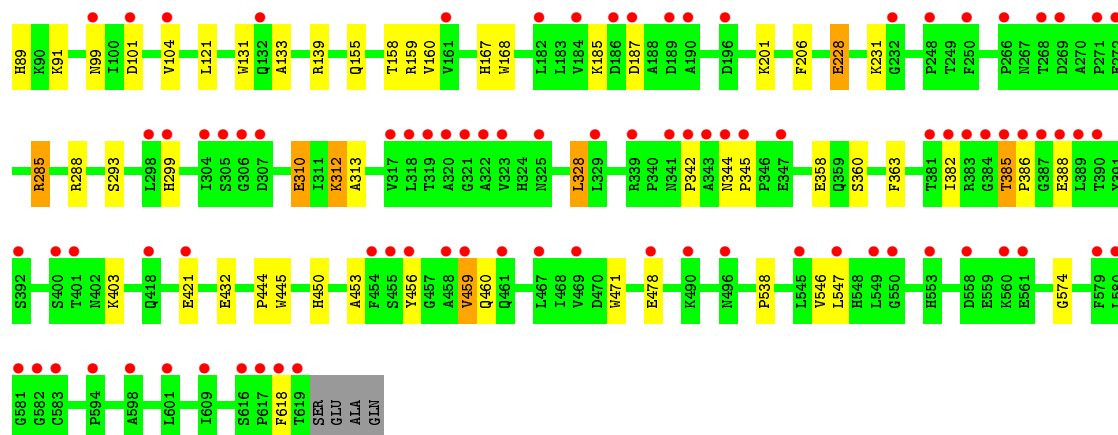


#### • Molecule 1: Pyranose oxidase

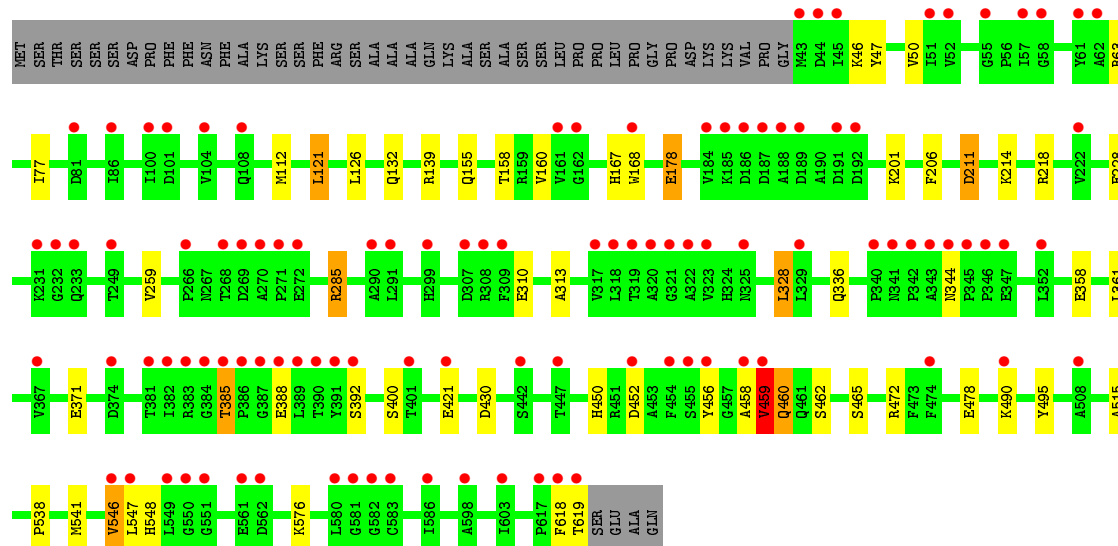
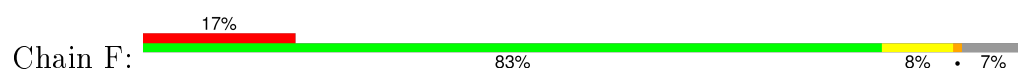




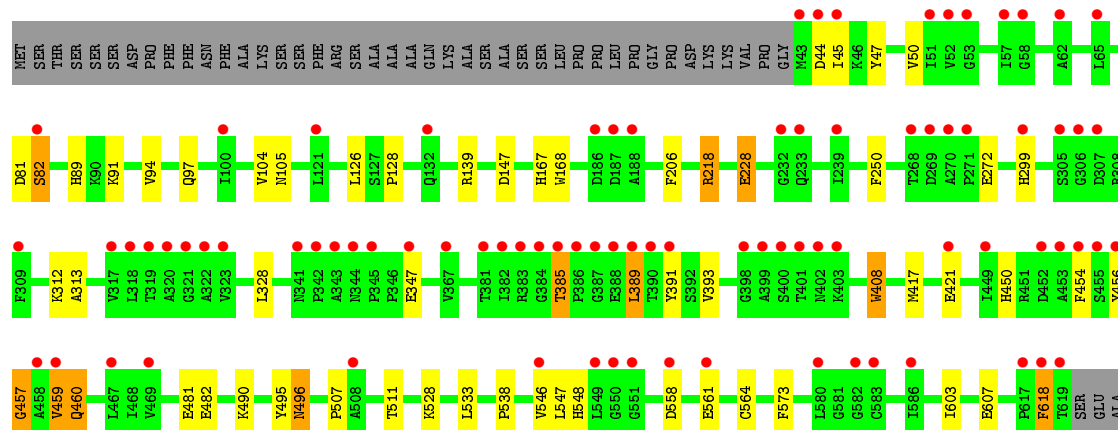
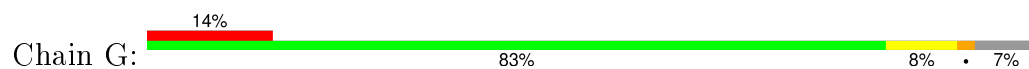




• Molecule 1: Pyranose oxidase

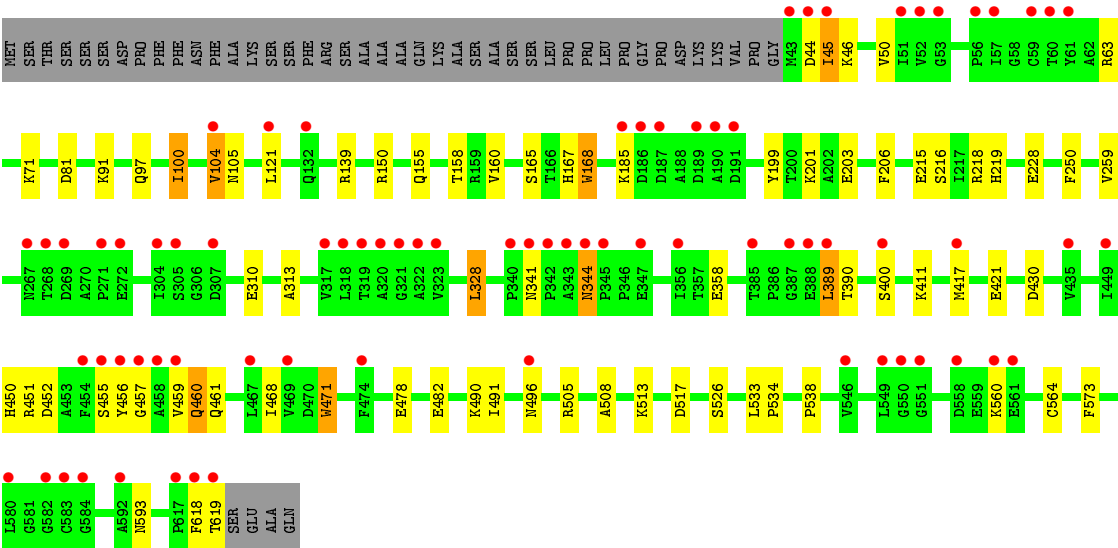
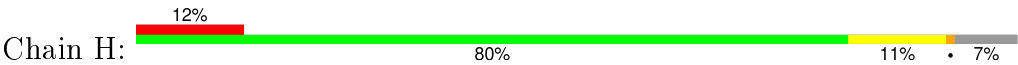


• Molecule 1: Pyranose oxidase



GLN

• Molecule 1: Pyranose oxidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	168.54Å 103.18Å 169.34Å 90.00° 106.45° 90.00°	Depositor
Resolution (Å)	29.72 – 2.10 29.72 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.72-2.10) 99.1 (29.72-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.07 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.156 , 0.204 0.168 , 0.215	Depositor DCC
$R_{free}$ test set	3262 reflections (1.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.8	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 56.2	EDS
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 321135 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	38641	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.48% 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, 0.375 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: FAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	1.12	11/4661 (0.2%)	0.97	11/6337 (0.2%)
1	B	1.13	10/4661 (0.2%)	1.00	17/6337 (0.3%)
1	C	0.99	5/4661 (0.1%)	0.90	9/6337 (0.1%)
1	D	1.01	6/4661 (0.1%)	0.90	8/6337 (0.1%)
1	E	0.98	9/4661 (0.2%)	0.86	6/6337 (0.1%)
1	F	0.95	7/4661 (0.2%)	0.87	5/6337 (0.1%)
1	G	1.06	9/4661 (0.2%)	0.91	7/6337 (0.1%)
1	H	1.04	9/4661 (0.2%)	0.92	6/6337 (0.1%)
All	All	1.04	66/37288 (0.2%)	0.92	69/50696 (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	2
1	B	0	1
1	C	0	1
1	F	0	1
1	G	0	1
All	All	0	6

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	228	GLU	CG-CD	10.91	1.68	1.51
1	D	310	GLU	CG-CD	10.02	1.67	1.51
1	D	310	GLU	CB-CG	8.87	1.69	1.52
1	A	310	GLU	CB-CG	8.15	1.67	1.52
1	E	310	GLU	CG-CD	8.00	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	228	GLU	CG-CD	7.88	1.63	1.51
1	A	310	GLU	CG-CD	7.59	1.63	1.51
1	G	482	GLU	CG-CD	7.38	1.63	1.51
1	B	421	GLU	CB-CG	6.87	1.65	1.52
1	F	228	GLU	CG-CD	6.87	1.62	1.51
1	H	310	GLU	CG-CD	6.85	1.62	1.51
1	A	432	GLU	CD-OE2	6.84	1.33	1.25
1	E	310	GLU	CB-CG	6.78	1.65	1.52
1	D	482	GLU	CG-CD	6.58	1.61	1.51
1	F	310	GLU	CG-CD	6.51	1.61	1.51
1	G	421	GLU	CB-CG	6.49	1.64	1.52
1	F	310	GLU	CB-CG	6.47	1.64	1.52
1	D	228	GLU	CG-CD	6.45	1.61	1.51
1	G	228	GLU	CG-CD	6.39	1.61	1.51
1	H	482	GLU	CG-CD	6.32	1.61	1.51
1	E	312	LYS	CD-CE	6.30	1.67	1.51
1	E	228	GLU	CG-CD	6.23	1.61	1.51
1	B	310	GLU	CB-CG	6.22	1.64	1.52
1	A	482	GLU	CG-CD	6.21	1.61	1.51
1	H	228	GLU	CB-CG	6.18	1.63	1.52
1	B	310	GLU	CG-CD	6.16	1.61	1.51
1	G	460	GLN	CB-CG	6.16	1.69	1.52
1	A	371	GLU	CD-OE1	6.11	1.32	1.25
1	A	228	GLU	CG-CD	6.04	1.61	1.51
1	G	82	SER	CB-OG	6.03	1.50	1.42
1	A	228	GLU	CD-OE1	6.01	1.32	1.25
1	C	310	GLU	CB-CG	5.98	1.63	1.52
1	E	421	GLU	CG-CD	5.97	1.60	1.51
1	A	371	GLU	CG-CD	5.74	1.60	1.51
1	B	514	GLU	CG-CD	5.70	1.60	1.51
1	D	432	GLU	CG-CD	5.62	1.60	1.51
1	C	421	GLU	CB-CG	5.62	1.62	1.52
1	G	347	GLU	CG-CD	5.59	1.60	1.51
1	F	371	GLU	CG-CD	5.58	1.60	1.51
1	A	139	ARG	CD-NE	-5.57	1.36	1.46
1	B	49	VAL	CB-CG2	5.56	1.64	1.52
1	C	310	GLU	CG-CD	5.52	1.60	1.51
1	A	355	TYR	CD2-CE2	-5.50	1.31	1.39
1	D	323	VAL	CB-CG2	5.48	1.64	1.52
1	C	101	ASP	CB-CG	5.41	1.63	1.51
1	H	508	ALA	CA-CB	5.41	1.63	1.52
1	E	421	GLU	CB-CG	5.40	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	310	GLU	CB-CG	5.39	1.62	1.52
1	B	371	GLU	CG-CD	5.33	1.59	1.51
1	G	94	VAL	CB-CG2	5.32	1.64	1.52
1	H	104	VAL	CB-CG2	-5.26	1.41	1.52
1	F	478	GLU	CG-CD	5.25	1.59	1.51
1	E	101	ASP	CB-CG	5.24	1.62	1.51
1	G	490	LYS	CD-CE	5.23	1.64	1.51
1	H	471	TRP	CB-CG	-5.22	1.40	1.50
1	E	432	GLU	CG-CD	5.21	1.59	1.51
1	B	478	GLU	CG-CD	5.21	1.59	1.51
1	H	478	GLU	CD-OE1	5.18	1.31	1.25
1	B	104	VAL	CB-CG2	-5.14	1.42	1.52
1	B	432	GLU	CD-OE2	5.12	1.31	1.25
1	G	421	GLU	CG-CD	5.09	1.59	1.51
1	F	178	GLU	CG-CD	5.08	1.59	1.51
1	C	132	GLN	CG-CD	5.03	1.62	1.51
1	F	478	GLU	CD-OE1	5.03	1.31	1.25
1	E	478	GLU	CD-OE1	5.03	1.31	1.25
1	A	347	GLU	CB-CG	5.02	1.61	1.52

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	ARG	NE-CZ-NH2	-17.72	111.44	120.30
1	F	139	ARG	NE-CZ-NH2	-17.23	111.69	120.30
1	B	139	ARG	NE-CZ-NH2	-14.69	112.96	120.30
1	E	139	ARG	NE-CZ-NH2	-13.21	113.70	120.30
1	C	139	ARG	NE-CZ-NH2	-13.05	113.77	120.30
1	D	139	ARG	NE-CZ-NH2	-11.81	114.39	120.30
1	B	139	ARG	NE-CZ-NH1	11.66	126.13	120.30
1	C	139	ARG	NE-CZ-NH1	9.94	125.27	120.30
1	F	139	ARG	NE-CZ-NH1	9.79	125.20	120.30
1	G	139	ARG	NE-CZ-NH2	-9.36	115.62	120.30
1	H	139	ARG	NE-CZ-NH2	-9.20	115.70	120.30
1	A	139	ARG	NE-CZ-NH1	8.95	124.78	120.30
1	D	139	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	B	196	ASP	CB-CG-OD1	7.51	125.06	118.30
1	H	104	VAL	CB-CA-C	-7.38	97.38	111.40
1	B	261	ASP	CB-CG-OD1	7.27	124.84	118.30
1	A	139	ARG	CG-CD-NE	-7.18	96.71	111.80
1	B	245	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	H	139	ARG	NE-CZ-NH1	7.05	123.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	139	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	B	211	ASP	CB-CG-OD1	6.91	124.52	118.30
1	G	139	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	C	218	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	D	104	VAL	CB-CA-C	-6.63	98.80	111.40
1	C	245	ARG	NE-CZ-NH1	6.53	123.57	120.30
1	B	245	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	A	139	ARG	CD-NE-CZ	6.50	132.70	123.60
1	H	328	LEU	CA-CB-CG	6.41	130.04	115.30
1	D	288	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	C	470	ASP	CB-CG-OD1	6.15	123.84	118.30
1	H	81	ASP	CB-CG-OD1	-6.13	112.78	118.30
1	C	218	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	B	302	ASP	CB-CG-OD1	6.11	123.80	118.30
1	B	599	MET	CG-SD-CE	5.98	109.77	100.20
1	B	328	LEU	CB-CG-CD1	5.96	121.13	111.00
1	G	147	ASP	CB-CG-OD1	5.90	123.61	118.30
1	H	417	MET	CG-SD-CE	-5.86	90.83	100.20
1	G	218	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	D	310	GLU	OE1-CD-OE2	-5.82	116.31	123.30
1	F	211	ASP	CB-CG-OD1	5.79	123.51	118.30
1	A	63	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	245	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	B	139	ARG	CB-CA-C	-5.70	99.00	110.40
1	C	101	ASP	CB-CG-OD1	5.68	123.41	118.30
1	B	451	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	D	470	ASP	CB-CG-OD1	5.60	123.34	118.30
1	E	288	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	D	139	ARG	CG-CD-NE	-5.54	100.17	111.80
1	B	111	LEU	CB-CG-CD1	-5.42	101.80	111.00
1	C	139	ARG	CB-CA-C	-5.40	99.59	110.40
1	E	310	GLU	OE1-CD-OE2	-5.40	116.83	123.30
1	G	139	ARG	CB-CA-C	-5.38	99.63	110.40
1	C	470	ASP	CB-CG-OD2	-5.36	113.47	118.30
1	G	82	SER	CA-CB-OG	5.33	125.60	111.20
1	A	265	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	B	76	ASP	CB-CG-OD1	5.28	123.05	118.30
1	D	211	ASP	CB-CG-OD1	5.25	123.03	118.30
1	B	211	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	F	139	ARG	CG-CD-NE	-5.23	100.81	111.80
1	B	139	ARG	CD-NE-CZ	5.23	130.92	123.60
1	E	139	ARG	CB-CA-C	-5.18	100.04	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	337	LEU	CB-CG-CD2	-5.12	102.29	111.00
1	A	63	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	E	139	ARG	CG-CD-NE	-5.08	101.14	111.80
1	B	82	SER	CB-CA-C	-5.08	100.46	110.10
1	F	139	ARG	CD-NE-CZ	5.08	130.71	123.60
1	A	328	LEU	CA-CB-CG	5.06	126.94	115.30
1	A	265	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	G	139	ARG	CG-CD-NE	-5.02	101.26	111.80

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	390	THR	Peptide
1	A	459	VAL	Peptide
1	B	459	VAL	Peptide
1	C	459	VAL	Peptide
1	F	459	VAL	Peptide
1	G	81	ASP	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	4545	0	4387	58	0
1	B	4545	0	4387	77	0
1	C	4545	0	4387	67	0
1	D	4545	0	4387	52	0
1	E	4545	0	4387	60	0
1	F	4545	0	4387	52	0
1	G	4545	0	4387	54	0
1	H	4545	0	4387	62	0
2	A	53	0	28	6	0
2	B	53	0	30	14	0
2	C	53	0	27	5	0
2	D	53	0	29	8	0
2	E	53	0	28	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	53	0	28	5	0
2	G	53	0	28	9	0
2	H	53	0	28	5	0
3	A	257	0	0	4	0
3	B	279	0	0	6	0
3	C	209	0	0	3	0
3	D	231	0	0	2	0
3	E	197	0	0	3	0
3	F	197	0	0	1	0
3	G	231	0	0	5	0
3	H	256	0	0	2	0
All	All	38641	0	35322	416	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (416) 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	1.62
1:C:167:HIS:HE2	2:C:801:FAD:C8M	0.99	1.62
1:H:167:HIS:HE2	2:H:801:FAD:C8M	1.05	1.58
1:F:167:HIS:HE2	2:F:801:FAD:C8M	1.07	1.56
1:A:167:HIS:HE2	2:A:801:FAD:C8M	1.14	1.55
1:E:167:HIS:HE2	2:E:801:FAD:C8M	1.15	1.54
1:G:167:HIS:HE2	2:G:801:FAD:C8M	1.19	1.52
1:D:167:HIS:HE2	2:D:801:FAD:C8M	1.26	1.48
1:E:167:HIS:NE2	2:E:801:FAD:HM82	1.29	1.48
1:A:167:HIS:NE2	2:A:801:FAD:HM82	1.25	1.41
1:B:167:HIS:NE2	2:B:801:FAD:HM82	1.30	1.40
1:F:167:HIS:NE2	2:F:801:FAD:HM82	1.07	1.39
1:G:167:HIS:NE2	2:G:801:FAD:HM82	1.34	1.37
1:H:167:HIS:NE2	2:H:801:FAD:HM82	1.09	1.37
1:C:167:HIS:NE2	2:C:801:FAD:HM82	1.02	1.33
1:E:459:VAL:CG1	1:F:121:LEU:HD22	1.61	1.31
1:D:167:HIS:NE2	2:D:801:FAD:HM82	1.43	1.30
1:B:388:GLU:OE1	1:B:389:LEU:HD13	1.42	1.16
1:B:388:GLU:OE1	1:B:389:LEU:CD1	1.96	1.12
1:G:456:TYR:CD1	1:G:460:GLN:HB3	1.83	1.12
1:D:299:HIS:HB2	1:D:310:GLU:OE1	1.49	1.11
1:A:167:HIS:HE2	2:A:801:FAD:HM81	1.16	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:LEU:HD22	1:B:459:VAL:CG1	1.83	1.09
1:D:389:LEU:H	1:D:389:LEU:CD1	1.67	1.07
1:A:167:HIS:CD2	2:A:801:FAD:HM82	1.90	1.06
1:C:167:HIS:CD2	2:C:801:FAD:HM82	1.91	1.06
1:B:393:VAL:H	1:B:417:MET:HE2	1.19	1.05
1:D:389:LEU:HD12	1:D:389:LEU:H	0.86	1.01
1:D:389:LEU:N	1:D:389:LEU:HD12	1.71	1.00
1:E:459:VAL:HG11	1:F:121:LEU:HD22	1.00	0.98
1:C:167:HIS:HE2	2:C:801:FAD:HM81	1.29	0.98
1:F:167:HIS:CD2	2:F:801:FAD:HM82	1.99	0.97
1:D:167:HIS:HE2	2:D:801:FAD:HM81	1.30	0.96
1:A:459:VAL:HG13	1:B:121:LEU:HB3	1.47	0.96
1:A:121:LEU:HD22	1:B:459:VAL:HG11	1.43	0.96
1:D:167:HIS:HE2	2:D:801:FAD:HM82	0.82	0.95
1:A:121:LEU:HB3	1:B:459:VAL:CG1	1.96	0.95
1:E:459:VAL:HG11	1:F:121:LEU:CD2	1.96	0.95
1:C:121:LEU:HB3	1:D:459:VAL:CG1	1.96	0.95
1:C:121:LEU:HB3	1:D:459:VAL:HG13	1.47	0.94
1:H:167:HIS:CD2	2:H:801:FAD:HM82	2.02	0.94
1:E:459:VAL:CG1	1:F:121:LEU:CD2	2.46	0.94
1:C:459:VAL:CG1	1:D:121:LEU:HB3	1.99	0.93
1:B:393:VAL:H	1:B:417:MET:CE	1.83	0.90
1:H:167:HIS:HE2	2:H:801:FAD:HM81	1.34	0.90
1:A:121:LEU:HB3	1:B:459:VAL:HG12	1.52	0.89
1:C:389:LEU:H	1:C:389:LEU:HD13	1.36	0.89
1:E:167:HIS:HE2	2:E:801:FAD:HM81	1.35	0.89
1:B:167:HIS:HE2	2:B:801:FAD:HM81	1.38	0.88
1:G:167:HIS:HE2	2:G:801:FAD:C8	1.87	0.87
1:A:121:LEU:HD22	1:B:459:VAL:HG13	1.57	0.87
1:H:341:ASN:HD22	1:H:344:ASN:CB	1.89	0.86
1:A:458:ALA:O	1:B:121:LEU:HD12	1.76	0.86
1:H:341:ASN:HD22	1:H:344:ASN:HB3	1.42	0.85
1:G:456:TYR:HD1	1:G:460:GLN:HB3	1.42	0.84
1:B:167:HIS:HE2	2:B:801:FAD:HM82	0.68	0.84
1:A:459:VAL:HG13	1:B:121:LEU:CB	2.07	0.84
1:E:121:LEU:CD2	1:H:121:LEU:CD2	2.57	0.83
1:B:167:HIS:HE2	2:B:801:FAD:C8	1.90	0.82
1:F:167:HIS:HE2	2:F:801:FAD:HM81	1.43	0.82
1:D:299:HIS:CB	1:D:310:GLU:OE1	2.26	0.82
1:A:341:ASN:HD22	1:A:343:ALA:H	1.28	0.81
1:A:459:VAL:CG1	1:B:121:LEU:HB3	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:167:HIS:HE2	2:G:801:FAD:HM82	0.63	0.80
1:G:456:TYR:CD1	1:G:460:GLN:CB	2.65	0.80
1:F:285:ARG:HA	1:F:328:LEU:CD1	2.11	0.80
1:C:459:VAL:HG13	1:D:121:LEU:HB3	1.64	0.80
1:E:167:HIS:HE2	2:E:801:FAD:HM82	0.64	0.80
1:E:167:HIS:CD2	2:E:801:FAD:HM82	2.16	0.80
1:E:459:VAL:HG13	1:F:121:LEU:HD22	1.64	0.79
1:C:121:LEU:CB	1:D:459:VAL:HG13	2.12	0.79
1:E:459:VAL:HG13	1:F:121:LEU:CG	2.13	0.79
1:D:167:HIS:CD2	2:D:801:FAD:HM82	2.17	0.79
1:B:388:GLU:OE1	1:B:389:LEU:HD11	1.81	0.78
1:A:167:HIS:HE2	2:A:801:FAD:HM82	0.79	0.77
1:G:456:TYR:HD1	1:G:460:GLN:CB	1.97	0.77
1:D:312:LYS:HE3	3:D:880:HOH:O	1.82	0.77
1:D:100:ILE:HD13	1:D:100:ILE:O	1.85	0.77
1:C:478:GLU:OE2	1:C:480:LYS:HE2	1.83	0.77
1:F:63:ARG:HD2	1:F:259:VAL:O	1.85	0.76
1:B:393:VAL:N	1:B:417:MET:HE2	1.99	0.76
1:F:50:VAL:HG13	1:F:313:ALA:HB2	1.69	0.75
1:B:389:LEU:HD13	1:B:389:LEU:H	1.53	0.74
1:E:459:VAL:CG1	1:F:121:LEU:HB3	2.18	0.73
1:E:121:LEU:HD22	1:H:121:LEU:CD2	2.18	0.73
1:A:285:ARG:HA	1:A:328:LEU:HD13	1.71	0.73
1:D:285:ARG:HA	1:D:328:LEU:CD1	2.19	0.73
1:A:121:LEU:CD2	1:B:459:VAL:CG1	2.65	0.72
1:E:121:LEU:HB3	1:F:459:VAL:HG23	1.68	0.72
1:E:121:LEU:CD2	1:H:121:LEU:HD22	2.19	0.72
1:G:167:HIS:CE1	2:G:801:FAD:HM82	2.24	0.72
1:B:121:LEU:CD2	1:C:121:LEU:CD2	2.68	0.71
1:H:456:TYR:CD1	1:H:460:GLN:HB3	2.25	0.71
1:C:458:ALA:O	1:D:121:LEU:HD12	1.90	0.70
1:C:456:TYR:HB3	1:C:460:GLN:HB2	1.73	0.70
1:A:121:LEU:CB	1:B:459:VAL:CG1	2.70	0.69
1:H:460:GLN:HG2	1:H:533:LEU:HD21	1.73	0.69
1:C:459:VAL:O	1:C:462:SER:HB3	1.92	0.69
1:E:459:VAL:HG13	1:F:121:LEU:CD2	2.20	0.68
1:D:158:THR:HG22	1:D:160:VAL:HG22	1.76	0.68
1:A:341:ASN:ND2	1:A:343:ALA:H	1.92	0.68
1:G:393:VAL:H	1:G:417:MET:CE	2.07	0.67
1:C:101:ASP:O	1:C:104:VAL:HG23	1.95	0.67
1:E:459:VAL:HG12	1:F:121:LEU:HB3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:299:HIS:HB2	3:G:1133:HOH:O	1.94	0.67
1:D:285:ARG:HA	1:D:328:LEU:HD11	1.77	0.66
1:E:121:LEU:CB	1:F:459:VAL:HG23	2.26	0.66
1:E:299:HIS:HB2	1:E:310:GLU:OE1	1.96	0.66
1:C:359:GLN:NE2	1:C:591:GLY:O	2.29	0.66
1:E:459:VAL:HG13	1:F:121:LEU:HD13	1.76	0.66
1:A:121:LEU:CD2	1:B:459:VAL:HG13	2.24	0.66
1:C:617:PRO:O	1:C:619:THR:HG22	1.95	0.66
1:B:389:LEU:HD23	1:B:390:THR:HG23	1.77	0.66
1:H:619:THR:HG23	1:H:619:THR:O	1.95	0.66
1:B:121:LEU:HD21	1:C:121:LEU:CD2	2.26	0.66
1:B:121:LEU:CD2	1:C:121:LEU:HD21	2.26	0.66
1:C:389:LEU:H	1:C:389:LEU:CD1	2.04	0.65
1:B:45:ILE:H	1:B:45:ILE:HD13	1.61	0.65
1:H:167:HIS:HE2	2:H:801:FAD:HM82	0.49	0.65
1:G:547:LEU:CD1	2:G:801:FAD:HM83	2.27	0.65
1:C:158:THR:HG22	1:C:160:VAL:HG22	1.78	0.65
1:D:359:GLN:NE2	1:D:591:GLY:O	2.30	0.65
1:B:167:HIS:NE2	2:B:801:FAD:C8	2.57	0.64
1:H:158:THR:HG22	1:H:160:VAL:HG22	1.80	0.64
1:E:121:LEU:HD22	1:H:121:LEU:HD21	1.80	0.64
1:G:393:VAL:H	1:G:417:MET:HE2	1.63	0.64
1:C:459:VAL:HG13	1:D:121:LEU:CB	2.27	0.63
1:B:541:MET:HE3	3:B:959:HOH:O	1.97	0.63
1:B:178:GLU:HG3	3:B:972:HOH:O	1.97	0.63
1:H:490:LYS:HD2	1:H:491:ILE:HD13	1.79	0.63
1:E:459:VAL:HG13	1:F:121:LEU:CD1	2.28	0.63
1:C:121:LEU:CB	1:D:459:VAL:CG1	2.73	0.63
1:B:45:ILE:H	1:B:45:ILE:CD1	2.12	0.63
1:E:121:LEU:HD21	1:H:121:LEU:HD22	1.81	0.62
1:E:121:LEU:HD12	1:F:458:ALA:O	1.99	0.62
1:C:344:ASN:N	1:C:344:ASN:HD22	1.98	0.62
1:B:389:LEU:CD2	1:B:390:THR:HG23	2.29	0.61
1:E:89:HIS:CE1	1:E:91:LYS:HG2	2.35	0.61
1:H:201:LYS:NZ	3:H:906:HOH:O	2.27	0.61
1:G:167:HIS:NE2	2:G:801:FAD:C8	2.54	0.61
1:H:389:LEU:HD23	1:H:390:THR:N	2.15	0.61
1:H:341:ASN:HD22	1:H:344:ASN:HB2	1.65	0.61
1:F:328:LEU:HD12	1:F:328:LEU:O	2.00	0.61
1:G:89:HIS:CE1	1:G:91:LYS:HB2	2.35	0.61
1:B:359:GLN:OE1	1:B:548:HIS:ND1	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:285:ARG:HA	1:F:328:LEU:HD11	1.82	0.60
1:C:459:VAL:CG1	1:D:121:LEU:CB	2.77	0.59
1:C:359:GLN:OE1	1:C:548:HIS:HB2	2.02	0.59
1:G:547:LEU:HD12	2:G:801:FAD:HM83	1.84	0.59
1:E:344:ASN:N	1:E:345:PRO:HD3	2.16	0.59
1:F:538:PRO:HG2	1:H:538:PRO:HG2	1.85	0.59
1:A:91:LYS:NZ	3:A:963:HOH:O	2.35	0.59
1:E:385:THR:HG22	1:E:386:PRO:HD2	1.85	0.58
1:C:296:GLU:O	1:C:312:LYS:HD3	2.02	0.58
1:C:389:LEU:N	1:C:389:LEU:HD13	2.15	0.58
1:H:91:LYS:NZ	3:H:980:HOH:O	2.35	0.58
1:E:299:HIS:CB	1:E:310:GLU:OE1	2.52	0.58
1:A:157:VAL:HG21	1:A:324:HIS:HE1	1.67	0.58
1:G:558:ASP:HB3	1:G:561:GLU:HB3	1.86	0.58
1:A:121:LEU:CG	1:B:459:VAL:HG13	2.34	0.58
1:F:459:VAL:O	1:F:462:SER:HB3	2.04	0.57
1:B:459:VAL:HA	1:B:462:SER:HB2	1.86	0.57
1:C:459:VAL:O	1:C:462:SER:CB	2.53	0.57
1:A:50:VAL:HG13	1:A:313:ALA:HB2	1.85	0.57
1:B:167:HIS:NE2	2:B:801:FAD:HM81	2.08	0.57
1:G:456:TYR:HD1	1:G:460:GLN:CG	2.17	0.57
1:A:407:TRP:O	1:A:411:LYS:HG3	2.05	0.57
1:F:452:ASP:OD2	1:F:472:ARG:CZ	2.52	0.57
1:G:82:SER:HB2	3:G:1013:HOH:O	2.05	0.57
1:B:218:ARG:HG3	1:B:430:ASP:OD2	2.05	0.56
1:G:460:GLN:HG3	1:G:533:LEU:HD21	1.86	0.56
1:B:547:LEU:HD12	2:B:801:FAD:HM83	1.87	0.56
1:F:47:TYR:O	1:F:313:ALA:HA	2.05	0.56
1:E:104:VAL:CG2	1:E:453:ALA:HB1	2.35	0.56
1:H:460:GLN:HG2	1:H:533:LEU:CD2	2.34	0.56
1:H:389:LEU:HD23	1:H:390:THR:HG23	1.87	0.56
1:E:104:VAL:HG23	1:E:453:ALA:HB1	1.87	0.55
1:G:546:VAL:HG13	1:G:548:HIS:H	1.71	0.55
1:G:459:VAL:HG12	1:G:460:GLN:N	2.21	0.55
1:A:121:LEU:CB	1:B:459:VAL:HG13	2.36	0.55
1:C:459:VAL:HG12	1:D:121:LEU:HB3	1.83	0.54
1:A:104:VAL:CG2	1:A:454:PHE:N	2.70	0.54
1:C:218:ARG:HD2	3:C:882:HOH:O	2.06	0.54
1:C:158:THR:CG2	1:C:160:VAL:HG22	2.36	0.54
1:B:201:LYS:NZ	3:B:952:HOH:O	2.40	0.54
1:E:91:LYS:NZ	3:E:822:HOH:O	2.30	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:218:ARG:HG3	1:H:430:ASP:OD2	2.08	0.54
1:G:456:TYR:CG	1:G:460:GLN:HB3	2.41	0.54
1:E:50:VAL:HG13	1:E:313:ALA:HB2	1.90	0.54
1:G:481:GLU:HG2	3:G:1084:HOH:O	2.08	0.54
1:H:564:CYS:HG	1:H:573:PHE:HE2	1.55	0.54
1:C:343:ALA:C	1:C:344:ASN:HD22	2.11	0.54
1:B:167:HIS:CE1	2:B:801:FAD:HM82	2.28	0.53
1:C:293:SER:HA	1:C:574:GLY:O	2.08	0.53
1:C:121:LEU:HD12	1:D:458:ALA:O	2.08	0.53
1:D:456:TYR:HB3	1:D:460:GLN:HB2	1.91	0.53
1:G:89:HIS:ND1	1:G:91:LYS:HB2	2.23	0.53
1:G:44:ASP:OD1	1:G:45:ILE:N	2.42	0.53
1:E:121:LEU:HB3	1:F:459:VAL:CG2	2.37	0.53
1:H:460:GLN:CG	1:H:533:LEU:HD21	2.38	0.53
1:A:104:VAL:HG21	1:A:454:PHE:CA	2.39	0.53
1:A:564:CYS:HG	1:A:573:PHE:HE2	1.56	0.53
1:E:459:VAL:CG1	1:F:121:LEU:CB	2.87	0.53
1:G:456:TYR:HD1	1:G:460:GLN:HG2	1.73	0.52
1:A:167:HIS:CD2	2:A:801:FAD:C8M	2.73	0.52
1:A:481:GLU:HG2	3:A:1028:HOH:O	2.08	0.52
1:E:459:VAL:HG13	1:F:121:LEU:CB	2.39	0.52
1:C:47:TYR:O	1:C:313:ALA:HA	2.09	0.52
1:D:97:GLN:HG3	1:D:250:PHE:CE2	2.44	0.52
1:F:361:LEU:HD23	1:F:541:MET:HG3	1.92	0.52
1:B:388:GLU:HB3	1:B:389:LEU:HD22	1.92	0.52
1:C:97:GLN:HG3	1:C:250:PHE:CD2	2.44	0.52
1:H:490:LYS:HD3	1:H:490:LYS:O	2.08	0.52
1:E:285:ARG:HA	1:E:328:LEU:CD1	2.40	0.52
1:D:393:VAL:H	1:D:417:MET:CE	2.22	0.52
1:A:346:PRO:HG2	1:A:350:PRO:HA	1.92	0.52
1:A:218:ARG:HG3	1:A:430:ASP:OD2	2.10	0.52
1:B:167:HIS:CD2	2:B:801:FAD:HM82	2.32	0.52
1:F:456:TYR:HB3	1:F:460:GLN:HB2	1.92	0.52
1:A:121:LEU:CD2	1:B:459:VAL:HG11	2.28	0.51
1:H:44:ASP:OD2	1:H:71:LYS:NZ	2.34	0.51
1:H:619:THR:CG2	1:H:619:THR:O	2.59	0.51
1:D:50:VAL:HG13	1:D:313:ALA:HB2	1.92	0.51
1:F:459:VAL:O	1:F:462:SER:CB	2.59	0.51
1:D:89:HIS:ND1	1:D:91:LYS:HB3	2.26	0.51
1:E:459:VAL:CG1	1:F:121:LEU:CG	2.82	0.50
1:F:211:ASP:HB2	1:F:214:LYS:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:50:VAL:HG13	1:H:313:ALA:HB2	1.92	0.50
1:B:167:HIS:CE1	2:B:801:FAD:C8M	2.88	0.50
1:F:361:LEU:CD2	1:F:541:MET:HG3	2.42	0.50
1:E:456:TYR:HD1	1:E:460:GLN:HB3	1.76	0.50
1:H:471:TRP:CH2	1:H:526:SER:HA	2.47	0.50
1:H:45:ILE:C	1:H:45:ILE:HD12	2.32	0.50
1:A:299:HIS:HD1	1:A:310:GLU:CD	2.14	0.49
1:H:451:ARG:HD3	1:H:468:ILE:O	2.12	0.49
1:C:169:THR:O	1:C:169:THR:HG22	2.12	0.49
1:C:132:GLN:NE2	3:C:930:HOH:O	2.44	0.49
1:G:546:VAL:HG13	1:G:547:LEU:N	2.27	0.49
1:D:336:GLN:HB2	1:D:346:PRO:HG3	1.95	0.49
1:G:91:LYS:NZ	3:G:958:HOH:O	2.45	0.49
1:E:99:ASN:ND2	1:F:112:MET:SD	2.86	0.49
1:B:95:GLU:O	1:B:99:ASN:ND2	2.45	0.49
1:A:285:ARG:HA	1:A:328:LEU:CD1	2.41	0.49
1:D:218:ARG:HG3	1:D:430:ASP:OD2	2.12	0.48
1:B:81:ASP:C	1:B:81:ASP:OD1	2.51	0.48
1:C:617:PRO:O	1:C:619:THR:N	2.47	0.48
1:B:538:PRO:HG2	1:D:538:PRO:HG2	1.95	0.48
1:G:47:TYR:O	1:G:313:ALA:HA	2.14	0.48
1:H:63:ARG:HD2	1:H:259:VAL:O	2.14	0.48
1:B:341:ASN:OD1	1:B:343:ALA:HB3	2.14	0.48
1:F:619:THR:O	1:F:619:THR:HG23	2.13	0.48
1:E:360:SER:HB2	3:E:998:HOH:O	2.14	0.48
1:C:285:ARG:HA	1:C:328:LEU:CD1	2.43	0.48
1:F:201:LYS:NZ	3:F:964:HOH:O	2.46	0.47
1:C:312:LYS:HD2	1:C:316:TYR:OH	2.13	0.47
1:D:150:ARG:NH1	1:D:505:ARG:HG3	2.29	0.47
1:E:344:ASN:N	1:E:345:PRO:CD	2.77	0.47
1:B:558:ASP:HB3	1:B:561:GLU:HB2	1.96	0.47
1:G:44:ASP:OD1	1:G:45:ILE:HG13	2.14	0.47
1:G:393:VAL:H	1:G:417:MET:HE1	1.78	0.47
1:G:507:PRO:HD2	1:G:511:THR:HG21	1.96	0.47
1:F:218:ARG:HG3	1:F:430:ASP:OD2	2.14	0.47
1:G:459:VAL:O	1:G:460:GLN:C	2.53	0.47
1:H:456:TYR:CD1	1:H:460:GLN:CB	2.95	0.47
1:C:63:ARG:HD2	1:C:259:VAL:O	2.14	0.47
1:H:341:ASN:ND2	1:H:344:ASN:CB	2.69	0.47
1:D:299:HIS:CA	1:D:310:GLU:OE1	2.62	0.47
1:E:546:VAL:HG13	1:E:547:LEU:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:ILE:HG12	1:A:471:TRP:CE3	2.50	0.47
1:A:47:TYR:O	1:A:313:ALA:HA	2.15	0.46
1:E:444:PRO:HD2	1:E:445:TRP:CZ3	2.50	0.46
1:E:155:GLN:NE2	1:E:358:GLU:OE2	2.48	0.46
1:G:546:VAL:CG1	1:G:547:LEU:N	2.78	0.46
1:B:121:LEU:HD22	1:C:121:LEU:HD21	1.96	0.46
1:D:336:GLN:NE2	1:D:344:ASN:O	2.47	0.46
1:C:100:ILE:CD1	3:C:989:HOH:O	2.63	0.46
1:A:405:PRO:O	1:A:408:TRP:HB3	2.15	0.46
1:D:201:LYS:NZ	3:D:881:HOH:O	2.28	0.46
1:E:293:SER:HA	1:E:574:GLY:O	2.15	0.46
1:F:126:LEU:HD13	1:F:132:GLN:CG	2.45	0.46
1:B:459:VAL:O	1:B:462:SER:HB3	2.16	0.46
1:B:389:LEU:CD1	1:B:389:LEU:H	2.22	0.46
1:G:457:GLY:C	1:G:459:VAL:H	2.19	0.46
1:H:456:TYR:HD1	1:H:460:GLN:CB	2.28	0.46
1:E:47:TYR:O	1:E:313:ALA:HA	2.15	0.46
1:H:100:ILE:HD13	1:H:100:ILE:O	2.15	0.46
1:B:45:ILE:N	1:B:45:ILE:CD1	2.78	0.46
1:H:150:ARG:NH1	1:H:505:ARG:HG3	2.31	0.46
1:C:341:ASN:HD21	1:C:343:ALA:HB3	1.81	0.46
1:G:97:GLN:HG3	1:G:250:PHE:CE2	2.51	0.46
1:H:155:GLN:NE2	1:H:358:GLU:OE2	2.45	0.46
1:E:158:THR:HG22	1:E:160:VAL:HG22	1.99	0.46
1:A:206:PHE:CE2	1:A:599:MET:CE	2.99	0.46
1:C:206:PHE:CE2	1:C:599:MET:HE3	2.51	0.46
1:C:414:ASN:O	1:C:418:GLN:HG2	2.16	0.46
1:C:206:PHE:CE2	1:C:599:MET:CE	2.99	0.45
1:D:89:HIS:CE1	1:D:91:LYS:HB3	2.51	0.45
1:A:399:ALA:O	1:A:402:ASN:HB2	2.16	0.45
1:D:169:THR:O	1:D:170:CYS:HB2	2.17	0.45
1:B:63:ARG:HD2	1:B:259:VAL:O	2.17	0.45
1:G:167:HIS:CD2	1:G:167:HIS:C	2.89	0.45
1:H:456:TYR:HD1	1:H:460:GLN:HB3	1.79	0.45
1:G:104:VAL:HG21	1:G:454:PHE:C	2.36	0.45
1:D:159:ARG:HA	2:D:801:FAD:O2B	2.16	0.45
1:A:104:VAL:HG22	1:A:453:ALA:C	2.37	0.45
1:G:618:PHE:C	1:G:618:PHE:CD1	2.90	0.45
1:G:218:ARG:HD2	3:G:1014:HOH:O	2.15	0.45
1:B:159:ARG:HA	2:B:801:FAD:O2B	2.17	0.45
1:E:131:TRP:CH2	1:E:133:ALA:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LEU:CD1	1:A:132:GLN:CG	2.95	0.44
1:B:167:HIS:CD2	1:B:167:HIS:C	2.90	0.44
1:E:342:PRO:C	1:E:344:ASN:H	2.20	0.44
1:H:97:GLN:HG3	1:H:250:PHE:CD2	2.52	0.44
1:A:206:PHE:CE2	1:A:599:MET:HE3	2.53	0.44
1:B:64:GLU:OE2	1:B:205:TYR:OH	2.24	0.44
1:G:603:ILE:O	1:G:607:GLU:HG3	2.18	0.44
1:H:344:ASN:O	1:H:344:ASN:CG	2.55	0.44
1:A:341:ASN:C	1:A:341:ASN:HD22	2.21	0.44
1:D:358:GLU:OE1	1:D:546:VAL:HG13	2.17	0.44
1:A:158:THR:HG22	1:A:160:VAL:HG22	2.00	0.44
1:C:159:ARG:HA	2:C:801:FAD:O2B	2.17	0.44
1:E:459:VAL:HG13	1:F:121:LEU:HB3	1.97	0.44
1:D:319:THR:HG22	1:D:581:GLY:HA3	2.00	0.44
1:B:121:LEU:HD21	1:C:121:LEU:HD23	1.99	0.44
1:C:157:VAL:HG21	1:C:324:HIS:HE1	1.83	0.44
1:C:408:TRP:CD1	1:C:408:TRP:C	2.90	0.44
1:G:564:CYS:HG	1:G:573:PHE:HE2	1.66	0.43
1:B:157:VAL:HG21	1:B:324:HIS:HE1	1.83	0.43
1:C:344:ASN:N	1:C:344:ASN:ND2	2.64	0.43
1:F:515:ALA:HB3	1:G:128:PRO:HG2	2.00	0.43
1:A:495:TYR:O	1:A:496:ASN:CB	2.66	0.43
1:A:105:ASN:O	1:B:105:ASN:HB3	2.19	0.43
1:B:547:LEU:CD1	2:B:801:FAD:HM83	2.48	0.43
1:A:95:GLU:OE1	1:B:495:TYR:OH	2.29	0.43
1:F:328:LEU:HD12	1:F:328:LEU:C	2.37	0.43
1:F:77:ILE:HD11	1:F:495:TYR:CD2	2.54	0.43
1:G:328:LEU:HD12	1:G:328:LEU:O	2.18	0.43
1:E:538:PRO:HG2	1:G:538:PRO:HG2	2.01	0.43
1:F:546:VAL:HG13	1:F:548:HIS:H	1.83	0.43
1:B:408:TRP:CD1	1:B:408:TRP:C	2.92	0.43
1:C:618:PHE:C	1:C:618:PHE:CD1	2.92	0.43
1:H:100:ILE:C	1:H:100:ILE:HD13	2.39	0.43
1:C:541:MET:HE2	1:C:545:LEU:HD23	2.01	0.43
1:B:363:PHE:HA	1:B:471:TRP:O	2.19	0.43
1:F:158:THR:HG22	1:F:160:VAL:HG22	2.01	0.43
1:D:97:GLN:HG3	1:D:250:PHE:CD2	2.54	0.43
1:C:607:GLU:O	1:C:611:GLN:HG3	2.18	0.43
1:A:341:ASN:HD22	1:A:343:ALA:N	2.07	0.43
1:E:201:LYS:NZ	3:E:945:HOH:O	2.47	0.43
1:E:363:PHE:HA	1:E:471:TRP:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:167:HIS:NE2	2:E:801:FAD:HM81	2.10	0.42
1:F:285:ARG:HA	1:F:328:LEU:HD13	1.99	0.42
1:H:97:GLN:HG3	1:H:250:PHE:CE2	2.54	0.42
1:E:299:HIS:CA	1:E:310:GLU:OE1	2.68	0.42
1:B:47:TYR:O	1:B:313:ALA:HA	2.19	0.42
1:H:459:VAL:HG12	1:H:460:GLN:N	2.34	0.42
1:D:359:GLN:NE2	1:D:591:GLY:C	2.73	0.42
1:H:165:SER:HA	1:H:168:TRP:CD1	2.54	0.42
1:B:543:PRO:HG2	3:B:870:HOH:O	2.18	0.42
1:E:382:ILE:N	1:E:382:ILE:HD12	2.34	0.42
1:A:82:SER:O	3:A:995:HOH:O	2.22	0.42
1:D:285:ARG:CA	1:D:328:LEU:HD11	2.49	0.42
1:H:389:LEU:CD2	1:H:390:THR:HG23	2.50	0.42
1:F:385:THR:O	1:F:388:GLU:HB2	2.18	0.42
1:B:367:VAL:CG2	1:B:533:LEU:HD13	2.49	0.42
1:A:104:VAL:HG22	1:A:453:ALA:HB1	2.01	0.42
1:H:471:TRP:CD1	1:H:471:TRP:N	2.87	0.42
1:A:548:HIS:HA	3:A:1057:HOH:O	2.19	0.42
1:D:328:LEU:O	1:D:328:LEU:HD12	2.20	0.42
1:C:359:GLN:HE21	1:C:591:GLY:C	2.23	0.42
1:H:457:GLY:O	1:H:461:GLN:HG3	2.20	0.42
1:G:385:THR:O	1:G:391:TYR:HB2	2.19	0.42
1:H:215:GLU:O	1:H:411:LYS:NZ	2.53	0.42
1:G:389:LEU:N	1:G:389:LEU:CD1	2.83	0.42
1:H:513:LYS:NZ	1:H:517:ASP:OD2	2.50	0.42
1:D:167:HIS:CD2	2:D:801:FAD:C8M	2.90	0.41
1:A:126:LEU:HD13	1:A:132:GLN:CG	2.49	0.41
1:H:199:TYR:O	1:H:203:GLU:HG3	2.20	0.41
1:G:408:TRP:C	1:G:408:TRP:CD1	2.93	0.41
1:A:459:VAL:HG22	1:B:121:LEU:HD13	2.03	0.41
1:A:459:VAL:HA	1:A:462:SER:HB2	2.02	0.41
1:C:155:GLN:NE2	1:C:358:GLU:OE2	2.49	0.41
1:A:618:PHE:CD1	1:A:618:PHE:C	2.93	0.41
1:D:547:LEU:HD12	2:D:801:FAD:HM83	2.01	0.41
1:D:215:GLU:O	1:D:411:LYS:NZ	2.54	0.41
1:F:167:HIS:NE2	2:F:801:FAD:HM81	2.14	0.41
1:H:44:ASP:HB3	1:H:46:LYS:H	1.85	0.41
1:C:618:PHE:C	1:C:618:PHE:HD1	2.24	0.41
1:F:155:GLN:NE2	1:F:358:GLU:OE2	2.50	0.41
1:H:459:VAL:HG12	1:H:460:GLN:HG3	2.01	0.41
1:C:383:ARG:HB2	1:C:392:SER:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:344:ASN:OD1	1:H:344:ASN:O	2.39	0.41
1:B:218:ARG:HD2	3:B:873:HOH:O	2.20	0.41
1:E:546:VAL:HG13	1:E:547:LEU:H	1.85	0.41
1:E:167:HIS:NE2	2:E:801:FAD:C8	2.80	0.41
1:C:343:ALA:C	1:C:344:ASN:ND2	2.73	0.41
1:B:359:GLN:NE2	1:B:591:GLY:O	2.54	0.41
1:G:495:TYR:O	1:G:496:ASN:CB	2.69	0.41
1:B:56:PRO:HD3	1:B:165:SER:HB3	2.03	0.41
1:F:546:VAL:CG1	1:F:547:LEU:N	2.83	0.41
1:G:105:ASN:O	1:H:105:ASN:HB3	2.21	0.41
1:H:45:ILE:CD1	1:H:45:ILE:C	2.89	0.40
1:C:326:THR:HG22	1:C:487:PHE:HE2	1.86	0.40
1:G:167:HIS:CE1	2:G:801:FAD:C8M	2.90	0.40
1:B:167:HIS:CD2	2:B:801:FAD:C8	3.04	0.40
1:H:452:ASP:C	1:H:452:ASP:OD1	2.59	0.40
1:E:159:ARG:HA	2:E:801:FAD:O2B	2.20	0.40
1:B:459:VAL:O	1:B:462:SER:CB	2.70	0.40
1:G:50:VAL:HG13	1:G:313:ALA:HB2	2.03	0.40
1:B:83:GLY:N	3:B:908:HOH:O	2.24	0.40
1:C:285:ARG:HA	1:C:328:LEU:HD11	2.03	0.40
1:C:418:GLN:HB3	1:C:418:GLN:HE21	1.47	0.40
1:A:281:VAL:CG1	1:A:300:ILE:HB	2.51	0.40
1:G:126:LEU:HD23	1:H:534:PRO:HD3	2.03	0.40
1:H:216:SER:HB3	1:H:219:HIS:HB3	2.04	0.40
1:C:105:ASN:HB3	1:D:105:ASN:O	2.22	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	575/623 (92%)	553 (96%)	22 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	575/623 (92%)	556 (97%)	19 (3%)	0	100	100
1	C	575/623 (92%)	556 (97%)	19 (3%)	0	100	100
1	D	575/623 (92%)	557 (97%)	18 (3%)	0	100	100
1	E	575/623 (92%)	553 (96%)	21 (4%)	1 (0%)	52	53
1	F	575/623 (92%)	560 (97%)	15 (3%)	0	100	100
1	G	575/623 (92%)	552 (96%)	22 (4%)	1 (0%)	52	53
1	H	575/623 (92%)	555 (96%)	19 (3%)	1 (0%)	52	53
All	All	4600/4984 (92%)	4442 (97%)	155 (3%)	3 (0%)	56	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	344	ASN
1	E	187	ASP
1	G	457	GLY

### 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	504/541 (93%)	487 (97%)	17 (3%)	44	45
1	B	504/541 (93%)	487 (97%)	17 (3%)	44	45
1	C	504/541 (93%)	487 (97%)	17 (3%)	44	45
1	D	504/541 (93%)	488 (97%)	16 (3%)	46	48
1	E	504/541 (93%)	488 (97%)	16 (3%)	46	48
1	F	504/541 (93%)	483 (96%)	21 (4%)	36	35
1	G	504/541 (93%)	491 (97%)	13 (3%)	54	58
1	H	504/541 (93%)	487 (97%)	17 (3%)	44	45
All	All	4032/4328 (93%)	3898 (97%)	134 (3%)	45	47

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ILE
1	A	121	LEU
1	A	168	TRP
1	A	185	LYS
1	A	206	PHE
1	A	312	LYS
1	A	328	LEU
1	A	341	ASN
1	A	388	GLU
1	A	394	THR
1	A	400	SER
1	A	401	THR
1	A	450	HIS
1	A	459	VAL
1	A	461	GLN
1	A	618	PHE
1	A	619	THR
1	B	44	ASP
1	B	45	ILE
1	B	95	GLU
1	B	168	TRP
1	B	185	LYS
1	B	206	PHE
1	B	328	LEU
1	B	385	THR
1	B	389	LEU
1	B	408	TRP
1	B	421	GLU
1	B	450	HIS
1	B	455	SER
1	B	459	VAL
1	B	490	LYS
1	B	593	ASN
1	B	619	THR
1	C	104	VAL
1	C	168	TRP
1	C	185	LYS
1	C	206	PHE
1	C	336	GLN
1	C	344	ASN
1	C	385	THR
1	C	389	LEU

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Mol	Chain	Res	Type
1	C	418	GLN
1	C	450	HIS
1	C	459	VAL
1	C	461	GLN
1	C	490	LYS
1	C	576	LYS
1	C	593	ASN
1	C	618	PHE
1	C	619	THR
1	D	46	LYS
1	D	82	SER
1	D	100	ILE
1	D	104	VAL
1	D	168	TRP
1	D	206	PHE
1	D	285	ARG
1	D	328	LEU
1	D	385	THR
1	D	388	GLU
1	D	389	LEU
1	D	450	HIS
1	D	459	VAL
1	D	462	SER
1	D	560	LYS
1	D	618	PHE
1	E	44	ASP
1	E	45	ILE
1	E	168	TRP
1	E	185	LYS
1	E	206	PHE
1	E	228	GLU
1	E	231	LYS
1	E	285	ARG
1	E	312	LYS
1	E	328	LEU
1	E	385	THR
1	E	388	GLU
1	E	403	LYS
1	E	450	HIS
1	E	459	VAL
1	E	618	PHE
1	F	46	LYS

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Mol	Chain	Res	Type
1	F	121	LEU
1	F	168	TRP
1	F	178	GLU
1	F	206	PHE
1	F	285	ARG
1	F	328	LEU
1	F	336	GLN
1	F	344	ASN
1	F	385	THR
1	F	392	SER
1	F	400	SER
1	F	421	GLU
1	F	450	HIS
1	F	459	VAL
1	F	460	GLN
1	F	465	SER
1	F	490	LYS
1	F	546	VAL
1	F	576	LYS
1	F	618	PHE
1	G	168	TRP
1	G	206	PHE
1	G	228	GLU
1	G	272	GLU
1	G	312	LYS
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	528	LYS
1	G	618	PHE
1	H	45	ILE
1	H	100	ILE
1	H	104	VAL
1	H	168	TRP
1	H	185	LYS
1	H	206	PHE
1	H	328	LEU
1	H	389	LEU
1	H	400	SER

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Mol	Chain	Res	Type
1	H	421	GLU
1	H	450	HIS
1	H	455	SER
1	H	460	GLN
1	H	496	ASN
1	H	560	LYS
1	H	593	ASN
1	H	618	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	324	HIS
1	A	341	ASN
1	A	460	GLN
1	B	336	GLN
1	B	460	GLN
1	B	611	GLN
1	C	324	HIS
1	C	341	ASN
1	C	344	ASN
1	C	418	GLN
1	C	448	GLN
1	D	263	GLN
1	D	299	HIS
1	D	324	HIS
1	D	341	ASN
1	D	460	GLN
1	E	99	ASN
1	E	324	HIS
1	E	341	ASN
1	E	418	GLN
1	E	460	GLN
1	E	611	GLN
1	F	299	HIS
1	F	324	HIS
1	F	448	GLN
1	G	263	GLN
1	G	324	HIS
1	G	418	GLN
1	G	460	GLN
1	H	110	GLN

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Mol	Chain	Res	Type
1	H	341	ASN
1	H	460	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	FAD	A	801	1	48,58,58	1.34	7 (14%)	54,89,89	5.31	19 (35%)
2	FAD	B	801	1	48,58,58	1.25	8 (16%)	54,89,89	3.37	26 (48%)
2	FAD	C	801	1	48,58,58	1.35	6 (12%)	54,89,89	4.30	21 (38%)
2	FAD	D	801	1	48,58,58	1.37	8 (16%)	54,89,89	4.12	24 (44%)
2	FAD	E	801	1	48,58,58	1.34	5 (10%)	54,89,89	3.73	22 (40%)
2	FAD	F	801	1	48,58,58	1.20	3 (6%)	54,89,89	4.41	20 (37%)
2	FAD	G	801	1	48,58,58	1.37	8 (16%)	54,89,89	4.93	21 (38%)
2	FAD	H	801	1	48,58,58	1.28	4 (8%)	54,89,89	4.40	22 (40%)

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	-	0/30/50/50	0/6/6/6
2	FAD	B	801	1	-	0/30/50/50	0/6/6/6
2	FAD	C	801	1	-	0/30/50/50	0/6/6/6
2	FAD	D	801	1	-	0/30/50/50	0/6/6/6
2	FAD	E	801	1	-	0/30/50/50	0/6/6/6
2	FAD	F	801	1	-	0/30/50/50	0/6/6/6
2	FAD	G	801	1	-	0/30/50/50	0/6/6/6
2	FAD	H	801	1	-	0/30/50/50	0/6/6/6

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	801	FAD	C10-N10	-3.76	1.34	1.39
2	A	801	FAD	O2B-C2B	-3.41	1.34	1.43
2	A	801	FAD	C2B-C3B	-3.36	1.44	1.53
2	D	801	FAD	C10-N10	-3.34	1.35	1.39
2	G	801	FAD	O2B-C2B	-3.21	1.35	1.43
2	B	801	FAD	C2B-C3B	-2.97	1.45	1.53
2	G	801	FAD	O4B-C4B	-2.77	1.38	1.45
2	C	801	FAD	O3B-C3B	-2.69	1.36	1.43
2	F	801	FAD	O2B-C2B	-2.62	1.36	1.43
2	B	801	FAD	O2B-C2B	-2.55	1.36	1.43
2	D	801	FAD	C9A-C5X	-2.49	1.37	1.42
2	G	801	FAD	C2B-C3B	-2.37	1.46	1.53
2	G	801	FAD	O3B-C3B	-2.25	1.37	1.43
2	A	801	FAD	O2'-C2'	-2.25	1.38	1.43
2	D	801	FAD	PA-O2A	-2.21	1.45	1.54
2	D	801	FAD	O3B-C3B	-2.15	1.37	1.43
2	D	801	FAD	C3B-C4B	-2.08	1.47	1.53
2	G	801	FAD	O4B-C1B	-2.04	1.38	1.41
2	D	801	FAD	C2B-C3B	-2.04	1.47	1.53
2	B	801	FAD	O3B-C3B	-2.03	1.38	1.43
2	F	801	FAD	O3B-C3B	-2.02	1.38	1.43
2	B	801	FAD	PA-O2A	-2.02	1.46	1.54
2	E	801	FAD	O4'-C4'	-2.01	1.38	1.43
2	A	801	FAD	C4X-N5	-2.01	1.30	1.33
2	A	801	FAD	C4'-C3'	-2.00	1.49	1.53
2	E	801	FAD	O4B-C1B	2.01	1.43	1.41
2	H	801	FAD	C4-N3	2.01	1.36	1.33
2	G	801	FAD	C7M-C7	2.04	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	FAD	C9A-N10	2.14	1.41	1.38
2	D	801	FAD	C4-N3	2.26	1.37	1.33
2	B	801	FAD	C6-C5X	2.30	1.45	1.41
2	C	801	FAD	C2A-N3A	2.32	1.36	1.32
2	B	801	FAD	C2A-N3A	2.34	1.36	1.32
2	A	801	FAD	C4-C4X	2.35	1.46	1.41
2	B	801	FAD	C4-C4X	2.47	1.46	1.41
2	C	801	FAD	O4B-C1B	2.48	1.44	1.41
2	C	801	FAD	C6-C5X	2.58	1.45	1.41
2	G	801	FAD	C4-C4X	2.63	1.46	1.41
2	H	801	FAD	C4-C4X	2.67	1.46	1.41
2	B	801	FAD	C7M-C7	2.76	1.56	1.51
2	C	801	FAD	C4-C4X	2.80	1.46	1.41
2	D	801	FAD	C4-C4X	2.82	1.46	1.41
2	G	801	FAD	C10-N1	2.85	1.40	1.35
2	H	801	FAD	C9A-N10	3.24	1.43	1.38
2	C	801	FAD	C1'-N10	3.36	1.51	1.48
2	H	801	FAD	C6-C5X	3.37	1.46	1.41
2	E	801	FAD	C1'-N10	3.49	1.52	1.48
2	F	801	FAD	C4X-N5	3.55	1.38	1.33
2	E	801	FAD	C4-C4X	3.84	1.48	1.41

All (175) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	801	FAD	C4-C4X-C10	-20.06	107.11	119.94
2	A	801	FAD	C4X-C4-N3	-16.09	101.59	123.59
2	F	801	FAD	N3A-C2A-N1A	-15.15	117.29	128.89
2	A	801	FAD	N3A-C2A-N1A	-13.81	118.32	128.89
2	G	801	FAD	N3A-C2A-N1A	-13.54	118.52	128.89
2	C	801	FAD	N3A-C2A-N1A	-13.36	118.66	128.89
2	H	801	FAD	N3A-C2A-N1A	-13.05	118.90	128.89
2	D	801	FAD	C4X-C4-N3	-11.96	107.24	123.59
2	D	801	FAD	N3A-C2A-N1A	-11.93	119.76	128.89
2	E	801	FAD	N3A-C2A-N1A	-11.74	119.91	128.89
2	C	801	FAD	C4-C4X-C10	-11.44	112.62	119.94
2	H	801	FAD	C4X-C4-N3	-10.93	108.65	123.59
2	F	801	FAD	C4X-C4-N3	-10.72	108.94	123.59
2	B	801	FAD	N3A-C2A-N1A	-10.26	121.04	128.89
2	E	801	FAD	C4X-C4-N3	-8.92	111.39	123.59
2	C	801	FAD	C4X-C10-N10	-7.26	116.24	120.52
2	B	801	FAD	C4-C4X-C10	-7.00	115.46	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	801	FAD	C4X-C10-N10	-6.95	116.42	120.52
2	A	801	FAD	C4B-O4B-C1B	-6.42	102.66	109.72
2	C	801	FAD	C4X-C4-N3	-6.30	114.98	123.59
2	A	801	FAD	C4X-C10-N10	-6.15	116.90	120.52
2	H	801	FAD	C4X-C10-N10	-6.12	116.91	120.52
2	G	801	FAD	C4X-C4-N3	-5.99	115.39	123.59
2	B	801	FAD	C4X-C10-N10	-5.79	117.11	120.52
2	H	801	FAD	C4B-O4B-C1B	-5.64	103.53	109.72
2	B	801	FAD	C4X-C4-N3	-5.44	116.16	123.59
2	E	801	FAD	C4-C4X-C10	-4.85	116.83	119.94
2	D	801	FAD	C9A-C5X-N5	-3.98	116.47	122.36
2	B	801	FAD	C7-C6-C5X	-3.96	114.46	120.92
2	E	801	FAD	C4X-C10-N10	-3.63	118.38	120.52
2	D	801	FAD	C4B-O4B-C1B	-3.50	105.88	109.72
2	C	801	FAD	C9A-C5X-N5	-3.37	117.36	122.36
2	F	801	FAD	C9A-C5X-N5	-3.32	117.44	122.36
2	B	801	FAD	C1B-N9A-C4A	-3.29	121.98	126.94
2	D	801	FAD	C4X-C10-N10	-3.13	118.67	120.52
2	H	801	FAD	C9A-C5X-N5	-3.09	117.79	122.36
2	G	801	FAD	C4X-C10-N10	-3.05	118.72	120.52
2	E	801	FAD	C9A-C5X-N5	-3.02	117.89	122.36
2	G	801	FAD	C7-C6-C5X	-2.85	116.27	120.92
2	D	801	FAD	C4A-C5A-N7A	-2.81	106.89	109.48
2	A	801	FAD	C4-C4X-N5	-2.64	115.52	118.72
2	B	801	FAD	C4A-C5A-N7A	-2.63	107.06	109.48
2	B	801	FAD	C8M-C8-C9	-2.59	113.25	120.28
2	C	801	FAD	C7-C6-C5X	-2.49	116.86	120.92
2	D	801	FAD	O3'-C3'-C2'	-2.48	102.50	108.75
2	H	801	FAD	C4-C4X-N5	-2.46	115.73	118.72
2	A	801	FAD	C1B-N9A-C4A	-2.46	123.24	126.94
2	A	801	FAD	C9A-C5X-N5	-2.43	118.75	122.36
2	D	801	FAD	P-O3P-PA	-2.40	125.98	132.73
2	A	801	FAD	C7-C6-C5X	-2.38	117.03	120.92
2	D	801	FAD	O5'-P-O1P	-2.38	100.39	109.62
2	H	801	FAD	C4-C4X-C10	-2.38	118.42	119.94
2	B	801	FAD	C9A-C5X-N5	-2.32	118.93	122.36
2	H	801	FAD	C8M-C8-C9	-2.29	114.06	120.28
2	E	801	FAD	C6-C5X-C9A	-2.28	115.98	118.98
2	B	801	FAD	C4B-O4B-C1B	-2.27	107.22	109.72
2	A	801	FAD	O5'-P-O1P	-2.25	100.89	109.62
2	E	801	FAD	C7-C6-C5X	-2.22	117.30	120.92
2	G	801	FAD	C8M-C8-C9	-2.21	114.28	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	FAD	C4A-C5A-N7A	-2.15	107.50	109.48
2	C	801	FAD	O5'-P-O1P	-2.15	101.29	109.62
2	B	801	FAD	C8M-C8-C7	-2.14	116.02	120.73
2	E	801	FAD	C8M-C8-C7	-2.08	116.16	120.73
2	F	801	FAD	O5'-P-O1P	-2.07	101.59	109.62
2	G	801	FAD	O4'-C4'-C5'	-2.05	105.74	110.19
2	F	801	FAD	O3P-PA-O5B	-2.01	97.61	102.94
2	F	801	FAD	O2A-PA-O3P	2.00	114.17	105.09
2	B	801	FAD	O2A-PA-O3P	2.00	114.18	105.09
2	B	801	FAD	O2B-C2B-C3B	2.04	118.45	111.83
2	D	801	FAD	O2'-C2'-C1'	2.04	114.96	109.94
2	B	801	FAD	C5B-C4B-C3B	2.04	123.32	115.21
2	G	801	FAD	O4'-C4'-C3'	2.05	114.18	109.02
2	B	801	FAD	C4X-N5-C5X	2.07	119.15	116.76
2	E	801	FAD	O2A-PA-O3P	2.07	114.50	105.09
2	G	801	FAD	O4B-C4B-C3B	2.08	109.33	105.15
2	B	801	FAD	O2'-C2'-C3'	2.08	114.24	109.02
2	B	801	FAD	C9-C8-C7	2.08	124.01	120.04
2	F	801	FAD	O2A-PA-O1A	2.09	123.84	112.53
2	F	801	FAD	O3B-C3B-C2B	2.11	118.69	111.83
2	E	801	FAD	C1'-N10-C9A	2.12	121.24	118.86
2	D	801	FAD	O2P-P-O1P	2.17	124.28	112.53
2	H	801	FAD	O4B-C4B-C5B	2.19	117.17	109.32
2	E	801	FAD	O2A-PA-O1A	2.20	124.43	112.53
2	H	801	FAD	C5B-C4B-C3B	2.20	123.93	115.21
2	C	801	FAD	O4'-C4'-C3'	2.20	114.54	109.02
2	H	801	FAD	O2A-PA-O1A	2.20	124.48	112.53
2	C	801	FAD	C2A-N1A-C6A	2.23	122.76	118.77
2	F	801	FAD	C6-C5X-N5	2.24	121.84	118.96
2	C	801	FAD	O2A-PA-O1A	2.32	125.08	112.53
2	G	801	FAD	C4-C4X-N5	2.33	121.54	118.72
2	D	801	FAD	C5X-C9A-N10	2.33	119.39	117.62
2	G	801	FAD	C5B-C4B-C3B	2.33	124.46	115.21
2	C	801	FAD	C6-C5X-C9A	2.36	122.09	118.98
2	H	801	FAD	C2A-N1A-C6A	2.37	123.01	118.77
2	A	801	FAD	C1'-N10-C9A	2.38	121.53	118.86
2	D	801	FAD	O2A-PA-O3P	2.38	115.91	105.09
2	E	801	FAD	O3B-C3B-C2B	2.39	119.61	111.83
2	B	801	FAD	C4-C4X-N5	2.44	121.68	118.72
2	E	801	FAD	O4B-C4B-C3B	2.58	110.34	105.15
2	F	801	FAD	C5B-C4B-C3B	2.60	125.54	115.21
2	A	801	FAD	O2B-C2B-C3B	2.69	120.57	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	FAD	O2B-C2B-C3B	2.75	120.77	111.83
2	H	801	FAD	O4'-C4'-C3'	2.78	116.00	109.02
2	F	801	FAD	C9-C8-C7	2.78	125.35	120.04
2	G	801	FAD	O4B-C4B-C5B	2.80	119.32	109.32
2	C	801	FAD	C9-C8-C7	2.82	125.42	120.04
2	B	801	FAD	O3B-C3B-C4B	2.84	119.57	111.05
2	B	801	FAD	C2A-N1A-C6A	2.88	123.91	118.77
2	F	801	FAD	O2B-C2B-C3B	2.89	121.24	111.83
2	D	801	FAD	O4B-C4B-C5B	2.89	119.67	109.32
2	B	801	FAD	C5X-C9A-N10	2.92	119.84	117.62
2	D	801	FAD	O4B-C4B-C3B	2.94	111.07	105.15
2	C	801	FAD	C5B-C4B-C3B	2.98	127.03	115.21
2	H	801	FAD	C5X-C9A-N10	2.99	119.89	117.62
2	G	801	FAD	C1B-N9A-C4A	3.05	131.53	126.94
2	G	801	FAD	O2B-C2B-C3B	3.06	121.76	111.83
2	H	801	FAD	O4B-C4B-C3B	3.11	111.41	105.15
2	H	801	FAD	O4B-C1B-N9A	3.11	114.62	108.10
2	A	801	FAD	C2A-N1A-C6A	3.13	124.35	118.77
2	F	801	FAD	C4X-N5-C5X	3.18	120.42	116.76
2	D	801	FAD	C1'-N10-C9A	3.24	122.49	118.86
2	E	801	FAD	C2A-N1A-C6A	3.25	124.58	118.77
2	B	801	FAD	O4B-C1B-N9A	3.27	114.95	108.10
2	A	801	FAD	O4B-C4B-C3B	3.36	111.93	105.15
2	H	801	FAD	C1'-N10-C9A	3.41	122.69	118.86
2	C	801	FAD	O2B-C2B-C3B	3.44	123.03	111.83
2	H	801	FAD	C4X-N5-C5X	3.45	120.73	116.76
2	B	801	FAD	O4B-C4B-C5B	3.50	121.83	109.32
2	G	801	FAD	C2A-N1A-C6A	3.54	125.10	118.77
2	E	801	FAD	C4X-N5-C5X	3.62	120.93	116.76
2	D	801	FAD	C2A-N1A-C6A	3.66	125.31	118.77
2	E	801	FAD	C5X-C9A-N10	3.68	120.42	117.62
2	A	801	FAD	O4B-C4B-C5B	3.70	122.55	109.32
2	E	801	FAD	C5B-C4B-C3B	3.74	130.06	115.21
2	H	801	FAD	O2B-C2B-C3B	3.75	124.01	111.83
2	A	801	FAD	C4-C4X-C10	4.03	122.52	119.94
2	F	801	FAD	C5X-C9A-N10	4.03	120.68	117.62
2	G	801	FAD	C4X-N5-C5X	4.15	121.53	116.76
2	F	801	FAD	O3B-C3B-C4B	4.20	123.64	111.05
2	D	801	FAD	C4X-N5-C5X	4.25	121.65	116.76
2	A	801	FAD	C4X-N5-C5X	4.26	121.66	116.76
2	B	801	FAD	C1'-N10-C9A	4.40	123.80	118.86
2	G	801	FAD	C1'-N10-C9A	4.48	123.89	118.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	FAD	C4-C4X-C10	4.52	122.83	119.94
2	D	801	FAD	O3B-C3B-C4B	4.55	124.69	111.05
2	G	801	FAD	O4B-C1B-N9A	4.68	117.90	108.10
2	F	801	FAD	C2A-N1A-C6A	4.74	127.23	118.77
2	C	801	FAD	C4X-N5-C5X	4.84	122.33	116.76
2	E	801	FAD	O3B-C3B-C4B	4.86	125.63	111.05
2	E	801	FAD	O4B-C1B-N9A	4.95	118.46	108.10
2	E	801	FAD	O2B-C2B-C3B	5.01	128.12	111.83
2	C	801	FAD	O3B-C3B-C4B	5.02	126.12	111.05
2	H	801	FAD	O3B-C3B-C4B	5.26	126.84	111.05
2	G	801	FAD	O3B-C3B-C4B	5.40	127.25	111.05
2	F	801	FAD	O4B-C1B-N9A	5.41	119.42	108.10
2	A	801	FAD	O3B-C3B-C4B	5.83	128.53	111.05
2	D	801	FAD	O4B-C1B-N9A	6.01	120.68	108.10
2	C	801	FAD	O4B-C1B-N9A	6.07	120.81	108.10
2	A	801	FAD	C2B-C1B-N9A	6.65	124.46	114.29
2	D	801	FAD	C2B-C1B-N9A	6.82	124.71	114.29
2	C	801	FAD	C4-C4X-N5	6.93	127.13	118.72
2	G	801	FAD	C2B-C1B-N9A	7.38	125.56	114.29
2	B	801	FAD	C2B-C1B-N9A	7.44	125.67	114.29
2	C	801	FAD	C2B-C1B-N9A	7.57	125.86	114.29
2	E	801	FAD	C2B-C1B-N9A	7.95	126.43	114.29
2	H	801	FAD	C2B-C1B-N9A	8.62	127.47	114.29
2	F	801	FAD	C2B-C1B-N9A	8.89	127.88	114.29
2	B	801	FAD	C4-N3-C2	12.45	126.01	115.25
2	E	801	FAD	C4-N3-C2	14.97	128.19	115.25
2	C	801	FAD	C4-N3-C2	16.93	129.88	115.25
2	D	801	FAD	C4-N3-C2	17.79	130.62	115.25
2	F	801	FAD	C4-N3-C2	19.53	132.13	115.25
2	G	801	FAD	C4-N3-C2	20.56	133.02	115.25
2	H	801	FAD	C4-N3-C2	20.89	133.30	115.25
2	A	801	FAD	C4-N3-C2	27.81	139.28	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 60 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	FAD	6	0
2	B	801	FAD	14	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	801	FAD	5	0
2	D	801	FAD	8	0
2	E	801	FAD	8	0
2	F	801	FAD	5	0
2	G	801	FAD	9	0
2	H	801	FAD	5	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, 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	577/623 (92%)	0.90	76 (13%) 4 6	20, 32, 56, 75	1 (0%)
1	B	577/623 (92%)	0.90	68 (11%) 6 8	19, 33, 54, 77	2 (0%)
1	C	577/623 (92%)	1.02	91 (15%) 3 4	22, 38, 57, 83	2 (0%)
1	D	577/623 (92%)	1.01	90 (15%) 3 4	24, 36, 57, 77	2 (0%)
1	E	577/623 (92%)	1.11	100 (17%) 2 3	25, 39, 59, 81	2 (0%)
1	F	577/623 (92%)	1.09	106 (18%) 2 2	26, 40, 59, 83	1 (0%)
1	G	577/623 (92%)	0.95	85 (14%) 3 5	23, 36, 56, 78	3 (0%)
1	H	577/623 (92%)	0.88	76 (13%) 4 6	22, 35, 53, 78	3 (0%)
All	All	4616/4984 (92%)	0.98	692 (14%) 3 5	19, 36, 57, 83	16 (0%)

All (692) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	619	THR	12.7
1	G	619	THR	11.9
1	C	619	THR	11.4
1	H	619	THR	10.8
1	D	619	THR	10.5
1	A	619	THR	10.5
1	B	459	VAL	10.4
1	A	343	ALA	10.2
1	F	459	VAL	9.4
1	F	343	ALA	9.0
1	B	343	ALA	9.0
1	A	385	THR	8.8
1	E	619	THR	8.5
1	D	344	ASN	8.1
1	A	459	VAL	8.0
1	G	389	LEU	7.9

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Mol	Chain	Res	Type	RSRZ
1	E	385	THR	7.9
1	E	459	VAL	7.9
1	C	343	ALA	7.8
1	C	459	VAL	7.7
1	F	619	THR	7.7
1	E	44	ASP	7.4
1	H	343	ALA	7.4
1	C	385	THR	7.2
1	F	43	MET	7.2
1	D	343	ALA	7.2
1	F	342	PRO	7.2
1	F	44	ASP	7.1
1	B	44	ASP	7.1
1	A	458	ALA	7.0
1	G	43	MET	7.0
1	D	43	MET	7.0
1	H	132	GLN	6.9
1	E	389	LEU	6.9
1	C	389	LEU	6.8
1	B	43	MET	6.8
1	C	43	MET	6.7
1	G	186	ASP	6.7
1	F	232	GLY	6.7
1	F	345	PRO	6.7
1	E	618	PHE	6.6
1	C	384	GLY	6.6
1	D	345	PRO	6.5
1	G	388	GLU	6.5
1	B	385	THR	6.5
1	B	389	LEU	6.5
1	E	342	PRO	6.5
1	G	343	ALA	6.5
1	D	459	VAL	6.4
1	H	344	ASN	6.4
1	A	43	MET	6.4
1	D	45	ILE	6.3
1	F	344	ASN	6.3
1	D	458	ALA	6.3
1	D	132	GLN	6.2
1	E	43	MET	6.2
1	G	44	ASP	6.1
1	C	618	PHE	6.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	H	43	MET	6.0
1	E	132	GLN	6.0
1	C	344	ASN	6.0
1	E	45	ILE	6.0
1	G	345	PRO	6.0
1	A	384	GLY	5.9
1	G	385	THR	5.8
1	H	44	ASP	5.8
1	B	186	ASP	5.8
1	E	458	ALA	5.7
1	H	45	ILE	5.7
1	E	344	ASN	5.6
1	H	342	PRO	5.6
1	F	454	PHE	5.6
1	F	455	SER	5.6
1	B	458	ALA	5.6
1	E	455	SER	5.6
1	C	44	ASP	5.5
1	H	186	ASP	5.5
1	F	385	THR	5.5
1	B	456	TYR	5.5
1	C	132	GLN	5.5
1	F	187	ASP	5.5
1	A	383	ARG	5.4
1	A	388	GLU	5.4
1	D	389	LEU	5.4
1	A	390	THR	5.4
1	B	344	ASN	5.4
1	D	186	ASP	5.3
1	H	617	PRO	5.3
1	E	57	ILE	5.3
1	E	384	GLY	5.3
1	A	186	ASP	5.2
1	D	388	GLU	5.2
1	G	299	HIS	5.2
1	G	132	GLN	5.2
1	F	341	ASN	5.2
1	H	618	PHE	5.2
1	B	454	PHE	5.1
1	C	342	PRO	5.0
1	A	401	THR	5.0
1	D	385	THR	5.0

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Mol	Chain	Res	Type	RSRZ
1	G	45	ILE	5.0
1	C	383	ARG	5.0
1	C	51	ILE	4.9
1	H	57	ILE	4.9
1	C	186	ASP	4.8
1	E	186	ASP	4.8
1	F	546	VAL	4.8
1	C	341	ASN	4.8
1	G	344	ASN	4.8
1	B	45	ILE	4.8
1	G	382	ILE	4.8
1	D	549	LEU	4.8
1	A	344	ASN	4.8
1	G	618	PHE	4.7
1	E	549	LEU	4.7
1	C	388	GLU	4.7
1	G	268	THR	4.7
1	E	184	VAL	4.7
1	A	406	ASP	4.7
1	E	617	PRO	4.7
1	G	188	ALA	4.6
1	H	341	ASN	4.6
1	G	459	VAL	4.6
1	A	44	ASP	4.6
1	D	44	ASP	4.6
1	C	57	ILE	4.6
1	D	382	ILE	4.6
1	G	455	SER	4.6
1	E	388	GLU	4.6
1	E	400	SER	4.6
1	A	386	PRO	4.6
1	F	188	ALA	4.6
1	D	269	ASP	4.6
1	D	454	PHE	4.5
1	F	290	ALA	4.5
1	E	306	GLY	4.5
1	E	456	TYR	4.5
1	A	549	LEU	4.5
1	F	387	GLY	4.5
1	C	45	ILE	4.5
1	C	268	THR	4.5
1	C	456	TYR	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	381	THR	4.4
1	F	388	GLU	4.4
1	F	189	ASP	4.4
1	A	389	LEU	4.4
1	E	320	ALA	4.4
1	E	318	LEU	4.4
1	A	456	TYR	4.3
1	D	268	THR	4.3
1	C	390	THR	4.3
1	B	187	ASP	4.2
1	F	186	ASP	4.2
1	G	57	ILE	4.2
1	D	232	GLY	4.2
1	B	132	GLN	4.2
1	H	458	ALA	4.2
1	G	456	TYR	4.2
1	A	57	ILE	4.2
1	E	271	PRO	4.2
1	G	187	ASP	4.2
1	H	456	TYR	4.2
1	G	454	PHE	4.1
1	A	317	VAL	4.1
1	C	272	GLU	4.1
1	E	547	LEU	4.1
1	C	52	VAL	4.1
1	H	189	ASP	4.1
1	D	401	THR	4.1
1	E	187	ASP	4.0
1	E	341	ASN	4.0
1	E	268	THR	4.0
1	H	549	LEU	4.0
1	D	187	ASP	4.0
1	C	455	SER	4.0
1	G	549	LEU	4.0
1	C	184	VAL	4.0
1	G	401	THR	4.0
1	H	345	PRO	4.0
1	H	305	SER	4.0
1	F	45	ILE	4.0
1	D	618	PHE	3.9
1	G	421	GLU	3.9
1	D	189	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	341	ASN	3.9
1	E	269	ASP	3.9
1	F	268	THR	3.9
1	C	458	ALA	3.9
1	B	345	PRO	3.9
1	H	271	PRO	3.9
1	H	400	SER	3.9
1	E	343	ALA	3.9
1	B	390	THR	3.9
1	G	309	PHE	3.9
1	E	561	GLU	3.9
1	A	345	PRO	3.8
1	C	317	VAL	3.8
1	C	189	ASP	3.8
1	E	189	ASP	3.8
1	F	383	ARG	3.8
1	H	104	VAL	3.8
1	C	345	PRO	3.8
1	E	390	THR	3.8
1	F	347	GLU	3.8
1	B	52	VAL	3.7
1	F	269	ASP	3.7
1	B	51	ILE	3.7
1	F	384	GLY	3.7
1	D	188	ALA	3.7
1	G	387	GLY	3.7
1	A	318	LEU	3.7
1	B	341	ASN	3.7
1	G	400	SER	3.7
1	C	400	SER	3.7
1	F	458	ALA	3.7
1	H	417	MET	3.7
1	F	586	ILE	3.7
1	B	387	GLY	3.6
1	A	342	PRO	3.6
1	C	305	SER	3.6
1	F	101	ASP	3.6
1	D	317	VAL	3.6
1	A	51	ILE	3.6
1	G	386	PRO	3.6
1	E	329	LEU	3.6
1	E	99	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	549	LEU	3.6
1	E	272	GLU	3.6
1	G	342	PRO	3.6
1	H	389	LEU	3.5
1	H	347	GLU	3.5
1	H	187	ASP	3.5
1	A	561	GLU	3.5
1	G	453	ALA	3.5
1	H	454	PHE	3.5
1	E	104	VAL	3.5
1	H	320	ALA	3.5
1	H	561	GLU	3.5
1	C	318	LEU	3.5
1	E	545	LEU	3.5
1	H	268	THR	3.5
1	D	272	GLU	3.4
1	F	299	HIS	3.4
1	E	601	LEU	3.4
1	F	549	LEU	3.4
1	G	100	ILE	3.4
1	A	391	TYR	3.4
1	F	104	VAL	3.4
1	D	270	ALA	3.4
1	F	51	ILE	3.4
1	G	458	ALA	3.4
1	D	407	TRP	3.4
1	C	232	GLY	3.4
1	E	52	VAL	3.4
1	G	52	VAL	3.4
1	E	345	PRO	3.4
1	E	581	GLY	3.4
1	G	384	GLY	3.4
1	E	454	PHE	3.4
1	F	192	ASP	3.4
1	B	57	ILE	3.3
1	A	319	THR	3.3
1	D	319	THR	3.3
1	D	400	SER	3.3
1	B	546	VAL	3.3
1	D	320	ALA	3.3
1	F	389	LEU	3.3
1	G	383	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	392	SER	3.3
1	E	56	PRO	3.3
1	G	317	VAL	3.3
1	G	341	ASN	3.3
1	F	81	ASP	3.3
1	F	550	GLY	3.3
1	F	317	VAL	3.3
1	F	340	PRO	3.3
1	B	383	ARG	3.3
1	C	583	CYS	3.3
1	B	342	PRO	3.3
1	E	322	ALA	3.2
1	H	185	LYS	3.2
1	E	305	SER	3.2
1	E	317	VAL	3.2
1	B	618	PHE	3.2
1	B	388	GLU	3.2
1	C	356	ILE	3.2
1	E	583	CYS	3.2
1	G	583	CYS	3.2
1	D	561	GLU	3.2
1	D	387	GLY	3.2
1	F	401	THR	3.2
1	C	322	ALA	3.2
1	H	322	ALA	3.2
1	H	321	GLY	3.2
1	B	104	VAL	3.2
1	H	121	LEU	3.2
1	G	398	GLY	3.2
1	D	583	CYS	3.2
1	F	272	GLU	3.2
1	H	546	VAL	3.2
1	C	190	ALA	3.1
1	F	421	GLU	3.1
1	E	299	HIS	3.1
1	E	304	ILE	3.1
1	E	490	LYS	3.1
1	D	456	TYR	3.1
1	G	323	VAL	3.1
1	G	320	ALA	3.1
1	C	617	PRO	3.1
1	E	51	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	580	LEU	3.1
1	G	390	THR	3.1
1	B	231	LYS	3.1
1	H	323	VAL	3.1
1	C	323	VAL	3.1
1	D	104	VAL	3.1
1	A	189	ASP	3.1
1	A	581	GLY	3.1
1	H	319	THR	3.0
1	C	187	ASP	3.0
1	B	582	GLY	3.0
1	E	325	ASN	3.0
1	G	82	SER	3.0
1	H	459	VAL	3.0
1	E	383	ARG	3.0
1	D	396	THR	3.0
1	B	232	GLY	3.0
1	H	340	PRO	3.0
1	H	583	CYS	3.0
1	F	57	ILE	3.0
1	A	580	LEU	3.0
1	C	561	GLU	3.0
1	E	182	LEU	3.0
1	H	53	GLY	3.0
1	A	272	GLU	3.0
1	E	616	SER	3.0
1	F	322	ALA	3.0
1	A	382	ILE	3.0
1	A	469	VAL	3.0
1	B	318	LEU	3.0
1	A	269	ASP	3.0
1	A	320	ALA	3.0
1	G	305	SER	3.0
1	B	583	CYS	3.0
1	F	319	THR	3.0
1	C	347	GLU	3.0
1	D	318	LEU	3.0
1	E	421	GLU	3.0
1	F	191	ASP	3.0
1	G	322	ALA	3.0
1	G	51	ILE	2.9
1	C	104	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	322	ALA	2.9
1	D	581	GLY	2.9
1	F	508	ALA	2.9
1	A	455	SER	2.9
1	D	299	HIS	2.9
1	D	399	ALA	2.9
1	D	560	LYS	2.9
1	F	309	PHE	2.9
1	B	319	THR	2.9
1	C	401	THR	2.9
1	C	309	PHE	2.9
1	C	271	PRO	2.9
1	A	347	GLU	2.9
1	C	580	LEU	2.9
1	D	391	TYR	2.9
1	G	391	TYR	2.9
1	E	401	THR	2.9
1	A	421	GLU	2.9
1	C	53	GLY	2.9
1	G	321	GLY	2.9
1	E	323	VAL	2.9
1	D	558	ASP	2.9
1	D	342	PRO	2.8
1	F	346	PRO	2.8
1	A	161	VAL	2.8
1	F	233	GLN	2.8
1	C	307	ASP	2.8
1	G	558	ASP	2.8
1	F	382	ILE	2.8
1	G	318	LEU	2.8
1	A	546	VAL	2.8
1	H	52	VAL	2.8
1	F	490	LYS	2.8
1	B	455	SER	2.8
1	H	272	GLU	2.8
1	D	381	THR	2.8
1	H	584	GLY	2.8
1	F	61	TYR	2.8
1	C	549	LEU	2.8
1	C	550	GLY	2.8
1	F	100	ILE	2.8
1	B	188	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	390	THR	2.8
1	B	317	VAL	2.8
1	E	469	VAL	2.8
1	C	406	ASP	2.7
1	E	307	ASP	2.7
1	G	232	GLY	2.7
1	G	582	GLY	2.7
1	F	390	THR	2.7
1	E	580	LEU	2.7
1	C	82	SER	2.7
1	D	582	GLY	2.7
1	A	618	PHE	2.7
1	E	598	ALA	2.7
1	G	319	THR	2.7
1	C	547	LEU	2.7
1	C	392	SER	2.7
1	F	456	TYR	2.7
1	C	396	THR	2.7
1	E	319	THR	2.7
1	E	467	LEU	2.7
1	H	318	LEU	2.7
1	E	347	GLU	2.7
1	F	561	GLU	2.7
1	F	321	GLY	2.7
1	D	51	ILE	2.7
1	A	104	VAL	2.7
1	C	407	TRP	2.7
1	F	320	ALA	2.7
1	D	617	PRO	2.7
1	A	398	GLY	2.7
1	E	298	LEU	2.6
1	F	231	LYS	2.6
1	H	307	ASP	2.6
1	H	560	LYS	2.6
1	G	469	VAL	2.6
1	H	469	VAL	2.6
1	F	249	THR	2.6
1	H	190	ALA	2.6
1	D	305	SER	2.6
1	E	61	TYR	2.6
1	B	58	GLY	2.6
1	C	267	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	57	ILE	2.6
1	A	270	ALA	2.6
1	A	400	SER	2.6
1	F	291	LEU	2.6
1	F	452	ASP	2.6
1	H	387	GLY	2.6
1	F	474	PHE	2.6
1	C	467	LEU	2.6
1	G	580	LEU	2.6
1	A	188	ALA	2.6
1	A	584	GLY	2.6
1	D	321	GLY	2.6
1	H	582	GLY	2.6
1	D	546	VAL	2.6
1	D	460	GLN	2.6
1	E	558	ASP	2.6
1	G	551	GLY	2.6
1	F	325	ASN	2.6
1	D	586	ILE	2.6
1	H	356	ILE	2.6
1	H	191	ASP	2.6
1	F	391	TYR	2.5
1	E	386	PRO	2.5
1	B	561	GLU	2.5
1	H	388	GLU	2.5
1	C	320	ALA	2.5
1	C	72	VAL	2.5
1	G	586	ILE	2.5
1	F	307	ASP	2.5
1	E	560	LYS	2.5
1	D	347	GLU	2.5
1	A	321	GLY	2.5
1	E	594	PRO	2.5
1	F	581	GLY	2.5
1	E	250	PHE	2.5
1	F	618	PHE	2.5
1	G	269	ASP	2.5
1	B	468	ILE	2.5
1	F	184	VAL	2.5
1	E	496	ASN	2.5
1	C	319	THR	2.5
1	G	508	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	474	PHE	2.5
1	F	329	LEU	2.5
1	A	58	GLY	2.5
1	E	53	GLY	2.5
1	C	340	PRO	2.5
1	G	561	GLU	2.5
1	A	454	PHE	2.5
1	H	267	ASN	2.5
1	C	551	GLY	2.5
1	D	59	CYS	2.5
1	G	617	PRO	2.5
1	F	442	SER	2.5
1	E	58	GLY	2.5
1	F	55	GLY	2.5
1	F	318	LEU	2.5
1	F	547	LEU	2.5
1	H	580	LEU	2.5
1	B	161	VAL	2.5
1	E	382	ILE	2.5
1	D	457	GLY	2.4
1	E	582	GLY	2.4
1	D	271	PRO	2.4
1	F	266	PRO	2.4
1	D	194	GLU	2.4
1	D	490	LYS	2.4
1	A	52	VAL	2.4
1	A	249	THR	2.4
1	D	341	ASN	2.4
1	F	583	CYS	2.4
1	D	163	GLY	2.4
1	H	457	GLY	2.4
1	G	233	GLN	2.4
1	G	403	LYS	2.4
1	F	580	LEU	2.4
1	D	356	ILE	2.4
1	B	228	GLU	2.4
1	B	322	ALA	2.4
1	C	387	GLY	2.4
1	E	232	GLY	2.4
1	B	594	PRO	2.4
1	B	545	LEU	2.4
1	A	582	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	321	GLY	2.4
1	C	321	GLY	2.4
1	D	66	VAL	2.4
1	G	550	GLY	2.4
1	D	598	ALA	2.4
1	F	86	ILE	2.4
1	F	271	PRO	2.4
1	G	121	LEU	2.4
1	H	467	LEU	2.4
1	A	387	GLY	2.4
1	E	54	SER	2.4
1	F	551	GLY	2.4
1	D	256	ALA	2.4
1	A	53	GLY	2.4
1	E	550	GLY	2.4
1	F	381	THR	2.4
1	G	467	LEU	2.4
1	E	266	PRO	2.3
1	G	270	ALA	2.3
1	G	546	VAL	2.3
1	F	447	THR	2.3
1	B	59	CYS	2.3
1	E	579	PHE	2.3
1	C	193	ALA	2.3
1	E	418	GLN	2.3
1	C	558	ASP	2.3
1	A	56	PRO	2.3
1	D	65	LEU	2.3
1	E	248	PRO	2.3
1	H	56	PRO	2.3
1	B	270	ALA	2.3
1	C	231	LYS	2.3
1	C	546	VAL	2.3
1	H	455	SER	2.3
1	E	321	GLY	2.3
1	H	269	ASP	2.3
1	F	168	TRP	2.3
1	H	551	GLY	2.3
1	H	51	ILE	2.3
1	B	453	ALA	2.3
1	F	270	ALA	2.3
1	E	101	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	307	ASP	2.3
1	B	550	GLY	2.3
1	F	162	GLY	2.3
1	D	435	VAL	2.3
1	H	317	VAL	2.3
1	G	449	ILE	2.3
1	C	598	ALA	2.3
1	A	121	LEU	2.3
1	B	329	LEU	2.3
1	F	352	LEU	2.3
1	B	306	GLY	2.2
1	C	397	PRO	2.2
1	E	161	VAL	2.2
1	F	367	VAL	2.2
1	G	381	THR	2.2
1	A	392	SER	2.2
1	B	581	GLY	2.2
1	B	307	ASP	2.2
1	E	196	ASP	2.2
1	F	374	ASP	2.2
1	B	315	VAL	2.2
1	D	286	VAL	2.2
1	B	384	GLY	2.2
1	B	490	LYS	2.2
1	A	397	PRO	2.2
1	C	454	PHE	2.2
1	E	381	THR	2.2
1	D	52	VAL	2.2
1	H	435	VAL	2.2
1	C	581	GLY	2.2
1	A	449	ILE	2.2
1	F	598	ALA	2.2
1	G	62	ALA	2.2
1	A	617	PRO	2.2
1	C	248	PRO	2.2
1	A	548	HIS	2.2
1	E	387	GLY	2.2
1	G	58	GLY	2.2
1	H	550	GLY	2.2
1	B	367	VAL	2.2
1	D	469	VAL	2.2
1	A	602	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	601	LEU	2.2
1	D	580	LEU	2.2
1	C	58	GLY	2.2
1	F	562	ASP	2.2
1	G	452	ASP	2.2
1	D	602	ALA	2.2
1	E	190	ALA	2.2
1	B	586	ILE	2.2
1	G	271	PRO	2.2
1	C	121	LEU	2.1
1	E	553	HIS	2.1
1	A	232	GLY	2.1
1	A	307	ASP	2.1
1	A	550	GLY	2.1
1	D	58	GLY	2.1
1	H	60	THR	2.1
1	B	330	VAL	2.1
1	F	52	VAL	2.1
1	F	62	ALA	2.1
1	H	592	ALA	2.1
1	G	347	GLU	2.1
1	F	582	GLY	2.1
1	H	59	CYS	2.1
1	E	339	ARG	2.1
1	C	228	GLU	2.1
1	F	222	VAL	2.1
1	F	392	SER	2.1
1	H	449	ILE	2.1
1	G	65	LEU	2.1
1	E	461	GLN	2.1
1	E	478	GLU	2.1
1	A	583	CYS	2.1
1	C	490	LYS	2.1
1	A	187	ASP	2.1
1	D	181	PRO	2.1
1	D	309	PHE	2.1
1	F	386	PRO	2.1
1	D	551	GLY	2.1
1	F	161	VAL	2.1
1	G	53	GLY	2.1
1	G	306	GLY	2.1
1	A	239	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	121	LEU	2.1
1	D	467	LEU	2.1
1	H	558	ASP	2.1
1	F	617	PRO	2.1
1	B	592	ALA	2.1
1	B	55	GLY	2.1
1	C	421	GLU	2.1
1	F	58	GLY	2.1
1	E	392	SER	2.1
1	F	108	GLN	2.1
1	H	61	TYR	2.1
1	D	185	LYS	2.1
1	H	385	THR	2.1
1	A	609	ILE	2.1
1	D	383	ARG	2.1
1	B	418	GLN	2.1
1	D	592	ALA	2.1
1	G	402	ASN	2.1
1	C	562	ASP	2.1
1	D	178	GLU	2.0
1	C	449	ILE	2.0
1	E	609	ILE	2.0
1	C	185	LYS	2.0
1	G	399	ALA	2.0
1	D	473	PHE	2.0
1	C	614	THR	2.0
1	B	185	LYS	2.0
1	D	161	VAL	2.0
1	F	185	LYS	2.0
1	G	367	VAL	2.0
1	D	609	ILE	2.0
1	F	603	ILE	2.0
1	H	304	ILE	2.0
1	D	545	LEU	2.0
1	A	452	ASP	2.0
1	C	310	GLU	2.0
1	F	308	ARG	2.0
1	A	268	THR	2.0
1	A	326	THR	2.0
1	C	381	THR	2.0
1	H	496	ASN	2.0
1	C	49	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	323	VAL	2.0
1	C	582	GLY	2.0
1	C	382	ILE	2.0
1	G	239	ILE	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, 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FAD	D	801	53/53	0.95	0.22	0.66	23,27,31,35	0
2	FAD	G	801	53/53	0.92	0.22	0.62	20,24,30,33	0
2	FAD	F	801	53/53	0.93	0.20	0.35	16,28,33,35	0
2	FAD	H	801	53/53	0.94	0.21	0.20	19,27,31,32	0
2	FAD	A	801	53/53	0.95	0.19	-0.11	20,24,30,35	0
2	FAD	C	801	53/53	0.94	0.18	-0.18	23,29,35,43	0
2	FAD	E	801	53/53	0.92	0.19	-0.23	21,30,35,38	0
2	FAD	B	801	53/53	0.95	0.17	-0.43	18,23,28,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.