Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 07:53 am BST

PDB ID	:	5MGY
Title	:	Crystal structure of Pseudomonas stutzeri flavinyl transferase ApbE, apo form
Authors	:	Zhang, L.; Trncik, C.; Andrade, S.L.A.; Einsle, O.
Deposited on	:	2016-11-22
Resolution	:	2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

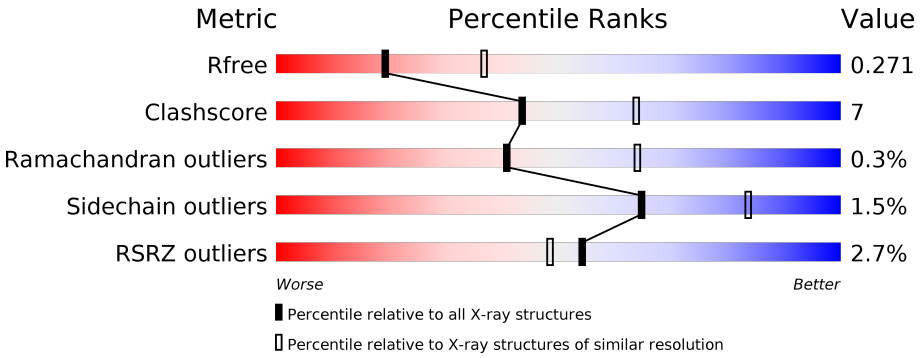
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	332	3% 80% 11% • 8%
1	B	332	2% 79% 11% • 9%
1	C	332	2% 83% 10% • 7%
1	D	332	% 80% 11% • 7%
1	E	332	2% 83% 11% • 5%
1	F	332	2% 79% 15% • 5%

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Mol	Chain	Length	Quality of chain
1	G	332	5% 72% 16% • 10%
1	H	332	3% 83% 12% • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18725 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 FAD:protein FMN transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	316	Total	C	N	O	S	0	0	0
			2388	1495	415	470	8			
1	B	303	Total	C	N	O	S	0	0	0
			2288	1431	392	457	8			
1	G	299	Total	C	N	O	S	0	0	0
			2261	1422	385	446	8			
1	A	305	Total	C	N	O	S	0	0	0
			2306	1444	395	459	8			
1	C	310	Total	C	N	O	S	0	0	0
			2334	1466	400	460	8			
1	D	309	Total	C	N	O	S	0	0	0
			2330	1464	399	459	8			
1	E	316	Total	C	N	O	S	0	0	0
			2388	1495	415	470	8			
1	F	315	Total	C	N	O	S	0	0	0
			2377	1489	411	469	8			

There are 256 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	27	MET	-	initiating methionine	UNP A0A2N8RKH1
H	28	ALA	-	expression tag	UNP A0A2N8RKH1
H	29	MET	-	expression tag	UNP A0A2N8RKH1
H	30	ASP	-	expression tag	UNP A0A2N8RKH1
H	31	LEU	-	expression tag	UNP A0A2N8RKH1
H	32	PHE	-	expression tag	UNP A0A2N8RKH1
H	33	GLN	-	expression tag	UNP A0A2N8RKH1
H	34	ASP	-	expression tag	UNP A0A2N8RKH1
H	35	LYS	-	expression tag	UNP A0A2N8RKH1
H	36	VAL	-	expression tag	UNP A0A2N8RKH1
H	37	GLU	-	expression tag	UNP A0A2N8RKH1
H	38	ALA	-	expression tag	UNP A0A2N8RKH1
H	39	PHE	-	expression tag	UNP A0A2N8RKH1

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Chain	Residue	Modelled	Actual	Comment	Reference
H	40	THR	-	expression tag	UNP A0A2N8RKH1
H	41	GLY	-	expression tag	UNP A0A2N8RKH1
H	42	PRO	-	expression tag	UNP A0A2N8RKH1
H	43	THR	-	expression tag	UNP A0A2N8RKH1
H	60	ALA	SER	conflict	UNP A0A2N8RKH1
H	63	VAL	MET	conflict	UNP A0A2N8RKH1
H	66	GLY	SER	conflict	UNP A0A2N8RKH1
H	71	ILE	LEU	conflict	UNP A0A2N8RKH1
H	74	GLN	GLU	conflict	UNP A0A2N8RKH1
H	114	SER	GLY	conflict	UNP A0A2N8RKH1
H	153	SER	ARG	conflict	UNP A0A2N8RKH1
H	351	VAL	-	expression tag	UNP A0A2N8RKH1
H	352	GLU	-	expression tag	UNP A0A2N8RKH1
H	353	HIS	-	expression tag	UNP A0A2N8RKH1
H	354	HIS	-	expression tag	UNP A0A2N8RKH1
H	355	HIS	-	expression tag	UNP A0A2N8RKH1
H	356	HIS	-	expression tag	UNP A0A2N8RKH1
H	357	HIS	-	expression tag	UNP A0A2N8RKH1
H	358	HIS	-	expression tag	UNP A0A2N8RKH1
B	27	MET	-	initiating methionine	UNP A0A2N8RKH1
B	28	ALA	-	expression tag	UNP A0A2N8RKH1
B	29	MET	-	expression tag	UNP A0A2N8RKH1
B	30	ASP	-	expression tag	UNP A0A2N8RKH1
B	31	LEU	-	expression tag	UNP A0A2N8RKH1
B	32	PHE	-	expression tag	UNP A0A2N8RKH1
B	33	GLN	-	expression tag	UNP A0A2N8RKH1
B	34	ASP	-	expression tag	UNP A0A2N8RKH1
B	35	LYS	-	expression tag	UNP A0A2N8RKH1
B	36	VAL	-	expression tag	UNP A0A2N8RKH1
B	37	GLU	-	expression tag	UNP A0A2N8RKH1
B	38	ALA	-	expression tag	UNP A0A2N8RKH1
B	39	PHE	-	expression tag	UNP A0A2N8RKH1
B	40	THR	-	expression tag	UNP A0A2N8RKH1
B	41	GLY	-	expression tag	UNP A0A2N8RKH1
B	42	PRO	-	expression tag	UNP A0A2N8RKH1
B	43	THR	-	expression tag	UNP A0A2N8RKH1
B	60	ALA	SER	conflict	UNP A0A2N8RKH1
B	63	VAL	MET	conflict	UNP A0A2N8RKH1
B	66	GLY	SER	conflict	UNP A0A2N8RKH1
B	71	ILE	LEU	conflict	UNP A0A2N8RKH1
B	74	GLN	GLU	conflict	UNP A0A2N8RKH1
B	114	SER	GLY	conflict	UNP A0A2N8RKH1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	153	SER	ARG	conflict	UNP A0A2N8RKH1
B	351	VAL	-	expression tag	UNP A0A2N8RKH1
B	352	GLU	-	expression tag	UNP A0A2N8RKH1
B	353	HIS	-	expression tag	UNP A0A2N8RKH1
B	354	HIS	-	expression tag	UNP A0A2N8RKH1
B	355	HIS	-	expression tag	UNP A0A2N8RKH1
B	356	HIS	-	expression tag	UNP A0A2N8RKH1
B	357	HIS	-	expression tag	UNP A0A2N8RKH1
B	358	HIS	-	expression tag	UNP A0A2N8RKH1
G	27	MET	-	initiating methionine	UNP A0A2N8RKH1
G	28	ALA	-	expression tag	UNP A0A2N8RKH1
G	29	MET	-	expression tag	UNP A0A2N8RKH1
G	30	ASP	-	expression tag	UNP A0A2N8RKH1
G	31	LEU	-	expression tag	UNP A0A2N8RKH1
G	32	PHE	-	expression tag	UNP A0A2N8RKH1
G	33	GLN	-	expression tag	UNP A0A2N8RKH1
G	34	ASP	-	expression tag	UNP A0A2N8RKH1
G	35	LYS	-	expression tag	UNP A0A2N8RKH1
G	36	VAL	-	expression tag	UNP A0A2N8RKH1
G	37	GLU	-	expression tag	UNP A0A2N8RKH1
G	38	ALA	-	expression tag	UNP A0A2N8RKH1
G	39	PHE	-	expression tag	UNP A0A2N8RKH1
G	40	THR	-	expression tag	UNP A0A2N8RKH1
G	41	GLY	-	expression tag	UNP A0A2N8RKH1
G	42	PRO	-	expression tag	UNP A0A2N8RKH1
G	43	THR	-	expression tag	UNP A0A2N8RKH1
G	60	ALA	SER	conflict	UNP A0A2N8RKH1
G	63	VAL	MET	conflict	UNP A0A2N8RKH1
G	66	GLY	SER	conflict	UNP A0A2N8RKH1
G	71	ILE	LEU	conflict	UNP A0A2N8RKH1
G	74	GLN	GLU	conflict	UNP A0A2N8RKH1
G	114	SER	GLY	conflict	UNP A0A2N8RKH1
G	153	SER	ARG	conflict	UNP A0A2N8RKH1
G	351	VAL	-	expression tag	UNP A0A2N8RKH1
G	352	GLU	-	expression tag	UNP A0A2N8RKH1
G	353	HIS	-	expression tag	UNP A0A2N8RKH1
G	354	HIS	-	expression tag	UNP A0A2N8RKH1
G	355	HIS	-	expression tag	UNP A0A2N8RKH1
G	356	HIS	-	expression tag	UNP A0A2N8RKH1
G	357	HIS	-	expression tag	UNP A0A2N8RKH1
G	358	HIS	-	expression tag	UNP A0A2N8RKH1
A	27	MET	-	initiating methionine	UNP A0A2N8RKH1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	28	ALA	-	expression tag	UNP A0A2N8RKH1
A	29	MET	-	expression tag	UNP A0A2N8RKH1
A	30	ASP	-	expression tag	UNP A0A2N8RKH1
A	31	LEU	-	expression tag	UNP A0A2N8RKH1
A	32	PHE	-	expression tag	UNP A0A2N8RKH1
A	33	GLN	-	expression tag	UNP A0A2N8RKH1
A	34	ASP	-	expression tag	UNP A0A2N8RKH1
A	35	LYS	-	expression tag	UNP A0A2N8RKH1
A	36	VAL	-	expression tag	UNP A0A2N8RKH1
A	37	GLU	-	expression tag	UNP A0A2N8RKH1
A	38	ALA	-	expression tag	UNP A0A2N8RKH1
A	39	PHE	-	expression tag	UNP A0A2N8RKH1
A	40	THR	-	expression tag	UNP A0A2N8RKH1
A	41	GLY	-	expression tag	UNP A0A2N8RKH1
A	42	PRO	-	expression tag	UNP A0A2N8RKH1
A	43	THR	-	expression tag	UNP A0A2N8RKH1
A	60	ALA	SER	conflict	UNP A0A2N8RKH1
A	63	VAL	MET	conflict	UNP A0A2N8RKH1
A	66	GLY	SER	conflict	UNP A0A2N8RKH1
A	71	ILE	LEU	conflict	UNP A0A2N8RKH1
A	74	GLN	GLU	conflict	UNP A0A2N8RKH1
A	114	SER	GLY	conflict	UNP A0A2N8RKH1
A	153	SER	ARG	conflict	UNP A0A2N8RKH1
A	351	VAL	-	expression tag	UNP A0A2N8RKH1
A	352	GLU	-	expression tag	UNP A0A2N8RKH1
A	353	HIS	-	expression tag	UNP A0A2N8RKH1
A	354	HIS	-	expression tag	UNP A0A2N8RKH1
A	355	HIS	-	expression tag	UNP A0A2N8RKH1
A	356	HIS	-	expression tag	UNP A0A2N8RKH1
A	357	HIS	-	expression tag	UNP A0A2N8RKH1
A	358	HIS	-	expression tag	UNP A0A2N8RKH1
C	27	MET	-	initiating methionine	UNP A0A2N8RKH1
C	28	ALA	-	expression tag	UNP A0A2N8RKH1
C	29	MET	-	expression tag	UNP A0A2N8RKH1
C	30	ASP	-	expression tag	UNP A0A2N8RKH1
C	31	LEU	-	expression tag	UNP A0A2N8RKH1
C	32	PHE	-	expression tag	UNP A0A2N8RKH1
C	33	GLN	-	expression tag	UNP A0A2N8RKH1
C	34	ASP	-	expression tag	UNP A0A2N8RKH1
C	35	LYS	-	expression tag	UNP A0A2N8RKH1
C	36	VAL	-	expression tag	UNP A0A2N8RKH1
C	37	GLU	-	expression tag	UNP A0A2N8RKH1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	38	ALA	-	expression tag	UNP A0A2N8RKH1
C	39	PHE	-	expression tag	UNP A0A2N8RKH1
C	40	THR	-	expression tag	UNP A0A2N8RKH1
C	41	GLY	-	expression tag	UNP A0A2N8RKH1
C	42	PRO	-	expression tag	UNP A0A2N8RKH1
C	43	THR	-	expression tag	UNP A0A2N8RKH1
C	60	ALA	SER	conflict	UNP A0A2N8RKH1
C	63	VAL	MET	conflict	UNP A0A2N8RKH1
C	66	GLY	SER	conflict	UNP A0A2N8RKH1
C	71	ILE	LEU	conflict	UNP A0A2N8RKH1
C	74	GLN	GLU	conflict	UNP A0A2N8RKH1
C	114	SER	GLY	conflict	UNP A0A2N8RKH1
C	153	SER	ARG	conflict	UNP A0A2N8RKH1
C	351	VAL	-	expression tag	UNP A0A2N8RKH1
C	352	GLU	-	expression tag	UNP A0A2N8RKH1
C	353	HIS	-	expression tag	UNP A0A2N8RKH1
C	354	HIS	-	expression tag	UNP A0A2N8RKH1
C	355	HIS	-	expression tag	UNP A0A2N8RKH1
C	356	HIS	-	expression tag	UNP A0A2N8RKH1
C	357	HIS	-	expression tag	UNP A0A2N8RKH1
C	358	HIS	-	expression tag	UNP A0A2N8RKH1
D	27	MET	-	initiating methionine	UNP A0A2N8RKH1
D	28	ALA	-	expression tag	UNP A0A2N8RKH1
D	29	MET	-	expression tag	UNP A0A2N8RKH1
D	30	ASP	-	expression tag	UNP A0A2N8RKH1
D	31	LEU	-	expression tag	UNP A0A2N8RKH1
D	32	PHE	-	expression tag	UNP A0A2N8RKH1
D	33	GLN	-	expression tag	UNP A0A2N8RKH1
D	34	ASP	-	expression tag	UNP A0A2N8RKH1
D	35	LYS	-	expression tag	UNP A0A2N8RKH1
D	36	VAL	-	expression tag	UNP A0A2N8RKH1
D	37	GLU	-	expression tag	UNP A0A2N8RKH1
D	38	ALA	-	expression tag	UNP A0A2N8RKH1
D	39	PHE	-	expression tag	UNP A0A2N8RKH1
D	40	THR	-	expression tag	UNP A0A2N8RKH1
D	41	GLY	-	expression tag	UNP A0A2N8RKH1
D	42	PRO	-	expression tag	UNP A0A2N8RKH1
D	43	THR	-	expression tag	UNP A0A2N8RKH1
D	60	ALA	SER	conflict	UNP A0A2N8RKH1
D	63	VAL	MET	conflict	UNP A0A2N8RKH1
D	66	GLY	SER	conflict	UNP A0A2N8RKH1
D	71	ILE	LEU	conflict	UNP A0A2N8RKH1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	74	GLN	GLU	conflict	UNP A0A2N8RKH1
D	114	SER	GLY	conflict	UNP A0A2N8RKH1
D	153	SER	ARG	conflict	UNP A0A2N8RKH1
D	351	VAL	-	expression tag	UNP A0A2N8RKH1
D	352	GLU	-	expression tag	UNP A0A2N8RKH1
D	353	HIS	-	expression tag	UNP A0A2N8RKH1
D	354	HIS	-	expression tag	UNP A0A2N8RKH1
D	355	HIS	-	expression tag	UNP A0A2N8RKH1
D	356	HIS	-	expression tag	UNP A0A2N8RKH1
D	357	HIS	-	expression tag	UNP A0A2N8RKH1
D	358	HIS	-	expression tag	UNP A0A2N8RKH1
E	27	MET	-	initiating methionine	UNP A0A2N8RKH1
E	28	ALA	-	expression tag	UNP A0A2N8RKH1
E	29	MET	-	expression tag	UNP A0A2N8RKH1
E	30	ASP	-	expression tag	UNP A0A2N8RKH1
E	31	LEU	-	expression tag	UNP A0A2N8RKH1
E	32	PHE	-	expression tag	UNP A0A2N8RKH1
E	33	GLN	-	expression tag	UNP A0A2N8RKH1
E	34	ASP	-	expression tag	UNP A0A2N8RKH1
E	35	LYS	-	expression tag	UNP A0A2N8RKH1
E	36	VAL	-	expression tag	UNP A0A2N8RKH1
E	37	GLU	-	expression tag	UNP A0A2N8RKH1
E	38	ALA	-	expression tag	UNP A0A2N8RKH1
E	39	PHE	-	expression tag	UNP A0A2N8RKH1
E	40	THR	-	expression tag	UNP A0A2N8RKH1
E	41	GLY	-	expression tag	UNP A0A2N8RKH1
E	42	PRO	-	expression tag	UNP A0A2N8RKH1
E	43	THR	-	expression tag	UNP A0A2N8RKH1
E	60	ALA	SER	conflict	UNP A0A2N8RKH1
E	63	VAL	MET	conflict	UNP A0A2N8RKH1
E	66	GLY	SER	conflict	UNP A0A2N8RKH1
E	71	ILE	LEU	conflict	UNP A0A2N8RKH1
E	74	GLN	GLU	conflict	UNP A0A2N8RKH1
E	114	SER	GLY	conflict	UNP A0A2N8RKH1
E	153	SER	ARG	conflict	UNP A0A2N8RKH1
E	351	VAL	-	expression tag	UNP A0A2N8RKH1
E	352	GLU	-	expression tag	UNP A0A2N8RKH1
E	353	HIS	-	expression tag	UNP A0A2N8RKH1
E	354	HIS	-	expression tag	UNP A0A2N8RKH1
E	355	HIS	-	expression tag	UNP A0A2N8RKH1
E	356	HIS	-	expression tag	UNP A0A2N8RKH1
E	357	HIS	-	expression tag	UNP A0A2N8RKH1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	358	HIS	-	expression tag	UNP A0A2N8RKH1
F	27	MET	-	initiating methionine	UNP A0A2N8RKH1
F	28	ALA	-	expression tag	UNP A0A2N8RKH1
F	29	MET	-	expression tag	UNP A0A2N8RKH1
F	30	ASP	-	expression tag	UNP A0A2N8RKH1
F	31	LEU	-	expression tag	UNP A0A2N8RKH1
F	32	PHE	-	expression tag	UNP A0A2N8RKH1
F	33	GLN	-	expression tag	UNP A0A2N8RKH1
F	34	ASP	-	expression tag	UNP A0A2N8RKH1
F	35	LYS	-	expression tag	UNP A0A2N8RKH1
F	36	VAL	-	expression tag	UNP A0A2N8RKH1
F	37	GLU	-	expression tag	UNP A0A2N8RKH1
F	38	ALA	-	expression tag	UNP A0A2N8RKH1
F	39	PHE	-	expression tag	UNP A0A2N8RKH1
F	40	THR	-	expression tag	UNP A0A2N8RKH1
F	41	GLY	-	expression tag	UNP A0A2N8RKH1
F	42	PRO	-	expression tag	UNP A0A2N8RKH1
F	43	THR	-	expression tag	UNP A0A2N8RKH1
F	60	ALA	SER	conflict	UNP A0A2N8RKH1
F	63	VAL	MET	conflict	UNP A0A2N8RKH1
F	66	GLY	SER	conflict	UNP A0A2N8RKH1
F	71	ILE	LEU	conflict	UNP A0A2N8RKH1
F	74	GLN	GLU	conflict	UNP A0A2N8RKH1
F	114	SER	GLY	conflict	UNP A0A2N8RKH1
F	153	SER	ARG	conflict	UNP A0A2N8RKH1
F	351	VAL	-	expression tag	UNP A0A2N8RKH1
F	352	GLU	-	expression tag	UNP A0A2N8RKH1
F	353	HIS	-	expression tag	UNP A0A2N8RKH1
F	354	HIS	-	expression tag	UNP A0A2N8RKH1
F	355	HIS	-	expression tag	UNP A0A2N8RKH1
F	356	HIS	-	expression tag	UNP A0A2N8RKH1
F	357	HIS	-	expression tag	UNP A0A2N8RKH1
F	358	HIS	-	expression tag	UNP A0A2N8RKH1

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

- Molecule 3 is water.

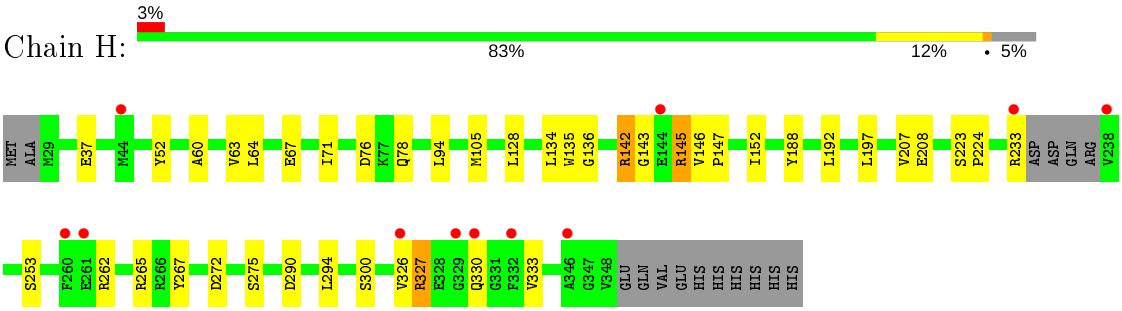
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	6	Total O 6 6	0	0
3	B	9	Total O 9 9	0	0
3	G	3	Total O 3 3	0	0
3	A	12	Total O 12 12	0	0
3	C	3	Total O 3 3	0	0
3	D	5	Total O 5 5	0	0
3	E	5	Total O 5 5	0	0
3	F	2	Total O 2 2	0	0

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

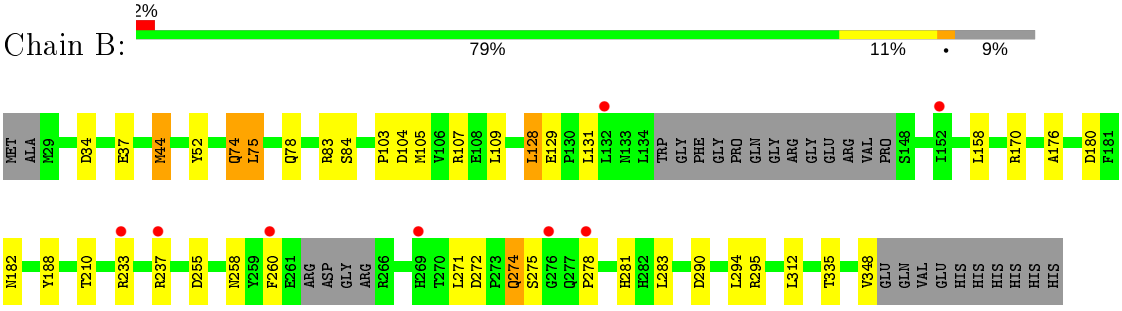
- Molecule 1: FAD:protein FMN transferase

Chain H:



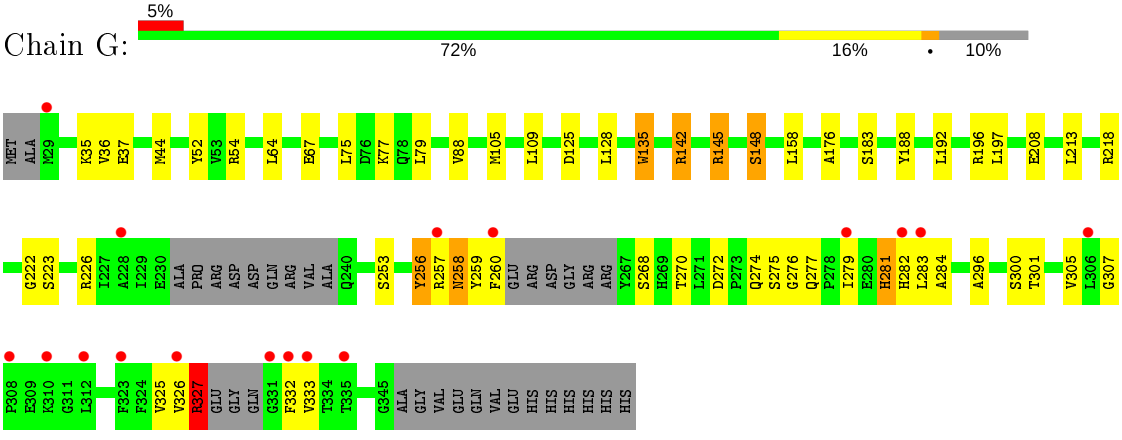
- Molecule 1: FAD:protein FMN transferase

Chain B:

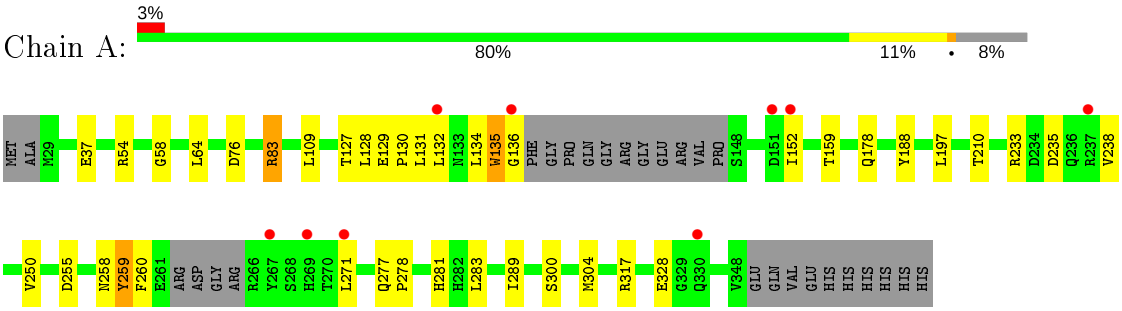


- Molecule 1: FAD:protein FMN transferase

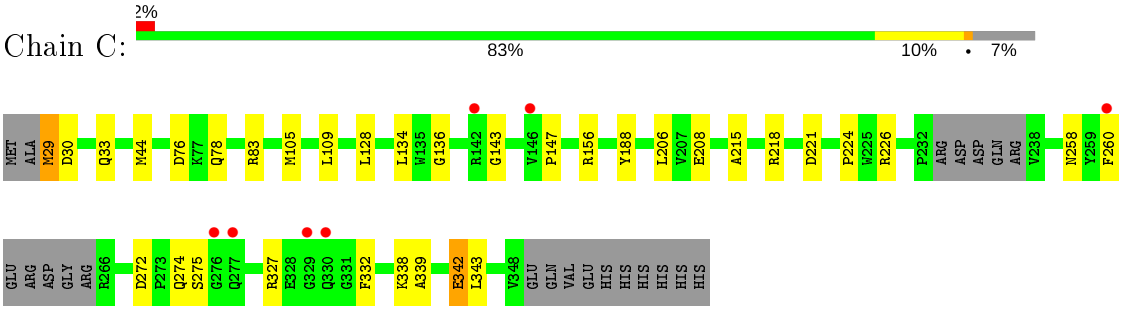
Chain G:



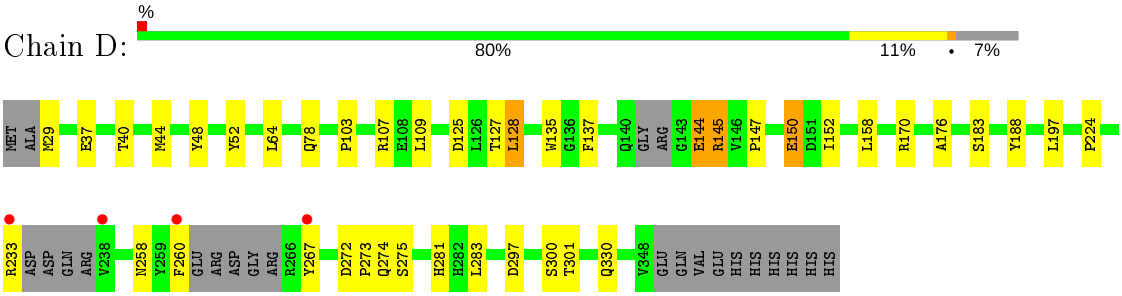
- Molecule 1: FAD:protein FMN transferase



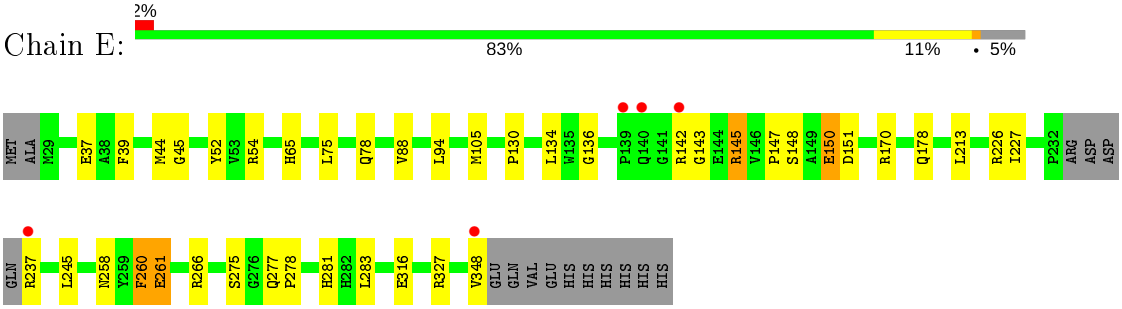
• Molecule 1: FAD:protein FMN transferase



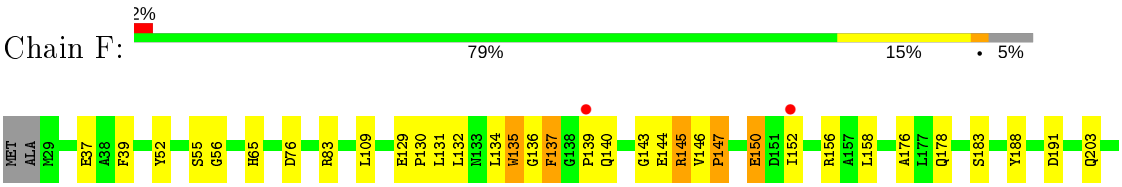
• Molecule 1: FAD:protein FMN transferase

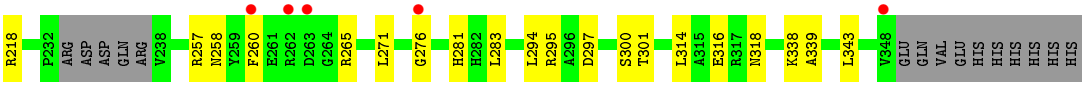


• Molecule 1: FAD:protein FMN transferase



• Molecule 1: FAD:protein FMN transferase




R218
P232
ARG
ASP
ASP
GLN
ARG
V238
R257
N258
Y259
F260
E261
R262
D263
G264
R265
L271
G276
H281
H282
L283
L294
R295
A296
D297
S300
T301
L314
A315
E316
R317
N318
K338
A339
L343
V348
GLU
GLN
VAL
GLU
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	135.66Å 91.98Å 138.06Å 90.00° 90.41° 90.00°	Depositor
Resolution (Å)	138.06 – 2.60 138.06 – 2.46	Depositor EDS
% Data completeness (in resolution range)	100.0 (138.06-2.60) 100.0 (138.06-2.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.232 , 0.274 0.233 , 0.271	Depositor DCC
R_{free} test set	5960 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	39.9	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 21.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.000 for h,-k,-l 0.000 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	18725	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.34 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.7302e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG

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	1.04	3/2343 (0.1%)	1.05	6/3171 (0.2%)
1	B	0.95	1/2323 (0.0%)	1.06	12/3143 (0.4%)
1	C	0.88	1/2374 (0.0%)	0.97	5/3214 (0.2%)
1	D	0.91	3/2369 (0.1%)	1.02	8/3206 (0.2%)
1	E	0.87	0/2429	1.04	10/3287 (0.3%)
1	F	0.92	2/2418 (0.1%)	1.10	10/3273 (0.3%)
1	G	1.04	3/2299 (0.1%)	1.08	11/3110 (0.4%)
1	H	0.92	1/2429 (0.0%)	1.05	11/3287 (0.3%)
All	All	0.94	14/18984 (0.1%)	1.05	73/25691 (0.3%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	281	HIS	C-N	24.09	1.89	1.34
1	A	259	TYR	C-N	18.56	1.76	1.34
1	D	150	GLU	CG-CD	8.63	1.64	1.51
1	C	342	GLU	CD-OE2	-7.88	1.17	1.25
1	B	74	GLN	CG-CD	-7.76	1.33	1.51
1	H	267	TYR	CE1-CZ	7.24	1.48	1.38
1	A	136	GLY	N-CA	7.18	1.56	1.46
1	F	300	SER	CB-OG	-6.96	1.33	1.42
1	A	300	SER	CB-OG	-6.49	1.33	1.42
1	G	135	TRP	CB-CG	6.06	1.61	1.50
1	G	135	TRP	CZ3-CH2	5.48	1.48	1.40
1	D	300	SER	CB-OG	-5.10	1.35	1.42
1	F	150	GLU	CD-OE2	-5.04	1.20	1.25
1	D	137	PHE	CG-CD1	5.03	1.46	1.38

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	145	ARG	NE-CZ-NH2	-17.41	111.60	120.30
1	G	145	ARG	NE-CZ-NH1	-13.63	113.48	120.30
1	D	145	ARG	NE-CZ-NH2	11.78	126.19	120.30
1	F	146	VAL	C-N-CD	-10.91	96.59	120.60
1	H	76	ASP	CB-CG-OD2	10.39	127.65	118.30
1	G	327	ARG	NE-CZ-NH1	9.95	125.27	120.30
1	A	255	ASP	CB-CG-OD2	8.92	126.33	118.30
1	H	142	ARG	NE-CZ-NH2	8.65	124.63	120.30
1	E	226	ARG	NE-CZ-NH1	-8.11	116.25	120.30
1	H	233	ARG	NE-CZ-NH2	-8.03	116.28	120.30
1	C	218	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	G	142	ARG	NE-CZ-NH2	7.64	124.12	120.30
1	B	295	ARG	NE-CZ-NH2	7.38	123.99	120.30
1	G	148	SER	N-CA-CB	7.29	121.43	110.50
1	G	145	ARG	NE-CZ-NH2	7.26	123.93	120.30
1	H	262	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	B	104	ASP	CB-CG-OD1	7.00	124.61	118.30
1	D	233	ARG	NE-CZ-NH1	-6.98	116.81	120.30
1	H	233	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	F	145	ARG	NH1-CZ-NH2	6.83	126.91	119.40
1	A	255	ASP	CB-CG-OD1	-6.59	112.37	118.30
1	H	208	GLU	OE1-CD-OE2	-6.58	115.41	123.30
1	E	226	ARG	NE-CZ-NH2	6.52	123.56	120.30
1	A	259	TYR	O-C-N	-6.50	112.30	122.70
1	G	327	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	B	295	ARG	NE-CZ-NH1	-6.45	117.07	120.30
1	F	295	ARG	NE-CZ-NH2	6.38	123.49	120.30
1	G	125	ASP	CB-CG-OD1	6.34	124.00	118.30
1	C	208	GLU	OE1-CD-OE2	-6.28	115.77	123.30
1	H	76	ASP	OD1-CG-OD2	-6.16	111.59	123.30
1	E	260	PHE	CB-CG-CD2	-6.05	116.57	120.80
1	G	77	LYS	CD-CE-NZ	5.99	125.48	111.70
1	A	233	ARG	NE-CZ-NH2	5.99	123.30	120.30
1	H	207	VAL	CG1-CB-CG2	-5.94	101.39	110.90
1	D	145	ARG	NE-CZ-NH1	-5.92	117.34	120.30
1	B	107	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	E	142	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	B	83	ARG	CB-CA-C	-5.82	98.75	110.40
1	F	191	ASP	CB-CG-OD1	5.81	123.53	118.30
1	C	44	MET	CG-SD-CE	5.76	109.42	100.20
1	C	226	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	E	170	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	B	255	ASP	CB-CG-OD2	5.73	123.45	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	170	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	F	265	ARG	NE-CZ-NH2	5.61	123.11	120.30
1	F	218	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	E	44	MET	CA-CB-CG	5.54	122.72	113.30
1	F	297	ASP	CB-CG-OD2	5.51	123.26	118.30
1	B	34	ASP	CB-CG-OD1	5.46	123.22	118.30
1	H	265	ARG	NE-CZ-NH2	5.41	123.00	120.30
1	F	257	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	D	107	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	E	45	GLY	N-CA-C	5.35	126.48	113.10
1	A	83	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	G	125	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	A	135	TRP	CA-C-N	5.23	126.65	116.20
1	F	137	PHE	CB-CG-CD2	5.21	124.45	120.80
1	B	75	LEU	CD1-CG-CD2	-5.20	94.91	110.50
1	D	44	MET	CG-SD-CE	5.19	108.50	100.20
1	B	290	ASP	CB-CG-OD1	-5.18	113.64	118.30
1	G	44	MET	CG-SD-CE	5.17	108.48	100.20
1	D	144	GLU	OE1-CD-OE2	-5.16	117.11	123.30
1	C	156	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	E	54	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	B	170	ARG	NE-CZ-NH2	5.13	122.87	120.30
1	H	290	ASP	CB-CG-OD1	-5.11	113.70	118.30
1	H	290	ASP	CB-CG-OD2	5.10	122.89	118.30
1	B	44	MET	CG-SD-CE	5.09	108.35	100.20
1	E	237	ARG	CG-CD-NE	-5.09	101.11	111.80
1	D	297	ASP	CB-CG-OD2	5.09	122.88	118.30
1	B	74	GLN	CB-CA-C	-5.00	100.39	110.40
1	G	54	ARG	NE-CZ-NH2	5.00	122.80	120.30
1	E	88	VAL	CG1-CB-CG2	-5.00	102.90	110.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2306	0	2261	31	1
1	B	2288	0	2250	26	1
1	C	2334	0	2295	19	0
1	D	2330	0	2292	21	0
1	E	2388	0	2349	30	0
1	F	2377	0	2336	53	0
1	G	2261	0	2220	61	0
1	H	2388	0	2349	34	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	12	0	0	1	0
3	B	9	0	0	0	0
3	C	3	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	2	0	0	0	0
3	G	3	0	0	0	0
3	H	6	0	0	0	0
All	All	18725	0	18352	248	1

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 7.

All (248) 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:F:134:LEU:HD11	1:F:147:PRO:CB	1.27	1.54
1:A:259:TYR:C	1:A:260:PHE:N	1.76	1.38
1:F:134:LEU:CD1	1:F:147:PRO:CB	2.02	1.37
1:G:281:HIS:C	1:G:282:HIS:N	1.89	1.24
1:F:134:LEU:CD1	1:F:147:PRO:CG	2.20	1.18
1:F:134:LEU:HD12	1:F:147:PRO:HG3	1.23	1.17
1:F:134:LEU:O	1:F:147:PRO:HG3	1.46	1.13
1:F:134:LEU:HD12	1:F:147:PRO:CG	1.82	1.09
1:H:142:ARG:HH22	1:H:145:ARG:HD2	1.14	1.08
1:H:142:ARG:NH2	1:H:145:ARG:CD	2.17	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:GLU:OE2	1:D:267:TYR:OH	1.71	1.05
1:H:142:ARG:NH2	1:H:145:ARG:HD3	1.75	1.01
1:H:142:ARG:HH22	1:H:145:ARG:CD	1.72	1.00
1:H:224:PRO:CD	1:E:260:PHE:CE2	2.46	0.98
1:G:272:ASP:OD2	1:G:274:GLN:HG2	1.63	0.98
1:F:134:LEU:CD1	1:F:147:PRO:HB3	1.91	0.98
1:G:258:ASN:HB2	1:G:260:PHE:CZ	2.00	0.96
1:G:259:TYR:OH	1:G:282:HIS:HA	1.64	0.96
1:F:134:LEU:HD11	1:F:147:PRO:HB3	1.47	0.96
1:H:224:PRO:HD3	1:E:260:PHE:CE2	2.04	0.91
1:F:134:LEU:CD1	1:F:147:PRO:HB2	1.84	0.91
1:F:134:LEU:HD11	1:F:147:PRO:HB2	0.88	0.86
1:G:282:HIS:HB3	1:G:327:ARG:HB3	1.61	0.83
1:F:134:LEU:CD1	1:F:147:PRO:HG3	1.96	0.83
1:G:327:ARG:HA	1:G:332:PHE:CE1	2.13	0.83
1:H:224:PRO:HD2	1:E:260:PHE:CE2	2.14	0.82
1:F:134:LEU:HD11	1:F:147:PRO:CG	1.97	0.82
1:H:142:ARG:NH2	1:H:145:ARG:HD2	1.88	0.81
1:H:142:ARG:HH21	1:H:145:ARG:HD3	1.46	0.79
1:B:260:PHE:CZ	1:C:224:PRO:HD3	2.18	0.79
1:G:281:HIS:CE1	1:G:307:GLY:CA	2.66	0.79
1:G:283:LEU:HD12	1:G:325:VAL:O	1.82	0.79
1:D:272:ASP:O	1:D:275:SER:O	2.01	0.79
1:A:260:PHE:CZ	1:D:224:PRO:HD3	2.19	0.78
1:G:135:TRP:NE1	1:G:276:GLY:O	2.17	0.77
1:B:233:ARG:HB2	1:B:237:ARG:HB3	1.67	0.76
1:G:226:ARG:HH12	1:F:260:PHE:HE2	1.32	0.75
1:G:326:VAL:O	1:G:332:PHE:HD1	1.69	0.75
1:G:256:TYR:CD2	1:G:257:ARG:N	2.56	0.74
1:H:272:ASP:O	1:H:275:SER:O	2.04	0.74
1:G:272:ASP:OD2	1:G:274:GLN:CG	2.36	0.73
1:A:132:LEU:HD23	1:A:271:LEU:HD11	1.70	0.73
1:A:132:LEU:HD23	1:A:271:LEU:CD1	2.19	0.73
1:F:134:LEU:HD21	1:F:152:ILE:HG13	1.69	0.72
1:G:258:ASN:CB	1:G:260:PHE:CZ	2.71	0.72
1:G:259:TYR:CD1	1:G:284:ALA:HB2	2.25	0.72
1:B:233:ARG:HB2	1:B:237:ARG:CB	2.22	0.70
1:G:268:SER:OG	1:G:279:ILE:HG12	1.92	0.69
1:H:64:LEU:HD13	1:H:197:LEU:HD22	1.76	0.68
1:C:272:ASP:O	1:C:275:SER:O	2.11	0.67
1:F:135:TRP:CZ2	1:F:152:ILE:HD11	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:259:TYR:HD1	1:G:284:ALA:HB2	1.59	0.66
1:F:134:LEU:O	1:F:134:LEU:HD12	1.95	0.66
1:G:327:ARG:CA	1:G:332:PHE:CE1	2.78	0.66
1:F:136:GLY:O	1:F:143:GLY:HA2	1.95	0.66
1:H:223:SER:HB2	1:E:260:PHE:HZ	1.61	0.65
1:F:135:TRP:CH2	1:F:152:ILE:HD11	2.31	0.65
1:E:145:ARG:O	1:E:147:PRO:HD3	1.98	0.64
1:F:134:LEU:O	1:F:147:PRO:CG	2.37	0.63
1:A:131:LEU:O	1:A:135:TRP:HD1	1.80	0.63
1:A:277:GLN:HB3	1:A:278:PRO:CD	2.28	0.63
1:H:224:PRO:HD3	1:E:260:PHE:CZ	2.33	0.62
1:G:326:VAL:O	1:G:332:PHE:CD1	2.53	0.61
1:G:281:HIS:CE1	1:G:307:GLY:HA3	2.34	0.61
1:C:258:ASN:HB3	1:C:260:PHE:CZ	2.36	0.61
1:H:224:PRO:CD	1:E:260:PHE:CZ	2.83	0.61
1:G:188:TYR:CE2	1:G:192:LEU:HD11	2.36	0.61
1:A:129:GLU:HA	1:A:132:LEU:HD12	1.83	0.60
1:B:260:PHE:CZ	1:C:224:PRO:CD	2.85	0.60
1:D:125:ASP:OD2	1:D:127:THR:OG1	2.14	0.60
1:H:223:SER:HA	1:E:260:PHE:CZ	2.37	0.59
1:H:224:PRO:HD3	1:E:260:PHE:CD2	2.37	0.59
1:F:131:LEU:HD11	1:F:156:ARG:CG	2.33	0.58
1:G:268:SER:OG	1:G:279:ILE:CG1	2.51	0.58
1:E:134:LEU:HG	1:E:147:PRO:HG3	1.84	0.58
1:B:258:ASN:HB3	1:B:260:PHE:CZ	2.40	0.57
1:H:223:SER:HA	1:E:260:PHE:CE1	2.39	0.57
1:H:223:SER:HB2	1:E:260:PHE:CZ	2.38	0.57
1:F:132:LEU:HA	1:F:271:LEU:HD11	1.85	0.56
1:B:271:LEU:HD23	1:B:278:PRO:N	2.20	0.56
1:G:281:HIS:CE1	1:G:307:GLY:N	2.74	0.56
1:G:327:ARG:HA	1:G:332:PHE:CD1	2.40	0.56
1:B:271:LEU:HD23	1:B:278:PRO:CA	2.36	0.56
1:G:274:GLN:HG3	1:G:275:SER:N	2.21	0.56
1:A:258:ASN:HB3	1:A:260:PHE:CZ	2.41	0.55
1:F:140:GLN:OE1	1:F:140:GLN:N	2.39	0.55
1:B:75:LEU:HD23	1:B:105:MET:SD	2.47	0.55
1:F:131:LEU:HD11	1:F:156:ARG:HG3	1.88	0.55
1:C:206:LEU:HD23	1:C:215:ALA:HB2	1.89	0.55
1:G:253:SER:HB2	1:G:300:SER:OG	2.06	0.55
1:E:78:GLN:OE1	1:E:105:MET:HB2	2.07	0.54
1:G:256:TYR:HD2	1:G:257:ARG:H	1.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:67:GLU:O	1:H:71:ILE:HG13	2.07	0.54
1:B:158:LEU:HD22	1:B:176:ALA:HB3	1.90	0.54
1:B:260:PHE:CE2	1:C:224:PRO:HD3	2.43	0.54
1:F:135:TRP:CD1	1:F:135:TRP:N	2.75	0.54
1:A:277:GLN:HB3	1:A:278:PRO:HD2	1.90	0.54
1:A:37:GLU:OE1	1:A:54:ARG:NH1	2.41	0.54
1:E:213:LEU:HD11	1:E:227:ILE:HG21	1.88	0.54
1:E:136:GLY:HA3	1:E:143:GLY:HA2	1.90	0.53
1:F:139:PRO:HG2	1:F:140:GLN:OE1	2.08	0.53
1:G:256:TYR:HA	1:G:284:ALA:HB1	1.90	0.53
1:H:136:GLY:HA3	1:H:143:GLY:HA2	1.90	0.52
1:H:142:ARG:HB2	1:F:203:GLN:OE1	2.09	0.52
1:A:134:LEU:O	1:A:134:LEU:HG	2.10	0.52
1:C:272:ASP:OD2	1:C:274:GLN:HB3	2.10	0.52
1:B:210:THR:HB	1:C:29:MET:HB2	1.92	0.52
1:G:258:ASN:HB2	1:G:260:PHE:HZ	1.66	0.52
1:D:272:ASP:OD2	1:D:274:GLN:HB3	2.10	0.52
1:C:76:ASP:OD1	1:C:83:ARG:HD3	2.10	0.51
1:B:260:PHE:CE2	1:C:224:PRO:CD	2.93	0.51
1:C:339:ALA:O	1:C:343:LEU:HD23	2.10	0.51
1:F:134:LEU:CG	1:F:147:PRO:CG	2.88	0.51
1:G:256:TYR:HE2	1:G:257:ARG:HE	1.59	0.51
1:G:259:TYR:HH	1:G:282:HIS:HA	1.75	0.51
1:F:134:LEU:HG	1:F:147:PRO:HG2	1.92	0.51
1:H:224:PRO:HD2	1:E:260:PHE:CZ	2.45	0.51
1:H:188:TYR:CE2	1:H:192:LEU:HD11	2.46	0.50
1:F:134:LEU:HD12	1:F:147:PRO:CB	2.07	0.50
1:G:223:SER:CB	1:F:260:PHE:CZ	2.94	0.50
1:G:259:TYR:OH	1:G:282:HIS:CA	2.48	0.50
1:A:135:TRP:HZ2	1:A:152:ILE:HD11	1.77	0.50
1:D:64:LEU:HD22	1:D:197:LEU:CD2	2.41	0.50
1:F:258:ASN:HB3	1:F:260:PHE:CZ	2.46	0.50
1:B:128:LEU:O	1:B:129:GLU:C	2.49	0.50
1:A:135:TRP:CZ2	1:A:152:ILE:HD11	2.47	0.50
1:G:183:SER:HB2	1:G:301:THR:HG21	1.93	0.49
1:G:281:HIS:ND1	1:G:307:GLY:HA3	2.26	0.49
1:D:78:GLN:OE1	1:D:103:PRO:HB2	2.13	0.49
1:G:327:ARG:NE	1:G:332:PHE:CZ	2.79	0.49
1:B:281:HIS:HD2	1:B:283:LEU:H	1.60	0.49
1:A:317:ARG:HD3	3:A:510:HOH:O	2.12	0.49
1:A:132:LEU:HD23	1:A:271:LEU:HD12	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:ARG:O	1:D:147:PRO:HD3	2.13	0.48
1:G:188:TYR:CZ	1:G:192:LEU:HD11	2.48	0.48
1:F:139:PRO:HB2	1:F:140:GLN:OE1	2.13	0.48
1:H:142:ARG:HA	1:F:203:GLN:HE22	1.78	0.48
1:G:259:TYR:CE1	1:G:282:HIS:O	2.66	0.48
1:A:260:PHE:CE2	1:D:224:PRO:HD3	2.48	0.48
1:D:128:LEU:HD11	1:D:273:PRO:HB3	1.94	0.48
1:G:270:THR:HB	1:G:279:ILE:HD13	1.96	0.48
1:B:272:ASP:OD2	1:B:274:GLN:HB3	2.14	0.48
1:E:75:LEU:HD23	1:E:105:MET:SD	2.54	0.48
1:C:109:LEU:HD21	1:C:188:TYR:CG	2.49	0.48
1:C:338:LYS:O	1:C:342:GLU:HG3	2.13	0.48
1:F:37:GLU:HB2	1:F:52:TYR:CE1	2.49	0.47
1:H:327:ARG:NH2	1:H:330:GLN:HA	2.29	0.47
1:E:281:HIS:HD2	1:E:283:LEU:H	1.62	0.47
1:G:67:GLU:OE1	1:G:196:ARG:NE	2.43	0.47
1:A:281:HIS:HD2	1:A:283:LEU:H	1.61	0.47
1:F:39:PHE:CD1	1:F:65:HIS:CD2	3.02	0.47
1:F:130:PRO:HD3	1:F:178:GLN:HB2	1.95	0.47
1:G:79:LEU:O	1:G:88:VAL:HG11	2.14	0.47
1:A:130:PRO:HD3	1:A:178:GLN:HB2	1.95	0.47
1:E:130:PRO:HD3	1:E:178:GLN:HB2	1.97	0.47
1:A:109:LEU:HD21	1:A:188:TYR:CG	2.50	0.47
1:F:131:LEU:HD11	1:F:156:ARG:HG2	1.97	0.47
1:G:296:ALA:O	1:G:300:SER:HB3	2.15	0.47
1:D:183:SER:HB2	1:D:301:THR:HG21	1.95	0.47
1:G:327:ARG:HD3	1:G:327:ARG:HA	1.68	0.47
1:G:281:HIS:HE1	1:G:305:VAL:O	1.98	0.46
1:H:37:GLU:HB2	1:H:52:TYR:CE1	2.50	0.46
1:A:64:LEU:HD22	1:A:197:LEU:HD22	1.98	0.46
1:G:259:TYR:HD1	1:G:284:ALA:CB	2.25	0.46
1:A:132:LEU:CD2	1:A:271:LEU:HD12	2.45	0.46
1:B:128:LEU:O	1:B:131:LEU:N	2.45	0.46
1:F:316:GLU:OE2	1:F:338:LYS:HB2	2.15	0.46
1:G:75:LEU:HD23	1:G:105:MET:SD	2.56	0.46
1:H:134:LEU:HG	1:H:147:PRO:HG3	1.98	0.46
1:B:294:LEU:HD23	1:B:294:LEU:C	2.35	0.46
1:D:258:ASN:HB3	1:D:260:PHE:CZ	2.51	0.46
1:E:150:GLU:CA	1:E:150:GLU:OE2	2.64	0.46
1:A:210:THR:HB	1:D:29:MET:HB2	1.97	0.45
1:G:223:SER:HB2	1:F:260:PHE:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:261:GLU:HA	1:E:266:ARG:HA	1.97	0.45
1:E:37:GLU:HB2	1:E:52:TYR:CE1	2.50	0.45
1:F:339:ALA:O	1:F:343:LEU:HD23	2.16	0.45
1:E:258:ASN:HB3	1:E:260:PHE:CZ	2.51	0.45
1:G:218:ARG:NH1	1:G:222:GLY:O	2.50	0.45
1:H:78:GLN:OE1	1:H:105:MET:HB2	2.16	0.45
1:B:272:ASP:HB3	1:B:275:SER:OG	2.16	0.45
1:G:109:LEU:HD21	1:G:188:TYR:CG	2.52	0.45
1:B:129:GLU:HG2	1:B:180:ASP:HB2	1.99	0.45
1:F:314:LEU:HG	1:F:318:ASN:HD22	1.82	0.45
1:F:316:GLU:OE2	1:F:338:LYS:CB	2.65	0.45
1:G:142:ARG:HG3	1:G:145:ARG:CZ	2.47	0.44
1:D:281:HIS:HD2	1:D:283:LEU:H	1.65	0.44
1:H:188:TYR:CZ	1:H:192:LEU:HD11	2.53	0.44
1:A:131:LEU:O	1:A:135:TRP:CD1	2.67	0.44
1:F:135:TRP:HB2	1:F:137:PHE:CE1	2.53	0.44
1:B:37:GLU:HB2	1:B:52:TYR:CE1	2.51	0.44
1:D:37:GLU:HB2	1:D:52:TYR:CE1	2.53	0.44
1:F:109:LEU:HD21	1:F:188:TYR:CG	2.53	0.44
1:E:277:GLN:HB3	1:E:278:PRO:CD	2.48	0.44
1:G:64:LEU:HD13	1:G:197:LEU:HD22	2.00	0.44
1:G:37:GLU:HB2	1:G:52:TYR:CE1	2.53	0.43
1:A:127:THR:O	1:A:159:THR:HG22	2.18	0.43
1:B:182:ASN:OD1	1:C:30:ASP:HB3	2.18	0.43
1:F:55:SER:O	1:F:56:GLY:C	2.57	0.43
1:D:109:LEU:HD21	1:D:188:TYR:CG	2.54	0.43
1:G:135:TRP:CZ2	1:G:277:GLN:HA	2.53	0.43
1:A:64:LEU:HD22	1:A:197:LEU:CD2	2.48	0.43
1:C:136:GLY:HA3	1:C:143:GLY:HA2	2.00	0.43
1:D:158:LEU:HD22	1:D:176:ALA:HB3	2.00	0.43
1:B:312:LEU:HD11	1:B:335:THR:HG21	2.00	0.43
1:E:148:SER:OG	1:E:151:ASP:OD1	2.31	0.43
1:G:208:GLU:HA	1:G:213:LEU:HB3	2.01	0.43
1:G:326:VAL:HB	1:G:333:VAL:CG2	2.48	0.43
1:B:78:GLN:OE1	1:B:103:PRO:HB2	2.19	0.43
1:E:227:ILE:HG12	1:E:245:LEU:HD11	2.01	0.42
1:C:78:GLN:OE1	1:C:105:MET:HB2	2.19	0.42
1:E:261:GLU:OE1	1:E:327:ARG:NH1	2.52	0.42
1:G:158:LEU:HD22	1:G:176:ALA:HB3	2.00	0.42
1:C:327:ARG:HD3	1:C:332:PHE:CE1	2.54	0.42
1:A:271:LEU:HA	1:A:278:PRO:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:TRP:CZ2	1:D:152:ILE:HD11	2.54	0.42
1:D:258:ASN:HB3	1:D:260:PHE:CE1	2.54	0.42
1:E:134:LEU:HG	1:E:147:PRO:CG	2.49	0.42
1:H:60:ALA:HB3	1:H:63:VAL:HG23	2.02	0.42
1:A:260:PHE:CZ	1:D:224:PRO:CD	2.95	0.42
1:F:136:GLY:HA3	1:F:143:GLY:HA2	2.00	0.42
1:F:183:SER:HB2	1:F:301:THR:HG21	2.02	0.41
1:G:35:LYS:HE2	1:G:36:VAL:O	2.20	0.41
1:A:277:GLN:CB	1:A:278:PRO:CD	2.94	0.41
1:A:76:ASP:OD1	1:A:83:ARG:HD3	2.20	0.41
1:B:272:ASP:OD2	1:B:274:GLN:N	2.53	0.41
1:H:135:TRP:CZ2	1:H:152:ILE:HD11	2.55	0.41
1:E:39:PHE:CD1	1:E:65:HIS:CD2	3.09	0.41
1:F:158:LEU:HD22	1:F:176:ALA:HB3	2.02	0.41
1:F:281:HIS:HD2	1:F:283:LEU:H	1.69	0.41
1:F:294:LEU:C	1:F:294:LEU:HD23	2.41	0.41
1:G:142:ARG:HG3	1:G:145:ARG:NH2	2.36	0.41
1:G:281:HIS:CE1	1:G:307:GLY:HA2	2.52	0.41
1:B:44:MET:HG3	1:C:33:GLN:O	2.21	0.41
1:F:139:PRO:CB	1:F:140:GLN:OE1	2.69	0.41
1:G:258:ASN:CB	1:G:260:PHE:HZ	2.26	0.41
1:H:294:LEU:C	1:H:294:LEU:HD23	2.41	0.41
1:H:253:SER:HB2	1:H:300:SER:OG	2.21	0.41
1:A:283:LEU:HD23	1:A:304:MET:HA	2.02	0.41
1:A:250:VAL:HG22	1:A:289:ILE:HG12	2.03	0.40
1:C:134:LEU:HG	1:C:147:PRO:HG3	2.03	0.40
1:F:76:ASP:OD1	1:F:83:ARG:HD3	2.21	0.40
1:H:326:VAL:HB	1:H:333:VAL:HG23	2.04	0.40
1:B:109:LEU:HD21	1:B:188:TYR:CG	2.57	0.40
1:D:40:THR:HB	1:D:48:TYR:O	2.22	0.40
1:E:261:GLU:H	1:E:261:GLU:HG2	1.79	0.40
1:F:129:GLU:N	1:F:130:PRO:HD2	2.36	0.40
1:G:105:MET:O	1:G:109:LEU:HG	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:SER:OG	1:A:328:GLU:OE1[2_646]	2.18	0.02

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	299/332 (90%)	283 (95%)	14 (5%)	2 (1%)	22	43
1	B	297/332 (90%)	279 (94%)	18 (6%)	0	100	100
1	C	304/332 (92%)	289 (95%)	14 (5%)	1 (0%)	41	64
1	D	301/332 (91%)	291 (97%)	9 (3%)	1 (0%)	41	64
1	E	312/332 (94%)	297 (95%)	15 (5%)	0	100	100
1	F	311/332 (94%)	298 (96%)	11 (4%)	2 (1%)	25	47
1	G	291/332 (88%)	275 (94%)	15 (5%)	1 (0%)	41	64
1	H	312/332 (94%)	301 (96%)	11 (4%)	0	100	100
All	All	2427/2656 (91%)	2313 (95%)	107 (4%)	7 (0%)	41	64

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	235	ASP
1	G	148	SER
1	F	276	GLY
1	C	221	ASP
1	D	330	GLN
1	F	147	PRO
1	A	58	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	243/265 (92%)	241 (99%)	2 (1%)	81 92
1	B	242/265 (91%)	238 (98%)	4 (2%)	60 81
1	C	245/265 (92%)	243 (99%)	2 (1%)	81 92
1	D	245/265 (92%)	243 (99%)	2 (1%)	81 92
1	E	250/265 (94%)	243 (97%)	7 (3%)	43 69
1	F	249/265 (94%)	245 (98%)	4 (2%)	62 82
1	G	239/265 (90%)	235 (98%)	4 (2%)	60 81
1	H	250/265 (94%)	245 (98%)	5 (2%)	55 78
All	All	1963/2120 (93%)	1933 (98%)	30 (2%)	65 83

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	94	LEU
1	H	128	LEU
1	H	145	ARG
1	H	146	VAL
1	H	327	ARG
1	B	74	GLN
1	B	128	LEU
1	B	274	GLN
1	B	348	VAL
1	G	128	LEU
1	G	256	TYR
1	G	258	ASN
1	G	327	ARG
1	A	128	LEU
1	A	238	VAL
1	C	29	MET
1	C	128	LEU
1	D	128	LEU
1	D	150	GLU
1	E	94	LEU
1	E	145	ARG
1	E	150	GLU
1	E	261	GLU
1	E	275	SER
1	E	316	GLU
1	E	348	VAL
1	F	135	TRP

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Mol	Chain	Res	Type
1	F	144	GLU
1	F	145	ARG
1	F	150	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	33	GLN
1	H	74	GLN
1	H	240	GLN
1	H	281	HIS
1	B	74	GLN
1	B	240	GLN
1	B	281	HIS
1	B	330	GLN
1	G	240	GLN
1	G	281	HIS
1	A	178	GLN
1	A	240	GLN
1	A	281	HIS
1	C	240	GLN
1	C	281	HIS
1	D	65	HIS
1	D	240	GLN
1	D	281	HIS
1	D	330	GLN
1	E	65	HIS
1	E	178	GLN
1	E	240	GLN
1	E	281	HIS
1	F	65	HIS
1	F	240	GLN
1	F	281	HIS
1	F	318	ASN
1	F	330	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

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	G	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	281:HIS	C	282:HIS	N	1.89
1	A	259:TYR	C	260:PHE	N	1.76

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	305/332 (91%)	-0.19	9 (2%)	50	43	26, 48, 106, 146	0
1	B	303/332 (91%)	-0.21	8 (2%)	56	50	25, 44, 109, 143	0
1	C	310/332 (93%)	-0.21	7 (2%)	60	54	29, 54, 106, 141	0
1	D	309/332 (93%)	-0.22	4 (1%)	77	73	28, 49, 106, 144	0
1	E	316/332 (95%)	-0.17	5 (1%)	72	68	31, 53, 113, 145	0
1	F	315/332 (94%)	-0.17	7 (2%)	62	56	27, 52, 131, 170	0
1	G	299/332 (90%)	0.11	17 (5%)	23	18	29, 69, 116, 154	0
1	H	316/332 (95%)	-0.20	11 (3%)	44	36	26, 50, 107, 154	0
All	All	2473/2656 (93%)	-0.16	68 (2%)	54	48	25, 51, 113, 170	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	331	GLY	9.4
1	G	282	HIS	8.6
1	G	326	VAL	5.1
1	D	260	PHE	4.9
1	E	140	GLN	4.7
1	B	237	ARG	4.7
1	G	260	PHE	4.2
1	A	269	HIS	4.0
1	A	267	TYR	3.9
1	D	238	VAL	3.9
1	G	312	LEU	3.9
1	D	233	ARG	3.8
1	A	136	GLY	3.8
1	G	335	THR	3.7
1	F	152	ILE	3.7
1	F	263	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	152	ILE	3.7
1	B	132	LEU	3.6
1	C	329	GLY	3.6
1	D	267	TYR	3.6
1	F	262	ARG	3.5
1	G	257	ARG	3.5
1	F	276	GLY	3.5
1	A	330	GLN	3.5
1	C	260	PHE	3.5
1	E	142	ARG	3.4
1	H	346	ALA	3.4
1	B	152	ILE	3.3
1	F	260	PHE	3.2
1	G	333	VAL	3.1
1	H	44	MET	3.0
1	C	142	ARG	2.9
1	B	276	GLY	2.9
1	G	323	PHE	2.9
1	E	237	ARG	2.8
1	G	29	MET	2.7
1	H	233	ARG	2.7
1	F	348	VAL	2.7
1	B	233	ARG	2.7
1	G	283	LEU	2.7
1	G	308	PRO	2.6
1	G	228	ALA	2.6
1	A	271	LEU	2.6
1	A	237	ARG	2.6
1	C	276	GLY	2.6
1	A	151	ASP	2.6
1	B	278	PRO	2.6
1	H	261	GLU	2.6
1	A	132	LEU	2.5
1	G	279	ILE	2.4
1	G	306	LEU	2.4
1	G	332	PHE	2.4
1	H	238	VAL	2.3
1	H	326	VAL	2.3
1	H	329	GLY	2.3
1	H	260	PHE	2.3
1	C	277	GLN	2.3
1	E	348	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	139	PRO	2.2
1	B	260	PHE	2.2
1	H	330	GLN	2.1
1	B	269	HIS	2.1
1	H	332	PHE	2.1
1	C	330	GLN	2.1
1	H	144	GLU	2.1
1	G	310	LYS	2.1
1	C	146	VAL	2.0
1	F	139	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	H	401	1/1	0.83	0.11	51,51,51,51	0
2	MG	F	401	1/1	0.83	0.07	46,46,46,46	0
2	MG	B	401	1/1	0.92	0.11	45,45,45,45	0
2	MG	G	401	1/1	0.94	0.08	61,61,61,61	0
2	MG	D	401	1/1	0.95	0.13	51,51,51,51	0
2	MG	E	401	1/1	0.95	0.11	51,51,51,51	0
2	MG	A	401	1/1	0.97	0.08	40,40,40,40	0
2	MG	C	401	1/1	0.99	0.05	38,38,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.