



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2017 – 01:44 PM EDT

PDB ID : 2IGM  
Title : Crystal structure of recombinant pyranose 2-oxidase H548N mutant  
Authors : Divne, C.  
Deposited on : unknown  
Resolution : 1.90 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

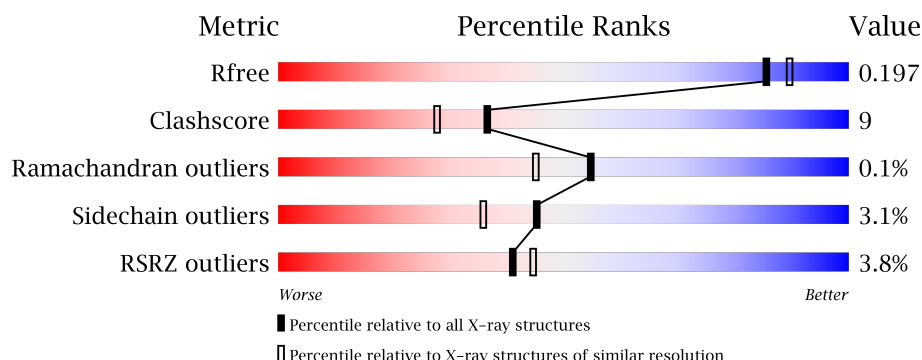
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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>4%</div> <div> <div></div> <div>81%</div> <div>10%</div> <div>7%</div> </div> </div>
1	B	623	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>11%</div> <div>7%</div> </div> </div>
1	C	623	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>11%</div> <div>7%</div> </div> </div>
1	D	623	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>12%</div> <div>7%</div> </div> </div>
1	E	623	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>11%</div> <div>7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	623	<div><div></div><div>4%</div><div>80%</div><div>11%</div><div>7%</div></div>
1	G	623	<div><div></div><div>4%</div><div>81%</div><div>11%</div><div>7%</div></div>
1	H	623	<div><div></div><div>3%</div><div>83%</div><div>9%</div><div>7%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 41255 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	2	0
			4561	2879	779	878	25			
1	B	577	Total	C	N	O	S	0	2	0
			4562	2881	779	877	25			
1	D	577	Total	C	N	O	S	0	3	0
			4569	2883	780	881	25			
1	C	577	Total	C	N	O	S	0	1	0
			4555	2876	778	876	25			
1	E	577	Total	C	N	O	S	0	2	0
			4561	2879	779	878	25			
1	F	577	Total	C	N	O	S	0	1	0
			4555	2876	778	876	25			
1	G	577	Total	C	N	O	S	0	2	0
			4562	2881	779	877	25			
1	H	577	Total	C	N	O	S	0	1	0
			4555	2876	778	876	25			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	548	ASN	HIS	ENGINEERED	UNP Q7ZA32
B	548	ASN	HIS	ENGINEERED	UNP Q7ZA32
C	548	ASN	HIS	ENGINEERED	UNP Q7ZA32
D	548	ASN	HIS	ENGINEERED	UNP Q7ZA32
E	548	ASN	HIS	ENGINEERED	UNP Q7ZA32
F	548	ASN	HIS	ENGINEERED	UNP Q7ZA32
G	548	ASN	HIS	ENGINEERED	UNP Q7ZA32
H	548	ASN	HIS	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	D	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	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 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	572	Total	O	0	0
			572	572		
4	B	570	Total	O	0	0
			570	570		
4	D	546	Total	O	0	0
			546	546		
4	C	514	Total	O	0	0
			514	514		

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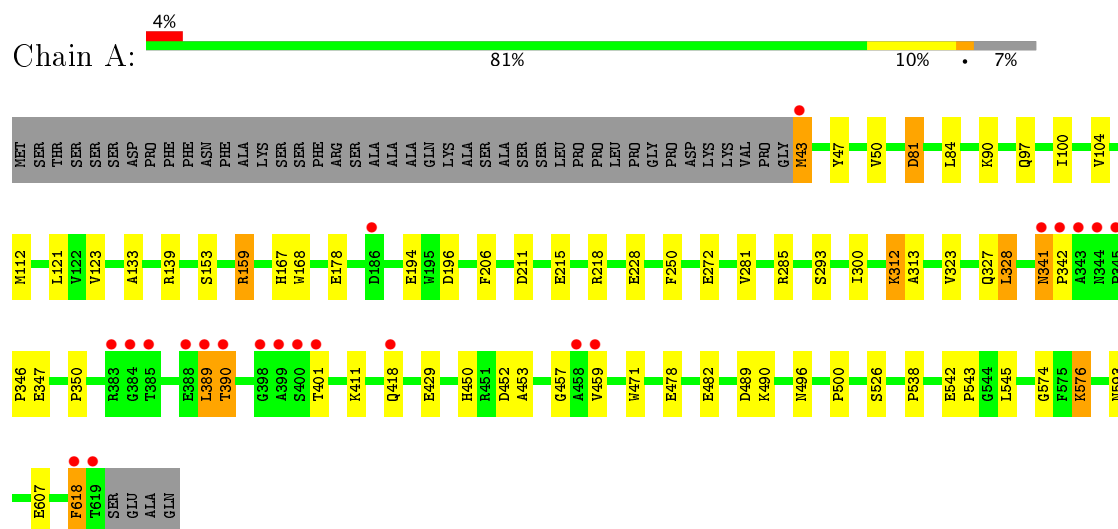
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	524	Total 524	O 524	0	0
4	F	472	Total 472	O 472	0	0
4	G	519	Total 519	O 519	0	0
4	H	538	Total 538	O 538	0	0

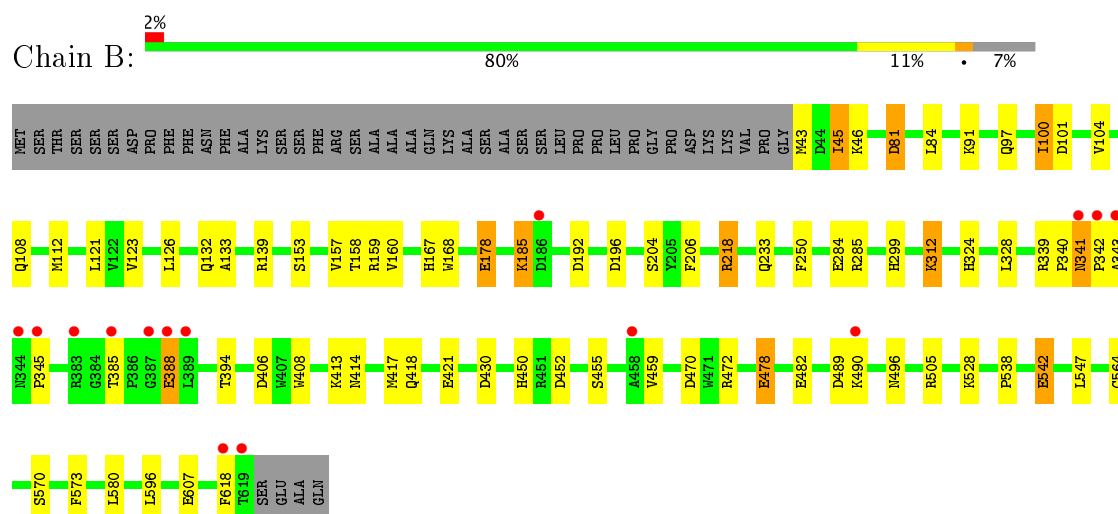
### 3 Residue-property plots [i](#)

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

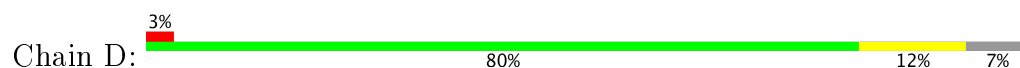
#### • Molecule 1: Pyranose oxidase



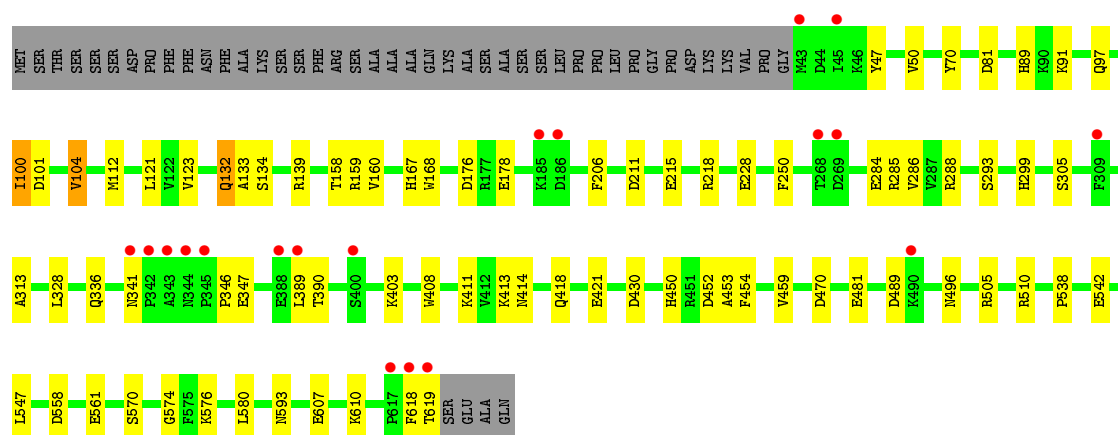
#### • Molecule 1: Pyranose oxidase



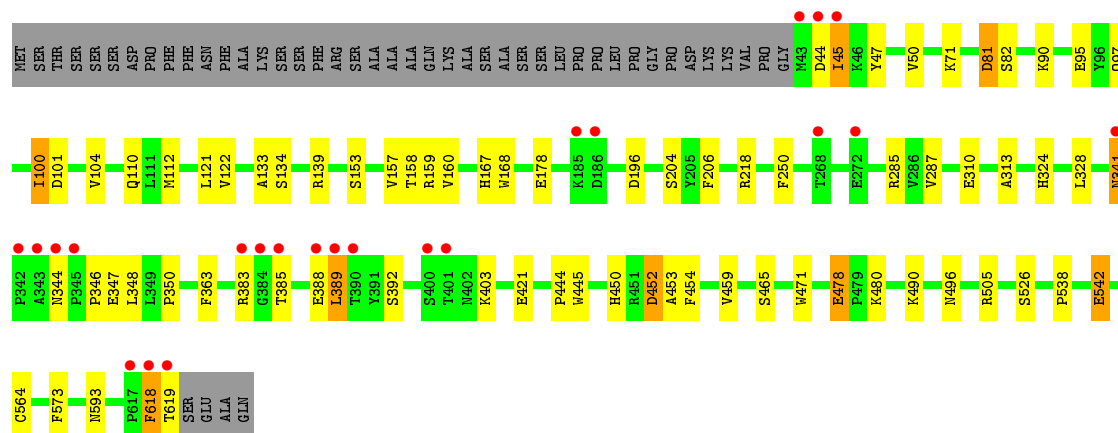
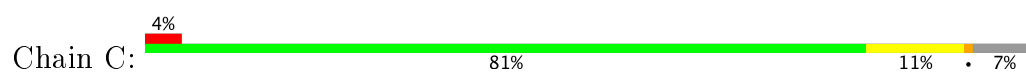
#### • Molecule 1: Pyranose oxidase



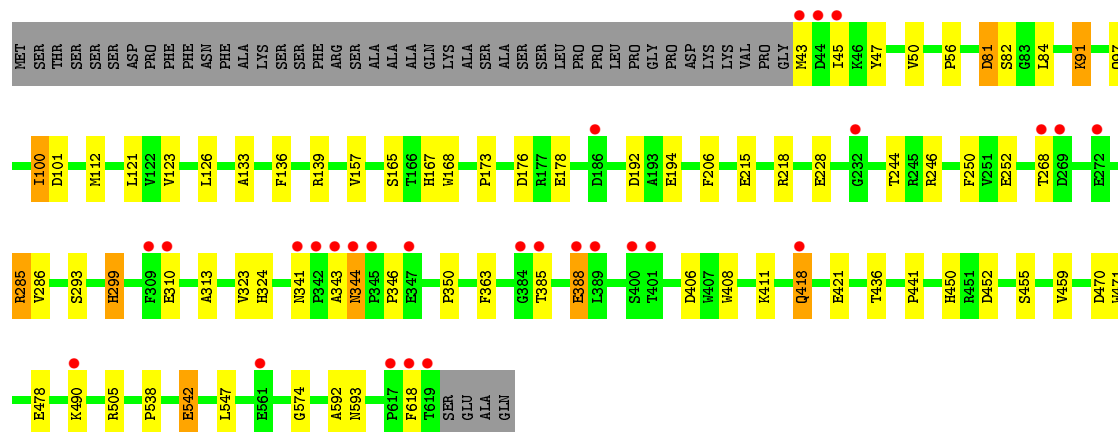
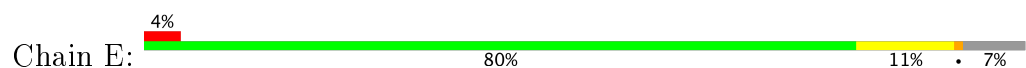




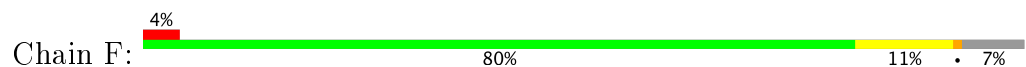
- Molecule 1: Pyranose oxidase

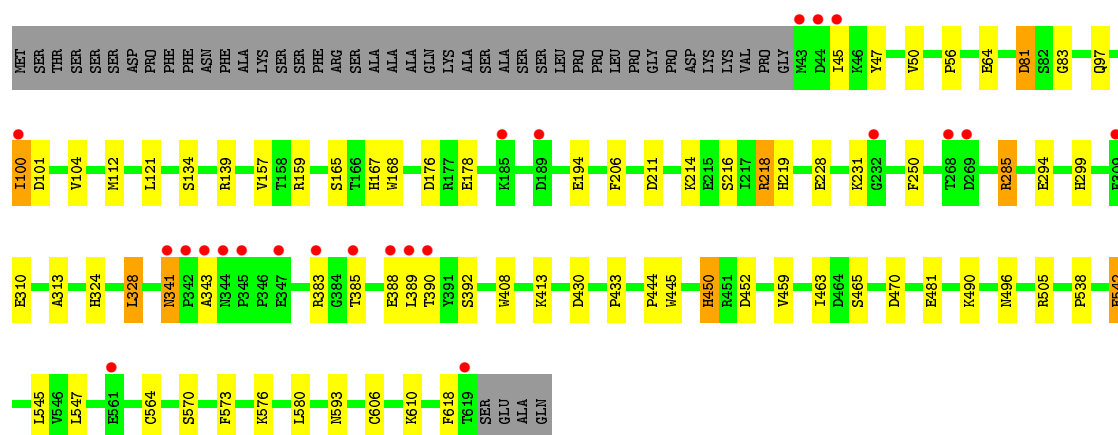


- Molecule 1: Pyranose oxidase

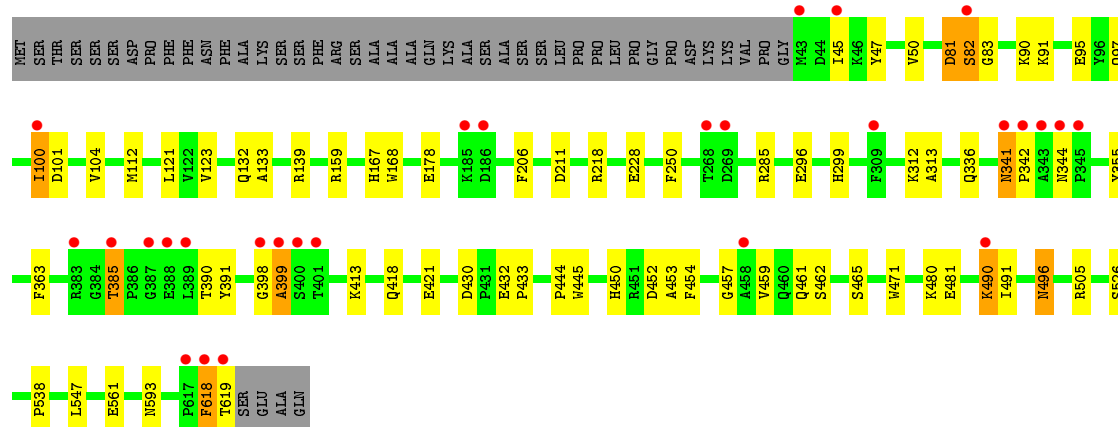
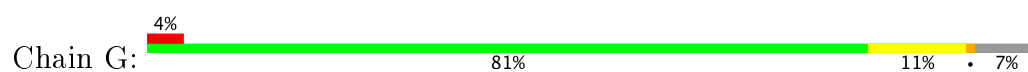


- Molecule 1: Pyranose oxidase

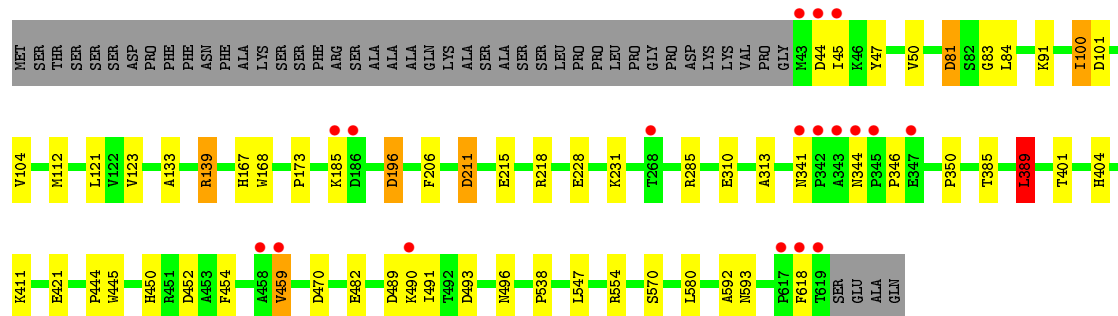
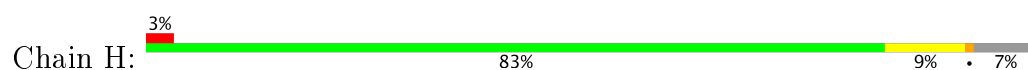




• Molecule 1: Pyranose oxidase



• Molecule 1: Pyranose oxidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	168.43Å 103.14Å 168.91Å 90.00° 106.08° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 19.99 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.7 (20.00-1.90) 96.8 (19.99-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.02 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.152 , 0.189 0.160 , 0.197	Depositor DCC
$R_{free}$ test set	4236 reflections (1.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.9	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 57.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	41255	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.67% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.90	3/4676 (0.1%)	0.87	6/6358 (0.1%)
1	B	0.90	5/4677 (0.1%)	0.90	16/6360 (0.3%)
1	C	0.86	5/4670 (0.1%)	0.90	8/6350 (0.1%)
1	D	0.86	3/4684 (0.1%)	0.90	12/6369 (0.2%)
1	E	0.84	3/4676 (0.1%)	0.82	7/6358 (0.1%)
1	F	0.84	3/4670 (0.1%)	0.87	9/6350 (0.1%)
1	G	0.87	2/4677 (0.0%)	0.88	9/6360 (0.1%)
1	H	0.86	1/4670 (0.0%)	0.88	13/6350 (0.2%)
All	All	0.87	25/37400 (0.1%)	0.88	80/50855 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	178	GLU	CB-CG	-7.40	1.38	1.52
1	B	542	GLU	CG-CD	6.54	1.61	1.51
1	D	104	VAL	CB-CG2	-6.25	1.39	1.52
1	B	482	GLU	CG-CD	6.15	1.61	1.51
1	D	542	GLU	CB-CG	-6.08	1.40	1.52
1	C	478	GLU	CD-OE1	6.04	1.32	1.25
1	G	228	GLU	CG-CD	5.97	1.60	1.51
1	E	542	GLU	CG-CD	5.92	1.60	1.51
1	E	228	GLU	CG-CD	5.89	1.60	1.51
1	B	421	GLU	CB-CG	5.74	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	482	GLU	CG-CD	5.72	1.60	1.51
1	D	139	ARG	CD-NE	-5.66	1.36	1.46
1	B	139	ARG	CD-NE	-5.61	1.36	1.46
1	F	228	GLU	CG-CD	5.46	1.60	1.51
1	C	465	SER	CB-OG	-5.44	1.35	1.42
1	F	542	GLU	CG-CD	5.42	1.60	1.51
1	H	139	ARG	CD-NE	-5.36	1.37	1.46
1	F	104	VAL	CB-CG2	-5.29	1.41	1.52
1	C	421	GLU	CB-CG	5.28	1.62	1.52
1	G	421	GLU	CB-CG	5.27	1.62	1.52
1	C	139	ARG	CD-NE	-5.23	1.37	1.46
1	C	542	GLU	CB-CG	-5.20	1.42	1.52
1	A	323	VAL	CB-CG2	5.18	1.63	1.52
1	E	478	GLU	CD-OE1	5.18	1.31	1.25
1	B	478	GLU	CD-OE1	5.12	1.31	1.25

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	139	ARG	NE-CZ-NH2	-23.67	108.46	120.30
1	C	139	ARG	NE-CZ-NH2	-23.61	108.49	120.30
1	F	139	ARG	NE-CZ-NH2	-22.77	108.92	120.30
1	G	139	ARG	NE-CZ-NH2	-21.96	109.32	120.30
1	H	139	ARG	NE-CZ-NH2	-19.62	110.49	120.30
1	C	139	ARG	NE-CZ-NH1	19.58	130.09	120.30
1	B	139	ARG	NE-CZ-NH2	-19.31	110.64	120.30
1	G	139	ARG	NE-CZ-NH1	18.64	129.62	120.30
1	A	139	ARG	NE-CZ-NH2	-18.49	111.06	120.30
1	E	139	ARG	NE-CZ-NH2	-17.63	111.48	120.30
1	H	139	ARG	NE-CZ-NH1	17.59	129.09	120.30
1	D	139	ARG	NE-CZ-NH1	17.27	128.93	120.30
1	B	139	ARG	NE-CZ-NH1	14.52	127.56	120.30
1	F	139	ARG	NE-CZ-NH1	13.77	127.18	120.30
1	A	139	ARG	NE-CZ-NH1	13.22	126.91	120.30
1	E	139	ARG	NE-CZ-NH1	12.56	126.58	120.30
1	G	81	ASP	CB-CG-OD1	-8.93	110.27	118.30
1	B	81	ASP	CB-CG-OD1	-8.87	110.32	118.30
1	C	81	ASP	CB-CG-OD1	-8.47	110.67	118.30
1	A	81	ASP	CB-CG-OD1	-8.18	110.94	118.30
1	F	218	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	H	81	ASP	CB-CG-OD1	-7.73	111.35	118.30
1	D	81	ASP	CB-CG-OD1	-7.32	111.72	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	81	ASP	CB-CG-OD2	7.14	124.73	118.30
1	G	505	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	C	139	ARG	CD-NE-CZ	7.09	133.53	123.60
1	G	139	ARG	CD-NE-CZ	7.06	133.48	123.60
1	E	81	ASP	CB-CG-OD1	-6.94	112.05	118.30
1	D	139	ARG	CD-NE-CZ	6.85	133.19	123.60
1	A	159	ARG	NE-CZ-NH1	6.81	123.71	120.30
1	D	470	ASP	CB-CG-OD1	6.80	124.42	118.30
1	D	470	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	H	139	ARG	CD-NE-CZ	6.26	132.36	123.60
1	E	470	ASP	CB-CG-OD1	6.23	123.91	118.30
1	B	489	ASP	CB-CG-OD1	6.23	123.91	118.30
1	D	139	ARG	CG-CD-NE	-6.22	98.73	111.80
1	C	452	ASP	CB-CA-C	6.21	122.83	110.40
1	D	81	ASP	CB-CG-OD2	6.13	123.82	118.30
1	H	470	ASP	CB-CG-OD1	6.11	123.80	118.30
1	H	285	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	C	81	ASP	CB-CG-OD2	6.03	123.73	118.30
1	G	81	ASP	CB-CG-OD2	5.96	123.67	118.30
1	B	218	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	F	139	ARG	CG-CD-NE	-5.92	99.36	111.80
1	B	472	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	D	211	ASP	CB-CG-OD1	5.89	123.60	118.30
1	A	489	ASP	CB-CG-OD1	5.86	123.57	118.30
1	B	192	ASP	CB-CG-OD1	5.85	123.57	118.30
1	D	489	ASP	CB-CG-OD1	5.84	123.56	118.30
1	B	196	ASP	CB-CG-OD1	5.83	123.55	118.30
1	B	470	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	B	406	ASP	CB-CG-OD1	5.80	123.52	118.30
1	G	211	ASP	CB-CG-OD1	5.66	123.40	118.30
1	C	139	ARG	CA-CB-CG	5.63	125.78	113.40
1	E	139	ARG	CG-CD-NE	-5.62	100.00	111.80
1	B	139	ARG	CG-CD-NE	-5.60	100.04	111.80
1	H	470	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	F	139	ARG	CD-NE-CZ	5.57	131.39	123.60
1	H	211	ASP	CB-CG-OD1	5.53	123.27	118.30
1	H	389	LEU	CA-CB-CG	5.51	127.97	115.30
1	G	139	ARG	CG-CD-NE	-5.47	100.31	111.80
1	D	104	VAL	CB-CA-C	-5.38	101.17	111.40
1	F	81	ASP	CB-CG-OD1	-5.38	113.46	118.30
1	E	406	ASP	CB-CG-OD1	5.38	123.14	118.30
1	H	554	ARG	NE-CZ-NH1	5.36	122.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	470	ASP	CB-CG-OD1	5.30	123.07	118.30
1	H	493	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	H	489	ASP	CB-CG-OD1	5.28	123.05	118.30
1	B	472	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	F	470	ASP	CB-CG-OD2	-5.24	113.59	118.30
1	B	139	ARG	CD-NE-CZ	5.22	130.91	123.60
1	E	192	ASP	CB-CG-OD1	5.20	122.98	118.30
1	D	288	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	B	406	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	A	211	ASP	CB-CG-OD1	5.08	122.87	118.30
1	G	505	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	F	159	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	C	139	ARG	CG-CD-NE	-5.02	101.27	111.80
1	H	196	ASP	CB-CG-OD1	5.02	122.81	118.30
1	F	139	ARG	CA-CB-CG	5.00	124.40	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	436	THR	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	4561	0	4408	91	0
1	B	4562	0	4412	112	0
1	C	4555	0	4404	85	0
1	D	4569	0	4411	87	0
1	E	4561	0	4408	100	0
1	F	4555	0	4404	93	0
1	G	4562	0	4412	104	0
1	H	4555	0	4404	74	0
2	A	53	0	30	6	0
2	B	53	0	29	13	0
2	C	53	0	28	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	53	0	29	8	0
2	E	53	0	30	11	0
2	F	53	0	29	9	0
2	G	53	0	29	10	0
2	H	53	0	28	6	0
3	A	12	0	12	1	0
3	B	12	0	12	1	0
3	C	12	0	12	0	0
3	D	12	0	12	2	0
3	E	12	0	12	4	0
3	F	12	0	12	0	0
3	G	12	0	12	2	0
3	H	12	0	12	1	0
4	A	572	0	0	40	0
4	B	570	0	0	37	0
4	C	514	0	0	22	0
4	D	546	0	0	46	0
4	E	524	0	0	43	0
4	F	472	0	0	30	0
4	G	519	0	0	38	0
4	H	538	0	0	30	0
All	All	41255	0	35591	648	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 9.

All (648) 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:G:167:HIS:HE2	2:G:801:FAD:C8M	0.98	1.61
1:E:167:HIS:HE2	2:E:801:FAD:C8M	1.01	1.60
1:D:167:HIS:HE2	2:D:801:FAD:C8M	0.97	1.59
1:B:167:HIS:HE2	2:B:801:FAD:C8M	0.97	1.57
1:F:167:HIS:HE2	2:F:801:FAD:C8M	0.96	1.54
1:C:167:HIS:HE2	2:C:801:FAD:C8M	0.92	1.53
1:A:167:HIS:HE2	2:A:801:FAD:C8M	0.90	1.52
1:H:167:HIS:HE2	2:H:801:FAD:C8M	0.98	1.52
1:E:121[B]:LEU:CD2	1:F:459:VAL:HG22	1.43	1.49
1:A:459:VAL:HG22	1:B:121[B]:LEU:CD2	1.52	1.40
1:E:167:HIS:NE2	2:E:801:FAD:HM82	1.09	1.38
1:H:167:HIS:NE2	2:H:801:FAD:HM82	1.06	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:VAL:CG2	1:B:121[B]:LEU:HD21	1.53	1.35
1:B:167:HIS:NE2	2:B:801:FAD:HM82	1.03	1.34
1:F:545:LEU:HD22	4:F:7392:HOH:O	1.26	1.33
1:G:167:HIS:NE2	2:G:801:FAD:HM82	1.00	1.32
1:A:104:VAL:HB	4:A:7508:HOH:O	1.26	1.31
1:B:452:ASP:HB2	4:B:7324:HOH:O	1.28	1.29
1:E:459:VAL:HG22	1:F:121[B]:LEU:CD2	1.62	1.29
1:E:121[B]:LEU:HD21	1:F:459:VAL:CG2	1.64	1.27
1:F:167:HIS:NE2	2:F:801:FAD:HM82	0.95	1.27
1:G:121[B]:LEU:CD2	1:H:459:VAL:HG23	1.62	1.26
1:B:204:SER:CB	4:B:7545:HOH:O	1.72	1.26
1:D:167:HIS:NE2	2:D:801:FAD:HM82	0.95	1.25
1:C:104:VAL:HB	4:C:7428:HOH:O	1.35	1.25
1:H:452:ASP:HB2	4:H:7281:HOH:O	1.33	1.24
1:H:389:LEU:HD12	4:H:7254:HOH:O	1.38	1.23
1:A:121[B]:LEU:CD2	1:B:459:VAL:HG22	1.70	1.21
1:C:167:HIS:NE2	2:C:801:FAD:HM82	0.88	1.21
1:A:327:GLN:NE2	4:A:7531:HOH:O	1.67	1.21
1:A:167:HIS:NE2	2:A:801:FAD:HM82	0.88	1.21
1:D:459:VAL:CG2	1:C:121[B]:LEU:HD21	1.70	1.20
1:D:459:VAL:HG22	1:C:121[B]:LEU:CD2	1.71	1.20
1:D:121[B]:LEU:CD2	1:C:459:VAL:HG22	1.71	1.20
1:G:465:SER:HB2	4:G:7441:HOH:O	1.06	1.19
1:C:100:ILE:HB	4:C:7356:HOH:O	1.41	1.19
1:G:453:ALA:HB1	4:G:7438:HOH:O	1.42	1.19
1:H:104:VAL:HB	4:H:7426:HOH:O	1.05	1.19
1:D:453:ALA:HB1	4:D:7506:HOH:O	1.43	1.18
1:B:417:MET:SD	4:B:7483:HOH:O	1.95	1.18
1:C:167:HIS:CD2	2:C:801:FAD:HM82	1.77	1.18
1:F:452:ASP:HB2	4:F:7275:HOH:O	1.41	1.17
1:G:452:ASP:HB2	4:G:7274:HOH:O	1.45	1.16
1:B:204:SER:HB2	4:B:7545:HOH:O	1.29	1.15
1:A:167:HIS:CD2	2:A:801:FAD:HM82	1.82	1.15
1:E:459:VAL:CG2	1:F:121[B]:LEU:HD21	1.79	1.12
1:D:121[B]:LEU:HD21	1:C:459:VAL:CG2	1.78	1.12
1:C:134:SER:HB2	4:C:7475:HOH:O	1.47	1.12
1:A:121[B]:LEU:HD21	1:B:459:VAL:HG22	1.23	1.10
1:A:97:GLN:HB2	4:A:7511:HOH:O	1.47	1.10
1:H:167:HIS:CD2	2:H:801:FAD:HM82	1.86	1.10
1:G:459:VAL:HG22	1:H:121[B]:LEU:HD21	1.19	1.10
1:C:178:GLU:OE1	4:C:7451:HOH:O	1.67	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:167:HIS:HE2	2:H:801:FAD:HM81	1.14	1.10
1:G:465:SER:CB	4:G:7441:HOH:O	1.66	1.09
1:G:121[B]:LEU:HD23	1:H:459:VAL:HA	1.19	1.09
1:C:452:ASP:HB2	4:C:7262:HOH:O	1.47	1.09
1:E:121[B]:LEU:HD23	1:F:459:VAL:HA	1.36	1.08
1:G:459:VAL:HG22	1:H:121[B]:LEU:CD2	1.84	1.07
1:G:121[B]:LEU:HD21	1:H:459:VAL:HG23	1.11	1.07
1:A:459:VAL:HA	1:B:121[B]:LEU:HD23	1.06	1.05
1:F:121[A]:LEU:CD2	1:G:121[A]:LEU:CD2	2.37	1.03
1:D:459:VAL:HG22	1:C:121[B]:LEU:HD21	1.07	1.03
3:D:7007:MES:H71	4:D:7447:HOH:O	1.56	1.03
1:G:121[B]:LEU:HD21	1:H:459:VAL:CG2	1.88	1.02
1:A:459:VAL:HA	1:B:121[B]:LEU:CD2	1.89	1.02
1:F:134:SER:HB2	4:F:7364:HOH:O	1.57	1.01
1:E:121[B]:LEU:CD2	1:F:459:VAL:CG2	2.32	1.00
1:B:285:ARG:HD3	4:B:7315:HOH:O	1.58	1.00
1:D:100:ILE:HD13	1:D:100:ILE:O	1.62	0.99
1:A:459:VAL:CA	1:B:121[B]:LEU:HD23	1.92	0.98
1:D:176:ASP:OD1	4:D:7499:HOH:O	1.81	0.98
1:F:167:HIS:CD2	2:F:801:FAD:HM82	1.98	0.98
1:E:452:ASP:CB	4:E:7267:HOH:O	2.09	0.97
1:E:452:ASP:HB3	4:E:7267:HOH:O	1.65	0.96
1:D:167:HIS:CD2	2:D:801:FAD:HM82	2.00	0.96
1:E:459:VAL:HG22	1:F:121[B]:LEU:HD21	0.97	0.96
1:B:121[A]:LEU:CD2	1:C:121[A]:LEU:CD2	2.43	0.96
1:A:167:HIS:HE2	2:A:801:FAD:HM81	1.31	0.96
1:A:418:GLN:HG3	4:A:7330:HOH:O	1.64	0.96
1:G:167:HIS:CD2	2:G:801:FAD:HM82	2.01	0.96
1:G:121[B]:LEU:CD2	1:H:459:VAL:HA	1.95	0.95
1:B:414:ASN:O	1:B:418:GLN:HG2	1.67	0.94
1:G:121[B]:LEU:CD2	1:H:459:VAL:CG2	2.45	0.94
1:G:418:GLN:HG3	4:G:7510:HOH:O	1.66	0.94
1:B:167:HIS:CD2	2:B:801:FAD:HM82	2.03	0.94
1:G:459:VAL:CG2	1:H:121[B]:LEU:HD21	1.97	0.94
1:E:126:LEU:HD11	4:E:7492:HOH:O	1.68	0.93
1:E:167:HIS:HE2	2:E:801:FAD:HM81	1.34	0.93
1:C:167:HIS:HE2	2:C:801:FAD:HM81	1.34	0.92
1:F:178:GLU:OE1	4:F:7427:HOH:O	1.87	0.92
1:A:121[B]:LEU:HD21	1:B:459:VAL:CG2	2.01	0.91
1:B:43:MET:N	4:B:7228:HOH:O	2.04	0.91
1:H:454:PHE:O	4:H:7503:HOH:O	1.89	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:HIS:CE1	2:D:801:FAD:HM82	2.07	0.90
1:E:167:HIS:CD2	2:E:801:FAD:HM82	2.07	0.89
1:G:100:ILE:HG12	4:G:7256:HOH:O	1.72	0.88
1:A:459:VAL:CB	1:B:121[B]:LEU:HD21	2.04	0.88
1:B:167:HIS:HE2	2:B:801:FAD:HM81	1.35	0.87
1:A:285:ARG:NH1	4:A:7463:HOH:O	2.06	0.87
1:A:194:GLU:HG2	4:A:7452:HOH:O	1.75	0.87
1:G:81:ASP:HA	4:G:7236:HOH:O	1.73	0.87
1:A:453:ALA:HB3	4:A:7490:HOH:O	1.76	0.85
4:A:7336:HOH:O	1:B:84:LEU:HD23	1.75	0.85
1:A:459:VAL:HG22	1:B:121[B]:LEU:HD21	0.85	0.85
4:D:7493:HOH:O	1:C:160:VAL:HG13	1.76	0.85
1:D:121[B]:LEU:HD21	1:C:459:VAL:HG22	0.89	0.85
1:F:167:HIS:CE1	2:F:801:FAD:HM82	2.08	0.85
1:D:178:GLU:HB3	4:D:7499:HOH:O	1.76	0.84
1:A:459:VAL:CG2	1:B:121[B]:LEU:CD2	2.30	0.83
1:B:121[A]:LEU:CD2	1:C:121[A]:LEU:HD23	2.08	0.83
1:G:121[B]:LEU:HD23	1:H:459:VAL:CA	2.04	0.83
1:E:459:VAL:CG2	1:F:121[B]:LEU:CD2	2.49	0.82
1:G:285:ARG:HD3	4:G:7371:HOH:O	1.80	0.81
4:E:7492:HOH:O	1:F:463:ILE:HD11	1.81	0.81
1:C:310:GLU:OE2	4:C:7438:HOH:O	1.99	0.81
1:G:167:HIS:HE2	2:G:801:FAD:HM81	1.39	0.80
1:F:176:ASP:OD2	4:F:7427:HOH:O	2.00	0.80
1:G:81:ASP:CA	4:G:7236:HOH:O	2.29	0.79
1:H:341:ASN:HD22	1:H:344:ASN:HB3	1.45	0.79
1:B:121[A]:LEU:HD21	1:C:121[A]:LEU:CD2	2.12	0.79
1:A:196:ASP:HB2	4:A:7411:HOH:O	1.83	0.79
1:D:286:VAL:HG22	4:D:7496:HOH:O	1.82	0.78
1:E:452:ASP:HB2	4:E:7267:HOH:O	1.77	0.78
1:A:121[B]:LEU:CD2	1:B:459:VAL:CG2	2.56	0.78
1:G:81:ASP:CA	4:G:7282:HOH:O	2.32	0.78
1:D:418:GLN:HG3	4:D:7275:HOH:O	1.83	0.77
1:B:133:ALA:O	4:B:7457:HOH:O	2.01	0.77
1:H:133:ALA:O	4:H:7369:HOH:O	2.02	0.77
1:D:101:ASP:OD1	4:D:7484:HOH:O	2.02	0.77
1:A:459:VAL:CB	1:B:121[B]:LEU:CD2	2.62	0.77
1:G:82:SER:N	4:G:7236:HOH:O	2.17	0.77
1:G:462:SER:OG	4:G:7489:HOH:O	2.03	0.76
1:A:500:PRO:HD3	4:A:7531:HOH:O	1.85	0.76
3:E:7004:MES:C7	4:E:7440:HOH:O	2.32	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:459:VAL:HG22	1:C:121[B]:LEU:CG	2.15	0.75
1:D:459:VAL:CG2	1:C:121[B]:LEU:CD2	2.47	0.75
1:F:81:ASP:HB2	4:F:7258:HOH:O	1.86	0.75
1:A:429:GLU:HG2	4:A:7455:HOH:O	1.86	0.74
1:C:619:THR:HG23	1:C:619:THR:O	1.86	0.74
1:F:121[A]:LEU:HD21	1:G:121[A]:LEU:CD2	2.17	0.74
1:D:176:ASP:CG	4:D:7499:HOH:O	2.24	0.74
1:D:178:GLU:CB	4:D:7499:HOH:O	2.32	0.74
1:E:121[B]:LEU:HD23	1:F:459:VAL:CA	2.16	0.74
1:A:459:VAL:HG22	1:B:121[B]:LEU:HD22	1.64	0.73
1:E:133:ALA:O	4:E:7440:HOH:O	2.05	0.73
1:E:121[B]:LEU:HD21	1:F:459:VAL:HG22	0.76	0.73
4:B:7457:HOH:O	1:C:505:ARG:NH2	2.22	0.73
1:G:167:HIS:CE1	2:G:801:FAD:HM82	2.12	0.72
1:B:167:HIS:CE1	2:B:801:FAD:HM82	2.14	0.72
1:B:542:GLU:HB2	4:B:7476:HOH:O	1.90	0.72
1:D:341:ASN:ND2	4:D:7479:HOH:O	2.19	0.72
1:E:176:ASP:OD2	4:E:7312:HOH:O	2.07	0.72
1:D:452[B]:ASP:OD1	4:D:7467:HOH:O	2.08	0.71
1:A:228:GLU:HG3	4:A:7294:HOH:O	1.90	0.71
1:B:285:ARG:CD	4:B:7315:HOH:O	2.24	0.71
3:E:7004:MES:H72	4:E:7440:HOH:O	1.88	0.71
1:F:121[A]:LEU:CD2	1:G:121[A]:LEU:HD21	2.19	0.71
1:B:478:GLU:HB2	4:B:7501:HOH:O	1.90	0.71
1:B:121[A]:LEU:HD21	1:C:121[A]:LEU:HD23	1.70	0.71
1:G:121[B]:LEU:HD23	1:H:459:VAL:HG23	1.68	0.70
1:D:178:GLU:OE1	4:D:7294:HOH:O	2.08	0.70
1:G:123:VAL:HG22	1:H:459:VAL:HG22	1.72	0.70
1:E:121[B]:LEU:CD2	1:F:459:VAL:HA	2.19	0.70
1:E:323:VAL:HG21	4:E:7494:HOH:O	1.91	0.70
1:H:100:ILE:HG12	4:H:7283:HOH:O	1.92	0.70
1:B:385:THR:HG22	4:B:7411:HOH:O	1.91	0.70
1:F:167:HIS:HE2	2:F:801:FAD:HM81	1.39	0.70
1:A:459:VAL:CA	1:B:121[B]:LEU:CD2	2.58	0.69
1:B:505:ARG:NH2	4:C:7327:HOH:O	2.25	0.69
1:F:81:ASP:CA	4:F:7258:HOH:O	2.39	0.69
1:D:459:VAL:HG23	1:C:121[B]:LEU:HD21	1.72	0.69
1:D:100:ILE:HD13	1:D:100:ILE:C	2.11	0.69
1:G:81:ASP:C	4:G:7236:HOH:O	2.29	0.69
3:D:7007:MES:C7	4:D:7447:HOH:O	2.24	0.69
1:F:299:HIS:HE2	1:F:310:GLU:CD	1.96	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:121[A]:LEU:CD2	1:H:121[A]:LEU:CD2	2.71	0.69
1:E:421:GLU:OE2	4:E:7504:HOH:O	2.11	0.68
1:E:121[B]:LEU:HD22	1:F:459:VAL:HG22	1.68	0.68
1:E:244:THR:O	4:E:7477:HOH:O	2.11	0.68
1:H:211:ASP:HB3	4:H:7331:HOH:O	1.93	0.68
1:B:178:GLU:HG3	4:B:7219:HOH:O	1.93	0.68
1:C:45:ILE:HG23	4:C:7267:HOH:O	1.92	0.68
1:G:101:ASP:O	1:G:104[A]:VAL:HG23	1.94	0.68
1:E:178:GLU:OE1	4:E:7312:HOH:O	2.11	0.68
1:F:121[A]:LEU:HD21	1:G:121[A]:LEU:HD22	1.74	0.68
1:A:496:ASN:CG	4:A:7509:HOH:O	2.32	0.68
1:A:104:VAL:CB	4:A:7508:HOH:O	2.04	0.67
1:E:133:ALA:C	4:E:7440:HOH:O	2.33	0.67
1:D:101:ASP:HA	4:D:7506:HOH:O	1.92	0.67
1:E:167:HIS:CE1	2:E:801:FAD:HM82	2.19	0.67
4:G:7299:HOH:O	1:H:84:LEU:HD23	1.95	0.67
1:A:250:PHE:CD2	4:A:7511:HOH:O	2.46	0.66
1:G:104[B]:VAL:HG13	4:G:7438:HOH:O	1.94	0.66
1:E:84:LEU:HD23	4:F:7219:HOH:O	1.94	0.66
1:B:339:ARG:HG3	4:B:7417:HOH:O	1.95	0.66
1:E:100:ILE:HB	4:E:7441:HOH:O	1.95	0.66
1:A:121[B]:LEU:HD23	1:B:459:VAL:HG22	1.72	0.66
1:D:418:GLN:CG	4:D:7275:HOH:O	2.41	0.66
1:E:133:ALA:CA	4:E:7440:HOH:O	2.43	0.66
1:E:82:SER:O	4:E:7256:HOH:O	2.14	0.66
1:C:82:SER:O	4:C:7311:HOH:O	2.12	0.66
1:F:97:GLN:HG3	1:F:250:PHE:CE2	2.30	0.66
1:B:528:LYS:HE3	4:B:7428:HOH:O	1.95	0.66
1:F:178:GLU:OE2	4:F:7347:HOH:O	2.14	0.66
1:E:121[B]:LEU:HD12	4:E:7181:HOH:O	1.95	0.66
1:E:133:ALA:HB3	4:E:7440:HOH:O	1.94	0.66
1:A:84:LEU:HD23	4:B:7307:HOH:O	1.95	0.66
1:C:133:ALA:O	4:C:7327:HOH:O	2.12	0.66
1:F:121[A]:LEU:CD2	1:G:121[A]:LEU:HD22	2.22	0.65
1:G:490:LYS:HD3	1:G:491:ILE:HD13	1.78	0.65
1:B:542:GLU:CB	4:B:7476:HOH:O	2.41	0.65
1:A:228:GLU:OE1	4:A:7390:HOH:O	2.15	0.65
1:E:97:GLN:HG3	1:E:250:PHE:CE2	2.32	0.65
1:H:310:GLU:OE1	4:H:7456:HOH:O	2.14	0.65
1:B:596:LEU:HD13	4:B:7543:HOH:O	1.97	0.65
1:G:121[B]:LEU:CD2	1:H:459:VAL:CA	2.70	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:7004:MES:H71	4:E:7440:HOH:O	1.94	0.64
1:E:167:HIS:HE2	2:E:801:FAD:HM82	0.50	0.64
1:D:91:LYS:CE	4:D:7373:HOH:O	2.45	0.64
1:G:81:ASP:C	4:G:7282:HOH:O	2.35	0.64
1:F:121[A]:LEU:HD23	1:G:121[A]:LEU:CD2	2.27	0.64
1:F:81:ASP:CB	4:F:7258:HOH:O	2.45	0.64
1:H:459:VAL:HG13	4:H:7517:HOH:O	1.97	0.64
1:E:286:VAL:HG22	4:E:7444:HOH:O	1.97	0.64
1:E:91:LYS:CE	4:E:7268:HOH:O	2.47	0.63
1:F:121[A]:LEU:HD22	1:G:121[A]:LEU:CD2	2.27	0.63
1:F:299:HIS:NE2	1:F:310:GLU:CD	2.51	0.63
1:E:97:GLN:HG3	1:E:250:PHE:CD2	2.34	0.63
1:A:121[B]:LEU:HD12	4:A:7267:HOH:O	1.96	0.63
1:C:97:GLN:HG3	1:C:250:PHE:CE2	2.34	0.63
1:D:133:ALA:HB3	4:D:7447:HOH:O	1.97	0.63
1:D:421:GLU:HG3	4:D:7367:HOH:O	1.99	0.63
1:B:91:LYS:CE	4:B:7302:HOH:O	2.47	0.62
1:C:100:ILE:HG12	4:C:7341:HOH:O	2.00	0.62
1:E:459:VAL:HA	1:F:121[B]:LEU:HD23	1.81	0.62
1:F:121[A]:LEU:HD22	1:G:121[A]:LEU:HD21	1.82	0.62
1:A:496:ASN:CG	4:A:7324:HOH:O	2.37	0.62
1:C:341:ASN:ND2	4:C:7416:HOH:O	2.32	0.62
1:G:459:VAL:CG2	1:H:121[B]:LEU:CD2	2.66	0.62
1:A:104:VAL:CG2	4:A:7508:HOH:O	2.42	0.62
1:B:121[A]:LEU:CD2	1:C:121[A]:LEU:HD21	2.29	0.62
1:G:101:ASP:HA	4:G:7438:HOH:O	1.99	0.62
1:A:194:GLU:CG	4:A:7452:HOH:O	2.39	0.62
1:B:91:LYS:NZ	4:B:7302:HOH:O	2.28	0.61
1:B:97:GLN:HG3	1:B:250:PHE:CE2	2.34	0.61
1:G:561:GLU:HG3	4:G:7264:HOH:O	2.00	0.61
1:G:97:GLN:HG3	1:G:250:PHE:CE2	2.36	0.61
1:G:496:ASN:HB2	4:G:7476:HOH:O	2.00	0.61
1:B:618:PHE:HB3	4:B:7490:HOH:O	2.01	0.61
1:E:167:HIS:HE2	2:E:801:FAD:C8	2.02	0.61
1:G:81:ASP:C	1:G:81:ASP:OD1	2.37	0.61
1:C:285:ARG:HD3	4:C:7309:HOH:O	2.01	0.60
1:D:561:GLU:HG2	4:D:7296:HOH:O	2.00	0.60
1:G:121[B]:LEU:HD21	1:H:459:VAL:CB	2.31	0.60
1:B:547:LEU:CD1	2:B:801:FAD:HM83	2.32	0.60
1:D:123:VAL:HG22	1:C:459:VAL:CG1	2.31	0.60
1:A:341:ASN:HD22	1:A:342:PRO:HD2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:505:ARG:NH2	4:E:7318:HOH:O	2.34	0.60
4:G:7261:HOH:O	1:H:81:ASP:HA	2.00	0.60
1:C:389:LEU:HD12	1:C:389:LEU:H	1.67	0.60
1:D:100:ILE:CD1	1:D:100:ILE:C	2.70	0.60
1:C:505:ARG:NH2	4:C:7312:HOH:O	2.35	0.59
1:A:133:ALA:O	4:A:7279:HOH:O	2.17	0.59
1:G:341:ASN:HB3	4:G:7527:HOH:O	2.03	0.59
1:B:413:LYS:HE3	4:B:7494:HOH:O	2.01	0.59
1:B:167:HIS:HE2	2:B:801:FAD:C8	2.01	0.58
1:B:121[A]:LEU:HD22	1:C:121[A]:LEU:CD2	2.31	0.58
1:G:104[A]:VAL:HG23	4:G:7438:HOH:O	2.03	0.58
1:G:121[B]:LEU:CD2	1:H:459:VAL:CB	2.80	0.58
1:E:246:ARG:NE	4:E:7477:HOH:O	2.36	0.58
1:F:81:ASP:C	4:F:7258:HOH:O	2.41	0.58
4:A:7279:HOH:O	1:D:505:ARG:NH2	2.35	0.58
1:H:346:PRO:HG2	1:H:350:PRO:HA	1.85	0.58
1:C:50:VAL:HG13	1:C:313:ALA:HB2	1.86	0.58
1:H:91:LYS:NZ	4:H:7301:HOH:O	2.17	0.58
4:D:7493:HOH:O	1:C:160:VAL:CG1	2.44	0.58
1:E:91:LYS:NZ	4:E:7268:HOH:O	2.34	0.58
1:B:341:ASN:HD22	1:B:342:PRO:N	2.03	0.57
1:E:299:HIS:CE1	1:E:310:GLU:HG2	2.39	0.57
1:F:83:GLY:N	4:F:7220:HOH:O	2.31	0.57
1:F:121[A]:LEU:CD2	1:G:121[A]:LEU:HD23	2.30	0.57
1:G:121[B]:LEU:HD23	1:H:459:VAL:CG2	2.27	0.57
1:A:50:VAL:HG13	1:A:313:ALA:HB2	1.86	0.57
1:D:121[B]:LEU:HD23	1:C:459:VAL:HA	1.86	0.57
1:E:505:ARG:NH2	4:H:7369:HOH:O	2.38	0.56
1:G:459:VAL:HA	1:H:121[B]:LEU:HD23	1.85	0.56
1:H:101:ASP:CG	4:H:7503:HOH:O	2.44	0.56
1:E:100:ILE:O	1:E:100:ILE:HD13	2.05	0.56
1:G:83:GLY:N	4:G:7261:HOH:O	2.21	0.56
4:F:7418:HOH:O	1:G:121[A]:LEU:HD11	2.03	0.56
1:B:167:HIS:HE2	2:B:801:FAD:HM82	0.40	0.56
1:B:121[A]:LEU:HD22	1:C:121[A]:LEU:HD21	1.87	0.56
1:F:505:ARG:NH2	4:G:7361:HOH:O	2.39	0.56
1:A:272:GLU:HG2	4:A:7368:HOH:O	2.04	0.56
1:F:481:GLU:HG2	4:F:7362:HOH:O	2.06	0.56
1:G:104[A]:VAL:CG2	4:G:7438:HOH:O	2.53	0.56
1:G:97:GLN:HG3	1:G:250:PHE:CD2	2.41	0.56
1:B:167:HIS:NE2	2:B:801:FAD:HM81	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:444:PRO:HD2	1:G:445:TRP:CZ3	2.41	0.55
1:F:50:VAL:HG13	1:F:313:ALA:HB2	1.88	0.55
1:H:231:LYS:HE3	4:H:7487:HOH:O	2.05	0.55
1:B:97:GLN:HG3	1:B:250:PHE:CD2	2.41	0.55
1:A:576:LYS:HE2	4:A:7432:HOH:O	2.07	0.55
1:B:341:ASN:ND2	1:B:343:ALA:H	2.04	0.55
1:H:45:ILE:HG22	4:H:7444:HOH:O	2.07	0.55
1:B:167:HIS:NE2	2:B:801:FAD:C8	2.66	0.54
1:B:284:GLU:C	1:B:285:ARG:HG2	2.27	0.54
1:B:81:ASP:C	1:B:81:ASP:OD1	2.44	0.54
1:E:441:PRO:HD3	4:E:7312:HOH:O	2.07	0.54
1:D:228:GLU:HG3	4:D:7312:HOH:O	2.07	0.54
1:G:418:GLN:CG	4:G:7510:HOH:O	2.36	0.54
1:D:97:GLN:HG3	1:D:250:PHE:CE2	2.43	0.54
1:E:323:VAL:CG2	4:E:7494:HOH:O	2.51	0.54
1:E:421:GLU:HG3	4:F:7340:HOH:O	2.07	0.54
1:A:390:THR:HG23	4:A:7528:HOH:O	2.08	0.54
1:B:101:ASP:O	1:B:104[B]:VAL:HG22	2.08	0.54
1:E:133:ALA:CB	4:E:7440:HOH:O	2.55	0.54
1:E:121[B]:LEU:CD2	1:F:459:VAL:CB	2.86	0.54
1:A:43:MET:HE3	4:A:7361:HOH:O	2.08	0.54
1:D:454:PHE:HB3	4:D:7484:HOH:O	2.08	0.54
1:A:121[A]:LEU:CD2	1:D:121[A]:LEU:CD2	2.86	0.53
1:E:246:ARG:HG2	4:E:7477:HOH:O	2.07	0.53
1:E:547:LEU:CD1	2:E:801:FAD:HM83	2.38	0.53
1:B:341:ASN:HD22	1:B:342:PRO:CD	2.21	0.53
1:D:305:SER:HB3	4:D:7472:HOH:O	2.06	0.53
1:B:43:MET:N	4:B:7389:HOH:O	2.40	0.53
1:A:121[B]:LEU:HD23	1:B:459:VAL:HA	1.90	0.53
1:D:133:ALA:CA	4:D:7447:HOH:O	2.56	0.53
1:D:576:LYS:CD	4:D:7295:HOH:O	2.55	0.53
1:B:45:ILE:HG23	4:B:7361:HOH:O	2.08	0.53
1:C:619:THR:CG2	1:C:619:THR:O	2.56	0.53
1:G:104[A]:VAL:HG21	1:G:454:PHE:C	2.29	0.53
1:H:211:ASP:CB	4:H:7331:HOH:O	2.56	0.53
1:D:123:VAL:HG22	1:C:459:VAL:HG12	1.90	0.53
1:C:97:GLN:HG3	1:C:250:PHE:CD2	2.43	0.53
1:E:418:GLN:HE21	1:E:418:GLN:HA	1.73	0.53
1:B:341:ASN:HD22	1:B:342:PRO:HD2	1.73	0.53
1:G:167:HIS:CE1	2:G:801:FAD:C8M	2.84	0.53
1:E:133:ALA:N	4:E:7440:HOH:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:81:ASP:HA	4:G:7282:HOH:O	2.02	0.53
1:A:496:ASN:CB	4:A:7324:HOH:O	2.57	0.52
1:G:341:ASN:HD22	1:G:342:PRO:HD2	1.75	0.52
1:E:244:THR:HB	4:E:7477:HOH:O	2.08	0.52
1:E:56:PRO:HD3	1:E:165:SER:HB3	1.91	0.52
1:H:618:PHE:HB3	4:H:7438:HOH:O	2.10	0.52
1:G:398:GLY:O	1:G:399:ALA:C	2.47	0.52
1:A:459:VAL:CG1	1:B:121[B]:LEU:HD21	2.39	0.52
1:A:121[B]:LEU:HD23	1:B:459:VAL:CG2	2.36	0.52
1:E:268:THR:HG22	4:E:7484:HOH:O	2.10	0.52
1:F:383:ARG:HB2	1:F:392:SER:HB3	1.92	0.52
1:F:157:VAL:HG21	1:F:324:HIS:HE1	1.74	0.51
1:G:481:GLU:HG2	4:G:7262:HOH:O	2.10	0.51
1:G:547:LEU:CD1	2:G:801:FAD:HM83	2.39	0.51
4:D:7493:HOH:O	1:C:110:GLN:HB2	2.09	0.51
1:E:167:HIS:NE2	2:E:801:FAD:C8	2.68	0.51
1:E:91:LYS:HE3	4:E:7268:HOH:O	2.10	0.51
1:C:218:ARG:HD2	4:C:7083:HOH:O	2.09	0.51
1:D:414:ASN:O	1:D:418:GLN:HG2	2.10	0.51
1:A:607:GLU:HG3	4:A:7438:HOH:O	2.09	0.51
1:B:104[B]:VAL:HG21	1:B:455:SER:HB3	1.93	0.51
1:E:459:VAL:HG22	1:F:121[B]:LEU:HD23	1.81	0.51
1:H:45:ILE:C	1:H:45:ILE:HD12	2.31	0.51
1:E:285:ARG:NH1	1:E:299:HIS:CD2	2.79	0.51
1:F:45:ILE:HG22	1:F:45:ILE:O	2.11	0.51
4:E:7492:HOH:O	1:F:463:ILE:CD1	2.47	0.51
1:B:121[A]:LEU:HD23	1:C:121[A]:LEU:HD23	1.92	0.51
1:A:81:ASP:OD1	1:A:81:ASP:C	2.45	0.51
1:C:153:SER:OG	1:C:542:GLU:HG3	2.11	0.51
1:A:285:ARG:HA	1:A:328:LEU:HD13	1.93	0.50
1:F:388:GLU:HB3	4:F:7431:HOH:O	2.10	0.50
1:D:121[B]:LEU:CD2	1:C:459:VAL:CG2	2.59	0.50
1:G:341:ASN:HD22	1:G:342:PRO:CD	2.25	0.50
1:G:81:ASP:CB	4:G:7282:HOH:O	2.59	0.50
1:F:385:THR:OG1	1:F:388:GLU:OE1	2.28	0.50
1:F:390:THR:HG23	4:F:7431:HOH:O	2.10	0.50
1:H:310:GLU:CD	4:H:7456:HOH:O	2.49	0.50
1:A:97:GLN:CB	4:A:7511:HOH:O	2.28	0.50
1:G:121[B]:LEU:CG	1:H:459:VAL:HG23	2.32	0.50
1:D:158:THR:HG22	1:D:160:VAL:HG22	1.93	0.50
1:F:121[A]:LEU:HD23	1:G:121[A]:LEU:HD23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:SER:HB2	4:D:7389:HOH:O	2.12	0.50
1:D:167:HIS:CE1	2:D:801:FAD:C8M	2.81	0.50
1:B:538:PRO:HG2	1:D:538:PRO:HG2	1.93	0.49
1:D:607:GLU:HG3	4:D:7304:HOH:O	2.12	0.49
1:F:285:ARG:HA	1:F:328:LEU:HD13	1.94	0.49
1:G:218:ARG:HD2	4:G:7043:HOH:O	2.12	0.49
1:B:45:ILE:O	1:B:45:ILE:HD12	2.12	0.49
1:F:97:GLN:HG3	1:F:250:PHE:CD2	2.47	0.49
1:H:44:ASP:HB3	4:H:7417:HOH:O	2.12	0.49
1:A:250:PHE:CE2	4:A:7511:HOH:O	2.65	0.49
1:A:542:GLU:OE1	1:A:545:LEU:HD13	2.12	0.49
1:B:564:CYS:HG	1:B:573:PHE:HE2	1.61	0.49
1:C:564:CYS:HG	1:C:573:PHE:HE2	1.60	0.49
1:E:346:PRO:HG2	1:E:350:PRO:HA	1.95	0.49
1:G:167:HIS:NE2	2:G:801:FAD:HM81	2.10	0.49
1:B:284:GLU:O	1:B:285:ARG:HG2	2.13	0.49
1:B:341:ASN:ND2	1:B:342:PRO:HD2	2.28	0.49
1:C:157:VAL:HG21	1:C:324:HIS:HE1	1.78	0.49
1:D:481:GLU:HG2	4:D:7272:HOH:O	2.13	0.49
1:E:167:HIS:NE2	2:E:801:FAD:HM81	2.07	0.49
1:H:459:VAL:CG1	4:H:7380:HOH:O	2.61	0.49
1:A:218:ARG:HD2	4:A:7091:HOH:O	2.13	0.49
1:D:453:ALA:HB3	4:D:7513:HOH:O	2.12	0.49
1:H:482:GLU:HG3	4:H:7357:HOH:O	2.12	0.49
1:H:547:LEU:CD1	2:H:801:FAD:HM83	2.43	0.48
1:C:385:THR:OG1	1:C:388:GLU:OE1	2.15	0.48
1:G:81:ASP:HB2	4:G:7282:HOH:O	2.12	0.48
1:G:91:LYS:HG2	4:G:7395:HOH:O	2.13	0.48
1:B:153:SER:OG	1:B:542:GLU:HG3	2.12	0.48
1:F:45:ILE:O	1:F:45:ILE:CG2	2.62	0.48
1:F:83:GLY:CA	4:F:7220:HOH:O	2.61	0.48
1:G:47:TYR:O	1:G:313:ALA:HA	2.13	0.48
1:G:457:GLY:O	1:G:461:GLN:HG3	2.13	0.48
1:A:312:LYS:HD2	4:A:7560:HOH:O	2.13	0.48
1:B:167:HIS:CE1	2:B:801:FAD:C8M	2.83	0.48
1:D:133:ALA:N	4:D:7447:HOH:O	2.46	0.48
1:A:194:GLU:CD	4:A:7452:HOH:O	2.51	0.48
1:E:100:ILE:CG2	1:E:101:ASP:N	2.77	0.48
1:H:91:LYS:CE	4:H:7301:HOH:O	2.60	0.48
1:D:101:ASP:O	1:D:104:VAL:HG23	2.13	0.48
1:E:459:VAL:HG22	1:F:121[B]:LEU:CG	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:411:LYS:HE3	4:H:7382:HOH:O	2.14	0.48
1:A:285:ARG:HA	1:A:328:LEU:CD1	2.44	0.48
1:A:389:LEU:H	1:A:389:LEU:HD12	1.79	0.48
1:C:287:VAL:HG22	4:C:7452:HOH:O	2.14	0.48
1:D:561:GLU:CG	4:D:7296:HOH:O	2.61	0.48
1:F:538:PRO:HG2	1:H:538:PRO:HG2	1.95	0.48
1:H:50:VAL:HG13	1:H:313:ALA:HB2	1.94	0.48
1:B:218:ARG:HD2	4:B:7023:HOH:O	2.14	0.47
1:B:233:GLN:CD	4:B:7569:HOH:O	2.52	0.47
1:C:619:THR:HG22	4:C:7283:HOH:O	2.13	0.47
1:F:47:TYR:O	1:F:313:ALA:HA	2.14	0.47
1:G:390:THR:HG23	4:G:7485:HOH:O	2.13	0.47
1:H:228:GLU:HG3	4:H:7256:HOH:O	2.14	0.47
4:G:7236:HOH:O	1:H:83:GLY:N	2.47	0.47
1:C:44:ASP:OD2	1:C:71:LYS:NZ	2.36	0.47
1:B:153:SER:OG	1:B:542:GLU:CG	2.61	0.47
1:E:100:ILE:HG23	1:E:101:ASP:N	2.28	0.47
1:E:547:LEU:HD12	2:E:801:FAD:HM83	1.96	0.47
1:G:459:VAL:HG22	1:H:121[B]:LEU:CG	2.43	0.47
1:D:133:ALA:C	4:D:7447:HOH:O	2.52	0.47
1:F:83:GLY:HA2	4:F:7220:HOH:O	2.13	0.47
1:A:123:VAL:HG22	1:B:459:VAL:CG1	2.44	0.47
1:A:81:ASP:O	1:A:90:LYS:HE2	2.14	0.47
1:H:401:THR:HG23	4:H:7440:HOH:O	2.13	0.47
1:B:46:LYS:HE2	4:B:7320:HOH:O	2.15	0.47
1:A:452:ASP:OD1	1:A:452:ASP:N	2.47	0.47
1:A:121[B]:LEU:CG	1:B:459:VAL:HG22	2.41	0.47
1:D:547:LEU:CD1	2:D:801:FAD:HM83	2.44	0.47
1:G:133:ALA:O	4:G:7361:HOH:O	2.20	0.47
1:H:215:GLU:O	1:H:411:LYS:NZ	2.47	0.47
1:C:618:PHE:C	1:C:618:PHE:HD1	2.17	0.47
1:C:81:ASP:OD1	1:C:81:ASP:C	2.51	0.47
1:C:478:GLU:HG2	1:C:480:LYS:HE2	1.96	0.47
1:C:618:PHE:C	1:C:618:PHE:CD1	2.88	0.46
1:G:50:VAL:HG13	1:G:313:ALA:HB2	1.98	0.46
1:A:123:VAL:HG22	1:B:459:VAL:HG12	1.97	0.46
1:F:167:HIS:CE1	2:F:801:FAD:C8M	2.83	0.46
1:G:490:LYS:CD	1:G:491:ILE:HD13	2.45	0.46
1:A:341:ASN:HD22	1:A:342:PRO:CD	2.28	0.46
1:F:100:ILE:HG23	1:F:101:ASP:N	2.31	0.46
1:F:490:LYS:HE2	4:F:7441:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:570:SER:HB3	1:H:580:LEU:O	2.16	0.46
1:C:100:ILE:HG23	1:C:101:ASP:N	2.30	0.46
1:C:196:ASP:HB2	4:C:7288:HOH:O	2.15	0.46
1:D:159:ARG:HA	2:D:801:FAD:O2B	2.16	0.46
1:E:388:GLU:HG2	4:E:7463:HOH:O	2.15	0.46
1:D:50:VAL:HG13	1:D:313:ALA:HB2	1.96	0.46
1:H:167:HIS:CD2	2:H:801:FAD:C8M	2.70	0.46
1:B:339:ARG:CG	4:B:7417:HOH:O	2.59	0.46
1:C:285:ARG:NH1	4:C:7362:HOH:O	2.48	0.46
1:C:47:TYR:O	1:C:313:ALA:HA	2.15	0.46
1:D:167:HIS:NE2	2:D:801:FAD:C8	2.71	0.46
1:B:340:PRO:HD2	4:B:7417:HOH:O	2.16	0.45
1:G:218:ARG:HG3	1:G:430:ASP:OD2	2.16	0.45
1:A:542:GLU:HB2	4:D:7486:HOH:O	2.16	0.45
1:C:285:ARG:HA	1:C:328:LEU:CD1	2.46	0.45
1:E:121[A]:LEU:CD2	1:H:121[A]:LEU:HD21	2.46	0.45
1:B:312:LYS:HE2	4:B:7320:HOH:O	2.17	0.45
1:E:215:GLU:O	1:E:411:LYS:NZ	2.47	0.45
1:F:218:ARG:HG3	1:F:430:ASP:OD2	2.16	0.45
1:D:215:GLU:CD	4:D:7508:HOH:O	2.55	0.45
1:D:215:GLU:O	1:D:411:LYS:NZ	2.45	0.45
1:E:538:PRO:HG2	1:G:538:PRO:HG2	1.97	0.45
1:B:45:ILE:C	1:B:45:ILE:HD12	2.37	0.45
1:D:218:ARG:HD2	4:D:7043:HOH:O	2.16	0.45
1:D:293:SER:HA	1:D:574:GLY:O	2.17	0.45
1:E:47:TYR:O	1:E:313:ALA:HA	2.17	0.45
1:E:121[B]:LEU:HD23	1:F:459:VAL:CB	2.46	0.45
1:A:459:VAL:HG13	1:B:121[B]:LEU:CD2	2.46	0.45
1:H:139:ARG:HD3	3:H:7002:MES:O3S	2.16	0.45
1:D:570:SER:HB3	1:D:580:LEU:O	2.16	0.45
1:F:64:GLU:OE1	4:F:7408:HOH:O	2.21	0.45
1:A:153:SER:OG	1:A:542:GLU:HG3	2.17	0.45
1:C:363:PHE:HA	1:C:471:TRP:O	2.17	0.45
1:F:211:ASP:HB2	1:F:214:LYS:HD3	1.98	0.45
1:A:459:VAL:CG1	1:B:123:VAL:HG22	2.46	0.45
1:D:505:ARG:NH2	4:D:7289:HOH:O	2.50	0.45
1:E:218:ARG:HD2	4:E:7084:HOH:O	2.17	0.45
1:F:121[A]:LEU:HD23	4:G:7292:HOH:O	2.16	0.45
1:F:167:HIS:NE2	2:F:801:FAD:HM81	2.12	0.45
1:B:185:LYS:HG2	4:B:7319:HOH:O	2.16	0.45
1:C:285:ARG:HA	1:C:328:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:GLN:HB2	4:D:7436:HOH:O	2.16	0.45
1:A:346:PRO:HG2	1:A:350:PRO:HA	1.99	0.44
1:C:383:ARG:HB3	1:C:392:SER:HB3	1.98	0.44
1:E:343:ALA:O	1:E:344:ASN:HB2	2.16	0.44
1:D:285:ARG:HG3	1:D:299:HIS:HB2	1.99	0.44
1:B:547:LEU:HD12	2:B:801:FAD:HM83	2.00	0.44
1:C:100:ILE:HG22	4:C:7271:HOH:O	2.17	0.44
1:C:285:ARG:CD	4:C:7309:HOH:O	2.64	0.44
1:F:167:HIS:NE2	2:F:801:FAD:C8	2.72	0.44
1:G:285:ARG:NH2	1:G:299:HIS:HD2	2.15	0.44
1:G:336:GLN:NE2	1:G:344:ASN:O	2.50	0.44
1:G:83:GLY:CA	4:G:7261:HOH:O	2.62	0.44
1:H:196:ASP:HB2	4:H:7258:HOH:O	2.17	0.44
3:A:7003:MES:O1S	3:A:7003:MES:H51	2.18	0.44
1:B:342:PRO:O	1:B:345:PRO:HD3	2.18	0.44
1:C:346:PRO:HG2	1:C:350:PRO:HA	1.99	0.44
1:D:413:LYS:HE2	1:D:414:ASN:OD1	2.17	0.44
1:D:284:GLU:C	1:D:328:LEU:CD1	2.86	0.44
1:E:136:PHE:HA	4:E:7426:HOH:O	2.17	0.44
1:G:121[A]:LEU:HD23	4:G:7292:HOH:O	2.18	0.44
1:G:81:ASP:OD1	1:G:81:ASP:O	2.35	0.44
1:B:394:THR:OG1	4:B:7370:HOH:O	2.21	0.44
1:C:104:VAL:HG21	1:C:454:PHE:CA	2.48	0.44
1:B:159:ARG:HA	2:B:801:FAD:O2B	2.18	0.44
1:E:81:ASP:HA	4:F:7220:HOH:O	2.16	0.44
1:H:104:VAL:CG2	4:H:7426:HOH:O	2.49	0.44
1:C:385:THR:N	4:C:7487:HOH:O	2.48	0.44
1:E:43:MET:HE2	4:E:7461:HOH:O	2.17	0.44
1:E:459:VAL:CA	1:F:121[B]:LEU:HD23	2.48	0.44
1:H:444:PRO:HD2	1:H:445:TRP:CZ3	2.53	0.44
1:A:496:ASN:ND2	4:A:7509:HOH:O	2.51	0.43
1:G:81:ASP:O	1:G:90:LYS:HE2	2.17	0.43
1:H:173:PRO:HG2	1:H:592:ALA:HB1	1.99	0.43
1:A:496:ASN:HB3	4:A:7324:HOH:O	2.17	0.43
1:E:246:ARG:CD	4:E:7477:HOH:O	2.66	0.43
1:A:167:HIS:CE1	2:A:801:FAD:C8M	2.80	0.43
1:D:91:LYS:NZ	4:D:7373:HOH:O	2.34	0.43
1:E:285:ARG:HH12	1:E:299:HIS:CD2	2.36	0.43
1:A:478:GLU:HB2	4:A:7366:HOH:O	2.18	0.43
1:E:293:SER:HA	1:E:574:GLY:O	2.17	0.43
1:E:452:ASP:OD1	1:E:452:ASP:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:LEU:HD12	1:B:132:GLN:HG3	2.01	0.43
1:E:45:ILE:HG22	1:E:45:ILE:O	2.18	0.43
1:D:89:HIS:CE1	1:D:91:LYS:HG2	2.54	0.43
3:E:7004:MES:H72	4:E:7426:HOH:O	2.19	0.43
1:B:218:ARG:HG3	1:B:430:ASP:OD2	2.18	0.43
1:C:81:ASP:O	1:C:90:LYS:HE2	2.18	0.43
1:E:123:VAL:HB	4:E:7492:HOH:O	2.18	0.43
1:E:363:PHE:HA	1:E:471:TRP:O	2.19	0.43
1:F:564:CYS:HG	1:F:573:PHE:HE2	1.67	0.43
1:A:538:PRO:HG2	1:C:538:PRO:HG2	2.00	0.43
1:B:158:THR:HG22	1:B:160:VAL:HG22	2.00	0.43
1:E:50:VAL:HG13	1:E:313:ALA:HB2	1.99	0.43
1:E:459:VAL:CG2	1:F:121[B]:LEU:HD23	2.45	0.43
1:B:100:ILE:CG1	4:B:7296:HOH:O	2.67	0.43
1:D:100:ILE:HG23	1:D:101:ASP:N	2.34	0.43
1:D:510:ARG:NH2	4:D:7443:HOH:O	2.52	0.43
4:A:7336:HOH:O	1:B:84:LEU:CD2	2.48	0.42
1:E:100:ILE:C	1:E:100:ILE:HD13	2.39	0.42
1:A:418:GLN:CG	4:A:7330:HOH:O	2.43	0.42
1:A:457:GLY:HA3	4:A:7285:HOH:O	2.19	0.42
1:C:104:VAL:CG2	1:C:453:ALA:C	2.87	0.42
1:E:121[A]:LEU:CD2	1:H:121[A]:LEU:HD23	2.48	0.42
1:G:167:HIS:NE2	2:G:801:FAD:C8	2.72	0.42
1:H:218:ARG:HD2	4:H:7077:HOH:O	2.19	0.42
1:A:47:TYR:O	1:A:313:ALA:HA	2.19	0.42
1:B:100:ILE:HG12	4:B:7296:HOH:O	2.17	0.42
1:E:173:PRO:HG2	1:E:592:ALA:HB1	2.01	0.42
1:F:194:GLU:HG2	4:F:7320:HOH:O	2.18	0.42
1:D:47:TYR:O	1:D:313:ALA:HA	2.19	0.42
1:D:347:GLU:HG3	4:D:7423:HOH:O	2.20	0.42
1:E:121[B]:LEU:CD2	1:F:459:VAL:CA	2.90	0.42
1:F:214:LYS:HB2	4:F:7455:HOH:O	2.20	0.42
1:F:231:LYS:NZ	4:F:7384:HOH:O	2.50	0.42
1:D:459:VAL:HA	1:C:121[B]:LEU:HD23	2.02	0.42
1:B:132:GLN:NE2	3:B:7006:MES:C3	2.83	0.42
1:D:132:GLN:HA	1:D:132:GLN:HE21	1.85	0.42
1:F:542:GLU:HB3	4:F:7392:HOH:O	2.19	0.42
1:A:281:VAL:CG1	1:A:300:ILE:HB	2.50	0.42
1:C:471:TRP:CH2	1:C:526:SER:HA	2.55	0.42
1:B:157:VAL:HG21	1:B:324:HIS:HE1	1.85	0.42
1:A:538:PRO:HG2	1:C:538:PRO:CG	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:ARG:HG3	1:D:430:ASP:OD2	2.20	0.42
1:E:81:ASP:HB2	4:F:7266:HOH:O	2.19	0.42
1:G:296:GLU:O	1:G:312:LYS:HD3	2.20	0.42
1:G:132:GLN:NE2	3:G:7008:MES:C3	2.83	0.42
1:D:619:THR:HG22	4:D:7311:HOH:O	2.20	0.41
1:G:432:GLU:HB2	1:G:433:PRO:HD2	2.01	0.41
3:G:7008:MES:H51	3:G:7008:MES:O1S	2.19	0.41
1:H:404:HIS:HE1	4:H:7279:HOH:O	2.02	0.41
1:B:413:LYS:NZ	1:B:414:ASN:OD1	2.51	0.41
1:A:312:LYS:CD	4:A:7560:HOH:O	2.67	0.41
1:F:328:LEU:HD12	1:F:328:LEU:C	2.41	0.41
1:F:433:PRO:O	1:F:450:HIS:HA	2.20	0.41
1:G:471:TRP:CH2	1:G:526:SER:HA	2.55	0.41
1:B:385:THR:OG1	1:B:388:GLU:HG3	2.20	0.41
1:C:159:ARG:HA	2:C:801:FAD:O2B	2.19	0.41
1:E:505:ARG:HD2	4:E:7360:HOH:O	2.20	0.41
1:A:159:ARG:HA	2:A:801:FAD:O2B	2.21	0.41
1:D:454:PHE:N	4:D:7484:HOH:O	2.53	0.41
1:F:341:ASN:HD21	1:F:343:ALA:HB3	1.86	0.41
1:F:56:PRO:HD3	1:F:165:SER:HB3	2.02	0.41
1:F:547:LEU:CD1	2:F:801:FAD:HM83	2.50	0.41
1:B:570:SER:HB3	1:B:580:LEU:O	2.20	0.41
1:C:158:THR:HG22	1:C:160:VAL:HG22	2.03	0.41
1:G:101:ASP:O	1:G:104[B]:VAL:HG22	2.20	0.41
1:G:385:THR:O	1:G:391:TYR:HB2	2.20	0.41
1:G:618:PHE:C	1:G:618:PHE:CD1	2.94	0.41
1:A:471:TRP:CH2	1:A:526:SER:HA	2.56	0.41
1:F:214:LYS:HG3	4:F:7451:HOH:O	2.19	0.41
1:F:606:CYS:O	1:F:610:LYS:HG3	2.20	0.41
1:H:459:VAL:HG11	4:H:7380:HOH:O	2.21	0.41
1:D:576:LYS:HD3	4:D:7295:HOH:O	2.18	0.41
1:E:157:VAL:HG21	1:E:324:HIS:HE1	1.86	0.41
1:B:285:ARG:NH1	1:B:299:HIS:HD2	2.18	0.41
1:C:444:PRO:HD2	1:C:445:TRP:CZ3	2.56	0.41
1:E:252:GLU:HB3	4:E:7477:HOH:O	2.21	0.41
1:E:45:ILE:HG23	1:E:310:GLU:O	2.20	0.41
1:F:216:SER:HB3	1:F:219:HIS:HB3	2.03	0.41
1:H:47:TYR:O	1:H:313:ALA:HA	2.21	0.41
1:A:215:GLU:O	1:A:411:LYS:NZ	2.53	0.40
1:B:108:GLN:HG2	4:B:7505:HOH:O	2.22	0.40
1:F:444:PRO:HD2	1:F:445:TRP:CZ3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:355:TYR:HA	1:G:480:LYS:O	2.20	0.40
1:A:293:SER:HA	1:A:574:GLY:O	2.21	0.40
1:D:510:ARG:CZ	4:D:7443:HOH:O	2.69	0.40
1:C:121[B]:LEU:HD12	1:C:122:VAL:N	2.37	0.40
1:C:347:GLU:HG2	1:C:348:LEU:HG	2.02	0.40
1:G:459:VAL:CG1	1:H:123:VAL:HG22	2.52	0.40
1:H:452:ASP:CB	4:H:7281:HOH:O	2.20	0.40
1:D:558:ASP:HB3	1:D:561:GLU:HB2	2.02	0.40
1:F:214:LYS:HE2	4:F:7415:HOH:O	2.21	0.40
1:F:505:ARG:NH2	4:F:7223:HOH:O	2.53	0.40
1:F:570:SER:HB3	1:F:580:LEU:O	2.21	0.40
1:G:159:ARG:HA	2:G:801:FAD:O2B	2.22	0.40
1:A:542:GLU:HA	1:A:543:PRO:HD3	1.97	0.40
1:A:618:PHE:CD1	1:A:618:PHE:C	2.94	0.40
1:B:233:GLN:HG2	4:B:7569:HOH:O	2.21	0.40
1:B:607:GLU:HG3	4:B:7364:HOH:O	2.21	0.40
1:C:100:ILE:HD13	1:C:453:ALA:HA	2.02	0.40
1:D:336:GLN:HB2	1:D:346:PRO:HG3	2.04	0.40
1:D:70:TYR:OH	1:D:610:LYS:HA	2.22	0.40
1:G:363:PHE:HA	1:G:471:TRP:O	2.21	0.40
1:H:490:LYS:HD3	1:H:491:ILE:HD13	2.04	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	577/623 (93%)	557 (96%)	20 (4%)	0	100	100
1	B	577/623 (93%)	564 (98%)	13 (2%)	0	100	100
1	C	576/623 (92%)	561 (97%)	14 (2%)	1 (0%)	51	41
1	D	578/623 (93%)	564 (98%)	14 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	577/623 (93%)	562 (97%)	14 (2%)	1 (0%)	51	41
1	F	576/623 (92%)	560 (97%)	16 (3%)	0	100	100
1	G	577/623 (93%)	561 (97%)	15 (3%)	1 (0%)	51	41
1	H	576/623 (92%)	559 (97%)	17 (3%)	0	100	100
All	All	4614/4984 (93%)	4488 (97%)	123 (3%)	3 (0%)	55	45

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	344	ASN
1	G	399	ALA
1	C	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	507/542 (94%)	490 (97%)	17 (3%)	42	32
1	B	507/542 (94%)	492 (97%)	15 (3%)	46	37
1	C	506/542 (93%)	491 (97%)	15 (3%)	46	37
1	D	508/542 (94%)	495 (97%)	13 (3%)	51	43
1	E	507/542 (94%)	488 (96%)	19 (4%)	39	28
1	F	506/542 (93%)	489 (97%)	17 (3%)	42	32
1	G	507/542 (94%)	490 (97%)	17 (3%)	42	32
1	H	506/542 (93%)	494 (98%)	12 (2%)	54	47
All	All	4054/4336 (94%)	3929 (97%)	125 (3%)	45	36

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	MET

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Mol	Chain	Res	Type
1	A	100	ILE
1	A	112	MET
1	A	168	TRP
1	A	206	PHE
1	A	312	LYS
1	A	328	LEU
1	A	341	ASN
1	A	347	GLU
1	A	389	LEU
1	A	390	THR
1	A	401	THR
1	A	450	HIS
1	A	490	LYS
1	A	576	LYS
1	A	593	ASN
1	A	618	PHE
1	B	45	ILE
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	328	LEU
1	B	341	ASN
1	B	388	GLU
1	B	408	TRP
1	B	450	HIS
1	B	490	LYS
1	B	496	ASN
1	D	100	ILE
1	D	112	MET
1	D	132	GLN
1	D	168	TRP
1	D	206	PHE
1	D	389	LEU
1	D	390	THR
1	D	403	LYS
1	D	408	TRP
1	D	450	HIS
1	D	496	ASN

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Mol	Chain	Res	Type
1	D	593	ASN
1	D	618	PHE
1	C	45	ILE
1	C	95	GLU
1	C	100	ILE
1	C	112	MET
1	C	168	TRP
1	C	204	SER
1	C	206	PHE
1	C	341	ASN
1	C	389	LEU
1	C	403	LYS
1	C	450	HIS
1	C	490	LYS
1	C	496	ASN
1	C	593	ASN
1	C	618	PHE
1	E	91	LYS
1	E	100	ILE
1	E	112	MET
1	E	168	TRP
1	E	194	GLU
1	E	206	PHE
1	E	285	ARG
1	E	299	HIS
1	E	341	ASN
1	E	385	THR
1	E	388	GLU
1	E	408	TRP
1	E	418	GLN
1	E	450	HIS
1	E	455	SER
1	E	490	LYS
1	E	542	GLU
1	E	593	ASN
1	E	618	PHE
1	F	100	ILE
1	F	112	MET
1	F	168	TRP
1	F	206	PHE
1	F	285	ARG
1	F	294	GLU

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Mol	Chain	Res	Type
1	F	328	LEU
1	F	341	ASN
1	F	389	LEU
1	F	408	TRP
1	F	413	LYS
1	F	450	HIS
1	F	465	SER
1	F	496	ASN
1	F	576	LYS
1	F	593	ASN
1	F	618	PHE
1	G	45	ILE
1	G	82	SER
1	G	95	GLU
1	G	100	ILE
1	G	112	MET
1	G	168	TRP
1	G	178	GLU
1	G	206	PHE
1	G	341	ASN
1	G	385	THR
1	G	413	LYS
1	G	450	HIS
1	G	490	LYS
1	G	496	ASN
1	G	593	ASN
1	G	618	PHE
1	G	619	THR
1	H	100	ILE
1	H	112	MET
1	H	168	TRP
1	H	185	LYS
1	H	206	PHE
1	H	385	THR
1	H	389	LEU
1	H	421	GLU
1	H	450	HIS
1	H	459	VAL
1	H	496	ASN
1	H	593	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	341	ASN
1	A	460	GLN
1	B	132	GLN
1	B	299	HIS
1	B	341	ASN
1	B	460	GLN
1	B	461	GLN
1	D	263	GLN
1	D	336	GLN
1	D	460	GLN
1	D	461	GLN
1	C	132	GLN
1	C	263	GLN
1	C	341	ASN
1	E	299	HIS
1	E	341	ASN
1	E	344	ASN
1	E	418	GLN
1	E	460	GLN
1	E	611	GLN
1	F	341	ASN
1	F	460	GLN
1	G	132	GLN
1	G	263	GLN
1	G	299	HIS
1	G	341	ASN
1	G	460	GLN
1	G	611	GLN
1	H	132	GLN
1	H	263	GLN
1	H	341	ASN
1	H	460	GLN
1	H	563	ASN
1	H	611	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	MES	A	7003	-	12,12,12	1.73	1 (8%)	14,16,16	6.35	8 (57%)
2	FAD	A	801	1	51,58,58	1.50	10 (19%)	54,89,89	4.30	17 (31%)
3	MES	B	7006	-	12,12,12	1.53	1 (8%)	14,16,16	6.05	8 (57%)
2	FAD	B	801	1	51,58,58	1.31	6 (11%)	54,89,89	3.13	17 (31%)
3	MES	C	7005	-	12,12,12	1.47	1 (8%)	14,16,16	6.30	9 (64%)
2	FAD	C	801	1	51,58,58	1.45	9 (17%)	54,89,89	3.48	15 (27%)
3	MES	D	7007	-	12,12,12	1.56	1 (8%)	14,16,16	7.59	8 (57%)
2	FAD	D	801	1	51,58,58	1.41	9 (17%)	54,89,89	3.41	15 (27%)
3	MES	E	7004	-	12,12,12	1.97	1 (8%)	14,16,16	8.15	8 (57%)
2	FAD	E	801	1	51,58,58	1.38	5 (9%)	54,89,89	3.72	19 (35%)
3	MES	F	7001	-	12,12,12	1.37	1 (8%)	14,16,16	5.56	7 (50%)
2	FAD	F	801	1	51,58,58	1.46	10 (19%)	54,89,89	3.47	20 (37%)
3	MES	G	7008	-	12,12,12	1.77	1 (8%)	14,16,16	6.51	6 (42%)
2	FAD	G	801	1	51,58,58	1.39	6 (11%)	54,89,89	3.59	16 (29%)
3	MES	H	7002	-	12,12,12	2.01	1 (8%)	14,16,16	5.66	8 (57%)
2	FAD	H	801	1	51,58,58	1.34	7 (13%)	54,89,89	4.40	16 (29%)

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
3	MES	A	7003	-	-	0/6/14/14	0/1/1/1
2	FAD	A	801	1	-	0/28/50/50	0/6/6/6
3	MES	B	7006	-	-	0/6/14/14	0/1/1/1
2	FAD	B	801	1	-	0/28/50/50	0/6/6/6
3	MES	C	7005	-	-	0/6/14/14	0/1/1/1
2	FAD	C	801	1	-	0/28/50/50	0/6/6/6
3	MES	D	7007	-	-	0/6/14/14	0/1/1/1
2	FAD	D	801	1	-	0/28/50/50	0/6/6/6
3	MES	E	7004	-	-	0/6/14/14	0/1/1/1
2	FAD	E	801	1	-	0/28/50/50	0/6/6/6
3	MES	F	7001	-	-	0/6/14/14	0/1/1/1
2	FAD	F	801	1	-	0/28/50/50	0/6/6/6
3	MES	G	7008	-	-	0/6/14/14	0/1/1/1
2	FAD	G	801	1	-	0/28/50/50	0/6/6/6
3	MES	H	7002	-	-	0/6/14/14	0/1/1/1
2	FAD	H	801	1	-	0/28/50/50	0/6/6/6

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	7002	MES	C8-S	-6.62	1.67	1.77
3	E	7004	MES	C8-S	-6.42	1.67	1.77
3	G	7008	MES	C8-S	-5.82	1.68	1.77
3	A	7003	MES	C8-S	-5.68	1.69	1.77
3	D	7007	MES	C8-S	-5.04	1.69	1.77
3	B	7006	MES	C8-S	-4.87	1.70	1.77
3	C	7005	MES	C8-S	-4.79	1.70	1.77
3	F	7001	MES	C8-S	-4.46	1.70	1.77
2	C	801	FAD	O4B-C4B	-3.24	1.37	1.45
2	H	801	FAD	C2B-C1B	-3.22	1.48	1.53
2	C	801	FAD	O3B-C3B	-2.90	1.36	1.43
2	H	801	FAD	C2-N1	-2.85	1.32	1.38
2	D	801	FAD	O3B-C3B	-2.77	1.36	1.43
2	B	801	FAD	O2B-C2B	-2.62	1.36	1.43
2	F	801	FAD	O3B-C3B	-2.58	1.37	1.43
2	B	801	FAD	O4B-C4B	-2.48	1.39	1.45
2	D	801	FAD	O4B-C4B	-2.46	1.39	1.45
2	F	801	FAD	C2-N1	-2.45	1.33	1.38
2	D	801	FAD	O2B-C2B	-2.42	1.37	1.43
2	E	801	FAD	O3B-C3B	-2.40	1.37	1.43
2	A	801	FAD	C2B-C3B	-2.37	1.47	1.53
2	G	801	FAD	O4B-C4B	-2.36	1.39	1.45
2	A	801	FAD	C2B-C1B	-2.29	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	FAD	C2B-C1B	-2.27	1.50	1.53
2	A	801	FAD	O3B-C3B	-2.27	1.37	1.43
2	F	801	FAD	O4B-C4B	-2.20	1.40	1.45
2	B	801	FAD	C2B-C3B	-2.17	1.47	1.53
2	D	801	FAD	C2B-C3B	-2.10	1.47	1.53
2	H	801	FAD	O2B-C2B	-2.09	1.38	1.43
2	C	801	FAD	C2B-C3B	-2.07	1.48	1.53
2	H	801	FAD	C4-N3	2.02	1.36	1.33
2	G	801	FAD	C4-N3	2.03	1.36	1.33
2	A	801	FAD	C9A-N10	2.04	1.41	1.38
2	C	801	FAD	C4-N3	2.08	1.36	1.33
2	F	801	FAD	C9A-N10	2.19	1.41	1.38
2	C	801	FAD	C6-C7	2.19	1.43	1.37
2	B	801	FAD	C1'-N10	2.27	1.50	1.48
2	A	801	FAD	C6-C5X	2.37	1.45	1.41
2	H	801	FAD	C10-N1	2.39	1.36	1.33
2	G	801	FAD	C5'-C4'	2.45	1.55	1.51
2	F	801	FAD	C4X-N5	2.48	1.36	1.33
2	E	801	FAD	C2A-N3A	2.49	1.36	1.32
2	G	801	FAD	C2A-N3A	2.53	1.36	1.32
2	C	801	FAD	O4B-C1B	2.60	1.44	1.41
2	F	801	FAD	C2A-N3A	2.64	1.36	1.32
2	A	801	FAD	C4-N3	2.68	1.37	1.33
2	A	801	FAD	C2A-N3A	2.79	1.36	1.32
2	F	801	FAD	C4-N3	2.79	1.38	1.33
2	C	801	FAD	C2A-N3A	2.81	1.36	1.32
2	H	801	FAD	C2A-N3A	2.86	1.36	1.32
2	D	801	FAD	C10-N1	2.87	1.37	1.33
2	A	801	FAD	C1'-N10	2.91	1.51	1.48
2	D	801	FAD	C4-N3	3.00	1.38	1.33
2	E	801	FAD	C4-N3	3.06	1.38	1.33
2	F	801	FAD	O4B-C1B	3.13	1.45	1.41
2	C	801	FAD	C10-N1	3.18	1.37	1.33
2	D	801	FAD	C2A-N3A	3.39	1.37	1.32
2	E	801	FAD	C4-C4X	3.40	1.47	1.41
2	B	801	FAD	C4-C4X	3.41	1.47	1.41
2	A	801	FAD	C10-N1	3.61	1.38	1.33
2	B	801	FAD	C10-N1	3.61	1.38	1.33
2	C	801	FAD	C4-C4X	3.76	1.48	1.41
2	G	801	FAD	C4-C4X	3.76	1.48	1.41
2	F	801	FAD	C10-N1	3.88	1.38	1.33
2	A	801	FAD	C4-C4X	4.09	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	801	FAD	C10-N1	4.11	1.39	1.33
2	H	801	FAD	C4-C4X	4.14	1.49	1.41
2	F	801	FAD	C4-C4X	4.17	1.49	1.41
2	D	801	FAD	C4-C4X	4.24	1.49	1.41
2	E	801	FAD	C10-N1	4.77	1.39	1.33

All (197) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	7004	MES	O2S-S-C8	-23.56	86.55	106.79
3	D	7007	MES	O2S-S-C8	-22.43	87.53	106.79
3	G	7008	MES	O1S-S-C8	-19.64	89.92	106.79
3	A	7003	MES	O1S-S-C8	-18.25	91.11	106.79
3	C	7005	MES	O2S-S-C8	-17.05	92.15	106.79
3	B	7006	MES	O1S-S-C8	-16.43	92.68	106.79
3	F	7001	MES	O2S-S-C8	-15.61	93.38	106.79
3	H	7002	MES	O1S-S-C8	-14.18	94.61	106.79
3	D	7007	MES	O1S-S-C8	-12.79	95.81	106.79
3	E	7004	MES	O1S-S-C8	-12.76	95.83	106.79
3	B	7006	MES	O2S-S-C8	-12.58	95.99	106.79
2	H	801	FAD	C4X-C4-N3	-11.91	106.52	123.48
2	C	801	FAD	N3A-C2A-N1A	-11.84	118.54	128.86
2	H	801	FAD	N3A-C2A-N1A	-11.59	118.76	128.86
2	G	801	FAD	N3A-C2A-N1A	-11.42	118.91	128.86
2	A	801	FAD	N3A-C2A-N1A	-11.03	119.25	128.86
2	A	801	FAD	C4X-C4-N3	-10.85	108.03	123.48
3	G	7008	MES	O2S-S-C8	-10.68	97.62	106.79
2	E	801	FAD	N3A-C2A-N1A	-10.61	119.62	128.86
3	E	7004	MES	O3S-S-C8	-10.45	93.21	106.06
2	F	801	FAD	N3A-C2A-N1A	-10.31	119.88	128.86
2	D	801	FAD	N3A-C2A-N1A	-10.26	119.92	128.86
2	B	801	FAD	N3A-C2A-N1A	-9.96	120.19	128.86
3	A	7003	MES	O2S-S-C8	-9.91	98.28	106.79
3	H	7002	MES	O2S-S-C8	-9.34	98.77	106.79
3	C	7005	MES	O1S-S-C8	-8.82	99.21	106.79
2	C	801	FAD	C4X-C4-N3	-8.78	110.98	123.48
3	C	7005	MES	O3S-S-C8	-8.55	95.54	106.06
3	H	7002	MES	O3S-S-C8	-8.33	95.81	106.06
2	E	801	FAD	C4X-C4-N3	-7.97	112.13	123.48
2	D	801	FAD	C4X-C4-N3	-7.32	113.05	123.48
2	F	801	FAD	C4X-C4-N3	-7.27	113.14	123.48
3	F	7001	MES	O1S-S-C8	-7.12	100.67	106.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	801	FAD	C4X-C4-N3	-6.56	114.14	123.48
3	F	7001	MES	O3S-S-C8	-6.50	98.06	106.06
3	A	7003	MES	O3S-S-C8	-6.38	98.21	106.06
2	G	801	FAD	C4-C4X-C10	-6.28	114.88	119.96
3	D	7007	MES	O3S-S-C8	-6.00	98.68	106.06
2	B	801	FAD	C4X-C4-N3	-5.63	115.47	123.48
2	F	801	FAD	C4-C4X-C10	-5.49	115.52	119.96
2	D	801	FAD	C4-C4X-C10	-5.35	115.63	119.96
2	B	801	FAD	C4-C4X-C10	-5.00	115.91	119.96
2	A	801	FAD	C4B-O4B-C1B	-4.49	104.99	109.77
2	E	801	FAD	C4B-O4B-C1B	-4.44	105.04	109.77
2	E	801	FAD	C4-C4X-C10	-4.42	116.39	119.96
2	H	801	FAD	C4B-O4B-C1B	-4.23	105.27	109.77
3	E	7004	MES	O1-C2-C3	-4.07	102.72	111.83
2	F	801	FAD	C4X-C10-N10	-3.76	117.91	120.52
2	H	801	FAD	C4X-C10-N10	-3.57	118.04	120.52
2	G	801	FAD	C4X-C10-N10	-3.13	118.35	120.52
3	D	7007	MES	O1-C6-C5	-2.85	105.45	111.83
2	B	801	FAD	C4B-O4B-C1B	-2.74	106.85	109.77
2	D	801	FAD	C4B-O4B-C1B	-2.64	106.96	109.77
2	C	801	FAD	C4B-O4B-C1B	-2.59	107.01	109.77
2	C	801	FAD	C4X-C10-N10	-2.52	118.77	120.52
2	F	801	FAD	C9A-C5X-N5	-2.51	118.50	122.24
2	B	801	FAD	C8M-C8-C9	-2.42	114.28	120.34
2	A	801	FAD	C8M-C8-C9	-2.39	114.34	120.34
2	E	801	FAD	C4X-C10-N10	-2.35	118.89	120.52
2	E	801	FAD	O5'-P-O1P	-2.35	99.79	109.25
3	C	7005	MES	O1-C2-C3	-2.27	106.75	111.83
2	F	801	FAD	C1'-N10-C10	-2.17	116.28	118.50
2	B	801	FAD	C1'-N10-C10	-2.11	116.34	118.50
2	F	801	FAD	O5'-P-O1P	-2.10	100.78	109.25
2	G	801	FAD	C8M-C8-C9	-2.05	115.21	120.34
2	C	801	FAD	O2A-PA-O1A	2.02	122.73	112.28
2	F	801	FAD	C5B-C4B-C3B	2.02	122.99	115.29
2	C	801	FAD	O4B-C4B-C3B	2.05	109.25	105.17
3	B	7006	MES	O3S-S-C8	2.06	108.58	106.06
2	D	801	FAD	O4'-C4'-C3'	2.07	114.23	109.09
3	A	7003	MES	O2S-S-O1S	2.09	121.10	113.86
2	H	801	FAD	C4-C4X-N5	2.09	120.97	118.68
2	H	801	FAD	O2'-C2'-C3'	2.12	114.34	109.09
2	F	801	FAD	O2A-PA-O1A	2.14	123.33	112.28
2	A	801	FAD	O2P-P-O1P	2.14	123.36	112.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	FAD	C7M-C7-C8	2.15	125.24	120.72
2	F	801	FAD	O4B-C4B-C5B	2.17	116.72	109.40
2	E	801	FAD	O2P-P-O1P	2.18	123.56	112.28
3	B	7006	MES	C2-C3-N4	2.22	113.21	110.11
3	B	7006	MES	O2S-S-O1S	2.23	121.59	113.86
3	D	7007	MES	O3S-S-O1S	2.23	116.49	111.37
2	E	801	FAD	C5B-C4B-C3B	2.27	123.94	115.29
2	F	801	FAD	C5A-C6A-N6A	2.28	125.13	120.47
2	A	801	FAD	C5A-C6A-N6A	2.34	125.23	120.47
2	F	801	FAD	C2B-C3B-C4B	2.37	107.23	102.62
2	B	801	FAD	O2B-C2B-C3B	2.37	119.42	111.83
2	G	801	FAD	O2P-P-O1P	2.38	124.58	112.28
2	H	801	FAD	O4B-C4B-C5B	2.39	117.48	109.40
2	E	801	FAD	O2A-PA-O1A	2.39	124.67	112.28
2	A	801	FAD	C5X-C9A-N10	2.40	119.44	117.66
2	D	801	FAD	C2A-N1A-C6A	2.40	122.97	118.77
2	C	801	FAD	C2B-C3B-C4B	2.42	107.32	102.62
2	E	801	FAD	C4X-N5-C5X	2.42	119.32	116.76
2	B	801	FAD	C7M-C7-C8	2.44	125.84	120.72
2	G	801	FAD	C2A-N1A-C6A	2.47	123.09	118.77
2	D	801	FAD	C4X-N5-C5X	2.50	119.40	116.76
2	H	801	FAD	C1'-N10-C9A	2.52	120.66	118.35
2	H	801	FAD	O4B-C4B-C3B	2.52	110.19	105.17
2	D	801	FAD	O4B-C4B-C3B	2.56	110.26	105.17
2	E	801	FAD	C4-C4X-N5	2.62	121.55	118.68
2	A	801	FAD	C2A-N1A-C6A	2.67	123.44	118.77
2	B	801	FAD	O4B-C4B-C3B	2.71	110.56	105.17
2	G	801	FAD	O2B-C2B-C3B	2.77	120.70	111.83
3	G	7008	MES	C6-C5-N4	2.79	114.02	110.11
2	B	801	FAD	C2A-N1A-C6A	2.80	123.67	118.77
2	A	801	FAD	O2B-C2B-C1B	2.81	120.40	111.61
2	C	801	FAD	C5B-C4B-C3B	2.82	126.03	115.29
3	H	7002	MES	C6-C5-N4	2.82	114.06	110.11
2	A	801	FAD	C5B-C4B-C3B	2.82	126.04	115.29
2	H	801	FAD	C5B-C4B-C3B	2.83	126.06	115.29
2	H	801	FAD	C2A-N1A-C6A	2.83	123.72	118.77
3	E	7004	MES	O3S-S-O1S	2.84	117.88	111.37
3	C	7005	MES	C6-C5-N4	2.84	114.09	110.11
3	A	7003	MES	C6-C5-N4	2.89	114.15	110.11
2	G	801	FAD	C5B-C4B-C3B	2.89	126.31	115.29
2	E	801	FAD	C2A-N1A-C6A	2.97	123.97	118.77
2	G	801	FAD	O4B-C4B-C5B	2.98	119.47	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	FAD	C4-C4X-N5	3.00	121.96	118.68
2	C	801	FAD	O2B-C2B-C3B	3.07	121.65	111.83
2	A	801	FAD	O3B-C3B-C4B	3.13	120.22	111.09
2	G	801	FAD	O2B-C2B-C1B	3.14	121.43	111.61
2	D	801	FAD	O2B-C2B-C3B	3.17	121.98	111.83
2	B	801	FAD	O4B-C4B-C5B	3.22	120.27	109.40
2	E	801	FAD	O4B-C4B-C3B	3.23	111.58	105.17
2	F	801	FAD	C2A-N1A-C6A	3.23	124.42	118.77
2	F	801	FAD	O2B-C2B-C1B	3.23	121.74	111.61
2	D	801	FAD	O4B-C4B-C5B	3.30	120.53	109.40
3	H	7002	MES	O3S-S-O2S	3.33	119.00	111.37
2	A	801	FAD	O4B-C4B-C5B	3.34	120.69	109.40
2	C	801	FAD	C2A-N1A-C6A	3.37	124.66	118.77
2	E	801	FAD	O4B-C4B-C5B	3.40	120.90	109.40
2	H	801	FAD	O2B-C2B-C1B	3.45	122.40	111.61
2	E	801	FAD	O2B-C2B-C3B	3.56	123.23	111.83
3	C	7005	MES	O3S-S-O1S	3.62	119.67	111.37
3	B	7006	MES	O3S-S-O2S	3.65	119.73	111.37
2	G	801	FAD	C4X-N5-C5X	3.65	120.62	116.76
2	E	801	FAD	O2B-C2B-C1B	3.66	123.07	111.61
2	E	801	FAD	C1'-N10-C9A	3.75	121.79	118.35
2	D	801	FAD	O2B-C2B-C1B	3.78	123.44	111.61
3	G	7008	MES	C7-N4-C5	3.87	121.17	111.26
2	A	801	FAD	C4X-N5-C5X	3.94	120.92	116.76
2	A	801	FAD	C1'-N10-C9A	3.98	122.00	118.35
2	C	801	FAD	O3B-C3B-C4B	4.01	122.80	111.09
2	A	801	FAD	O2B-C2B-C3B	4.07	124.85	111.83
3	F	7001	MES	C6-C5-N4	4.11	115.87	110.11
3	H	7002	MES	C7-N4-C5	4.16	121.92	111.26
2	C	801	FAD	C4X-N5-C5X	4.17	121.17	116.76
3	H	7002	MES	O3S-S-O1S	4.18	120.95	111.37
3	D	7007	MES	C7-N4-C3	4.19	122.00	111.26
3	E	7004	MES	C7-N4-C5	4.20	122.02	111.26
2	H	801	FAD	O2B-C2B-C3B	4.21	125.33	111.83
2	G	801	FAD	O3B-C3B-C4B	4.22	123.41	111.09
2	G	801	FAD	C1'-N10-C9A	4.27	122.26	118.35
3	E	7004	MES	O3S-S-O2S	4.29	121.21	111.37
3	B	7006	MES	C7-N4-C5	4.29	122.26	111.26
3	G	7008	MES	O3S-S-O2S	4.30	121.22	111.37
3	A	7003	MES	O3S-S-O2S	4.30	121.23	111.37
2	D	801	FAD	C1'-N10-C9A	4.33	122.31	118.35
2	C	801	FAD	C1'-N10-C9A	4.38	122.36	118.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	FAD	O3B-C3B-C4B	4.44	124.06	111.09
2	C	801	FAD	O2B-C2B-C1B	4.49	125.66	111.61
2	B	801	FAD	C4-C4X-N5	4.51	123.63	118.68
2	F	801	FAD	O2B-C2B-C3B	4.53	126.33	111.83
2	B	801	FAD	O2B-C2B-C1B	4.60	126.01	111.61
2	H	801	FAD	O3B-C3B-C4B	4.71	124.86	111.09
2	B	801	FAD	C1'-N10-C9A	4.72	122.67	118.35
2	F	801	FAD	O3B-C3B-C4B	4.73	124.89	111.09
2	F	801	FAD	C4X-N5-C5X	4.77	121.80	116.76
2	B	801	FAD	C4X-N5-C5X	4.78	121.81	116.76
3	F	7001	MES	O3S-S-O2S	4.78	122.34	111.37
2	F	801	FAD	C1'-N10-C9A	4.79	122.74	118.35
3	F	7001	MES	C7-N4-C5	4.86	123.71	111.26
3	F	7001	MES	C5-N4-C3	4.89	119.94	108.87
3	C	7005	MES	C7-N4-C5	4.97	124.00	111.26
3	A	7003	MES	C7-N4-C5	5.01	124.11	111.26
2	D	801	FAD	O3B-C3B-C4B	5.07	125.90	111.09
3	D	7007	MES	O3S-S-O2S	5.14	123.15	111.37
3	C	7005	MES	C5-N4-C3	5.14	120.52	108.87
2	E	801	FAD	O3B-C3B-C4B	5.20	126.28	111.09
3	B	7006	MES	C5-N4-C3	5.24	120.74	108.87
2	F	801	FAD	C4-C4X-N5	5.31	124.51	118.68
2	G	801	FAD	C4-C4X-N5	5.42	124.62	118.68
3	H	7002	MES	C5-N4-C3	5.62	121.60	108.87
3	A	7003	MES	C5-N4-C3	5.64	121.64	108.87
3	C	7005	MES	O3S-S-O2S	5.73	124.51	111.37
3	E	7004	MES	C5-N4-C3	5.87	122.16	108.87
3	D	7007	MES	C5-N4-C3	6.01	122.48	108.87
2	H	801	FAD	C4X-N5-C5X	6.08	123.19	116.76
3	G	7008	MES	C5-N4-C3	6.20	122.91	108.87
2	B	801	FAD	C4-N3-C2	12.83	126.38	115.16
2	F	801	FAD	C4-N3-C2	15.36	128.59	115.16
2	C	801	FAD	C4-N3-C2	16.21	129.34	115.16
2	D	801	FAD	C4-N3-C2	16.80	129.85	115.16
2	G	801	FAD	C4-N3-C2	17.44	130.41	115.16
2	E	801	FAD	C4-N3-C2	19.18	131.93	115.16
2	A	801	FAD	C4-N3-C2	23.88	136.04	115.16
2	H	801	FAD	C4-N3-C2	23.95	136.11	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 79 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	7003	MES	1	0
2	A	801	FAD	6	0
3	B	7006	MES	1	0
2	B	801	FAD	13	0
2	C	801	FAD	5	0
3	D	7007	MES	2	0
2	D	801	FAD	8	0
3	E	7004	MES	4	0
2	E	801	FAD	11	0
2	F	801	FAD	9	0
3	G	7008	MES	2	0
2	G	801	FAD	10	0
3	H	7002	MES	1	0
2	H	801	FAD	6	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%)	-0.31	22 (3%) 41 45	8, 13, 36, 57	0
1	B	577/623 (92%)	-0.35	15 (2%) 56 60	8, 14, 31, 49	0
1	C	577/623 (92%)	-0.20	23 (3%) 39 43	9, 17, 37, 54	0
1	D	577/623 (92%)	-0.28	19 (3%) 47 50	8, 15, 34, 54	0
1	E	577/623 (92%)	-0.24	28 (4%) 30 34	10, 17, 34, 53	0
1	F	577/623 (92%)	-0.23	23 (3%) 39 43	9, 18, 37, 53	0
1	G	577/623 (92%)	-0.22	28 (4%) 30 34	10, 16, 39, 52	0
1	H	577/623 (92%)	-0.32	18 (3%) 49 53	8, 15, 31, 53	0
All	All	4616/4984 (92%)	-0.27	176 (3%) 41 45	8, 16, 35, 57	0

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	619	THR	11.2
1	C	619	THR	9.9
1	A	619	THR	9.7
1	D	619	THR	9.3
1	B	619	THR	9.1
1	E	619	THR	8.7
1	H	343	ALA	8.5
1	F	343	ALA	7.4
1	F	619	THR	7.3
1	G	619	THR	7.3
1	A	389	LEU	7.1
1	C	389	LEU	7.0
1	C	343	ALA	6.5
1	A	343	ALA	6.5
1	D	343	ALA	6.0
1	G	343	ALA	5.9

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Mol	Chain	Res	Type	RSRZ
1	C	45	ILE	5.9
1	E	343	ALA	5.8
1	H	45	ILE	5.7
1	D	389	LEU	5.6
1	B	618	PHE	5.5
1	F	45	ILE	5.4
1	F	389	LEU	5.3
1	C	618	PHE	5.3
1	F	44	ASP	5.2
1	E	45	ILE	5.2
1	B	343	ALA	5.0
1	D	45	ILE	4.9
1	H	344	ASN	4.9
1	G	45	ILE	4.8
1	A	385	THR	4.7
1	C	385	THR	4.6
1	A	342	PRO	4.6
1	C	44	ASP	4.6
1	F	344	ASN	4.5
1	G	400	SER	4.5
1	C	384	GLY	4.4
1	C	383	ARG	4.3
1	F	342	PRO	4.3
1	C	390	THR	4.3
1	A	344	ASN	4.3
1	G	342	PRO	4.2
1	F	43	MET	4.2
1	H	342	PRO	4.2
1	G	388	GLU	4.1
1	G	344	ASN	4.0
1	F	388	GLU	4.0
1	G	389	LEU	3.9
1	G	401	THR	3.9
1	F	345	PRO	3.8
1	E	618	PHE	3.8
1	E	385	THR	3.8
1	A	390	THR	3.8
1	F	390	THR	3.8
1	A	384	GLY	3.8
1	F	385	THR	3.7
1	E	384	GLY	3.7
1	F	341	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	344	ASN	3.6
1	G	618	PHE	3.6
1	A	400	SER	3.5
1	A	399	ALA	3.5
1	H	618	PHE	3.5
1	B	342	PRO	3.5
1	B	344	ASN	3.5
1	E	232	GLY	3.5
1	A	388	GLU	3.5
1	A	383	ARG	3.4
1	C	43	MET	3.4
1	G	43	MET	3.4
1	A	401	THR	3.4
1	D	344	ASN	3.4
1	E	186	ASP	3.4
1	A	43	MET	3.3
1	E	272	GLU	3.3
1	B	383	ARG	3.3
1	G	186	ASP	3.2
1	C	341	ASN	3.2
1	H	186	ASP	3.2
1	D	186	ASP	3.1
1	C	345	PRO	3.1
1	H	43	MET	3.1
1	C	388	GLU	3.1
1	F	383	ARG	3.1
1	D	618	PHE	3.1
1	H	345	PRO	3.1
1	A	341	ASN	3.1
1	E	344	ASN	3.1
1	H	341	ASN	3.1
1	A	618	PHE	3.0
1	F	561	GLU	3.0
1	D	345	PRO	3.0
1	E	345	PRO	3.0
1	E	388	GLU	3.0
1	E	341	ASN	3.0
1	E	43	MET	2.9
1	D	388	GLU	2.9
1	A	345	PRO	2.9
1	D	309	PHE	2.9
1	E	342	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	401	THR	2.9
1	B	389	LEU	2.9
1	D	268	THR	2.8
1	G	100	ILE	2.8
1	H	44	ASP	2.8
1	G	398	GLY	2.8
1	E	400	SER	2.8
1	G	399	ALA	2.8
1	H	458	ALA	2.8
1	E	617	PRO	2.8
1	C	617	PRO	2.8
1	D	43	MET	2.8
1	D	342	PRO	2.7
1	E	269	ASP	2.6
1	G	458	ALA	2.6
1	E	44	ASP	2.6
1	E	490	LYS	2.6
1	F	269	ASP	2.6
1	G	341	ASN	2.6
1	A	459	VAL	2.6
1	D	400	SER	2.5
1	F	347	GLU	2.5
1	G	490	LYS	2.5
1	H	347	GLU	2.5
1	B	186	ASP	2.5
1	F	232	GLY	2.5
1	E	389	LEU	2.5
1	E	401	THR	2.5
1	H	490	LYS	2.4
1	B	388	GLU	2.4
1	C	400	SER	2.4
1	E	418	GLN	2.4
1	E	561	GLU	2.4
1	H	268	THR	2.3
1	D	185	LYS	2.3
1	G	309	PHE	2.3
1	G	345	PRO	2.3
1	D	341	ASN	2.3
1	G	617	PRO	2.3
1	H	185	LYS	2.3
1	B	458	ALA	2.3
1	C	342	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	268	THR	2.3
1	F	268	THR	2.3
1	C	268	THR	2.2
1	D	617	PRO	2.2
1	H	459	VAL	2.2
1	B	345	PRO	2.2
1	C	186	ASP	2.2
1	G	82	SER	2.2
1	A	398	GLY	2.2
1	G	268	THR	2.2
1	F	189	ASP	2.2
1	F	100	ILE	2.1
1	E	347	GLU	2.1
1	B	341	ASN	2.1
1	E	310	GLU	2.1
1	H	617	PRO	2.1
1	A	186	ASP	2.1
1	G	385	THR	2.1
1	G	269	ASP	2.1
1	A	418	GLN	2.1
1	A	458	ALA	2.1
1	G	383	ARG	2.1
1	B	490	LYS	2.1
1	D	490	LYS	2.1
1	E	309	PHE	2.1
1	G	185	LYS	2.1
1	B	385	THR	2.1
1	F	309	PHE	2.1
1	C	272	GLU	2.0
1	B	387	GLY	2.0
1	G	387	GLY	2.0
1	D	269	ASP	2.0
1	C	185	LYS	2.0
1	F	185	LYS	2.0

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

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

### 6.3 Carbohydrates [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(Å <sup>2</sup> )	Q<0.9
3	MES	C	7005	12/12	0.96	0.10	0.24	17,20,22,23	0
3	MES	H	7002	12/12	0.96	0.09	-0.16	18,20,21,22	0
3	MES	G	7008	12/12	0.97	0.08	-0.34	19,22,24,24	0
3	MES	B	7006	12/12	0.96	0.09	-0.39	22,23,26,26	0
2	FAD	C	801	53/53	0.98	0.07	-0.43	9,13,16,19	0
3	MES	D	7007	12/12	0.98	0.07	-0.65	20,24,25,25	0
2	FAD	F	801	53/53	0.98	0.06	-0.69	10,13,15,17	0
3	MES	E	7004	12/12	0.98	0.07	-0.70	19,22,25,27	0
2	FAD	D	801	53/53	0.98	0.06	-0.70	10,12,14,16	0
2	FAD	A	801	53/53	0.98	0.06	-0.85	7,10,14,16	0
3	MES	F	7001	12/12	0.98	0.07	-0.85	14,18,19,19	0
3	MES	A	7003	12/12	0.98	0.06	-0.95	16,17,19,20	0
2	FAD	E	801	53/53	0.98	0.06	-0.99	9,13,15,18	0
2	FAD	G	801	53/53	0.98	0.06	-1.01	10,12,15,17	0
2	FAD	H	801	53/53	0.98	0.05	-1.05	9,13,15,17	0
2	FAD	B	801	53/53	0.98	0.06	-1.08	8,11,13,19	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.