



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:05 PM GMT

PDB ID : 1RZ0  
Title : Flavín reductase PheA2 in native state  
Authors : van den Heuvel, R.H.; Westphal, A.H.; Heck, A.J.; Walsh, M.A.; Rovida, S.;  
van Berkel, W.J.; Mattevi, A.  
Deposited on : 2003-12-23  
Resolution : 2.20 Å(reported)

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

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

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

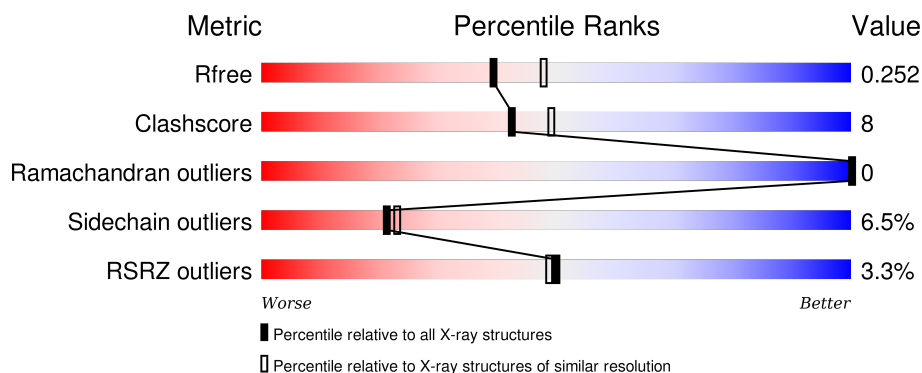
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



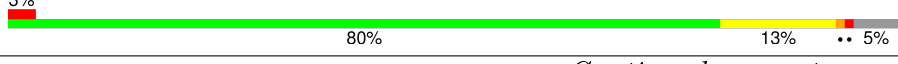
The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	161	
1	B	161	
1	C	161	
1	D	161	
1	E	161	

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Mol	Chain	Length	Quality of chain
1	F	161	<div><div>3%</div><div><div></div><div>75%</div><div>18%</div><div>• 5%</div></div></div>
1	G	161	<div><div>2%</div><div><div></div><div>74%</div><div>19%</div><div>•• 5%</div></div></div>
1	H	161	<div><div>5%</div><div><div></div><div>77%</div><div>16%</div><div>• 5%</div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10239 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 phenol 2-hydroxylase component B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	Se	0	0	0
			1176	749	196	224	1	6			
1	B	153	Total	C	N	O	S	Se	0	0	0
			1176	749	196	224	1	6			
1	C	153	Total	C	N	O	S	Se	0	0	0
			1176	749	196	224	1	6			
1	D	153	Total	C	N	O	S	Se	0	0	0
			1176	749	196	224	1	6			
1	E	153	Total	C	N	O	S	Se	0	0	0
			1176	749	196	224	1	6			
1	F	153	Total	C	N	O	S	Se	0	0	0
			1176	749	196	224	1	6			
1	G	153	Total	C	N	O	S	Se	0	0	0
			1176	749	196	224	1	6			
1	H	153	Total	C	N	O	S	Se	0	0	0
			1176	749	196	224	1	6			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
A	10	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
A	31	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
A	37	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
A	56	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
A	80	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
B	10	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
B	31	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
B	37	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
B	56	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
B	80	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	10	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
C	31	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
C	37	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
C	56	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
C	80	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
D	10	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
D	31	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
D	37	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
D	56	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
D	80	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
E	1	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
E	10	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
E	31	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
E	37	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
E	56	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
E	80	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
F	1	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
F	10	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
F	31	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
F	37	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
F	56	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
F	80	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
G	1	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
G	10	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
G	31	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
G	37	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
G	56	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
G	80	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
H	1	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
H	10	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
H	31	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
H	37	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
H	56	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2
H	80	MSE	MET	MODIFIED RESIDUE	UNP Q9LAG2

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	H	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	60	Total	O	0	0
			60	60		
3	B	55	Total	O	0	0
			55	55		
3	C	48	Total	O	0	0
			48	48		
3	D	56	Total	O	0	0
			56	56		

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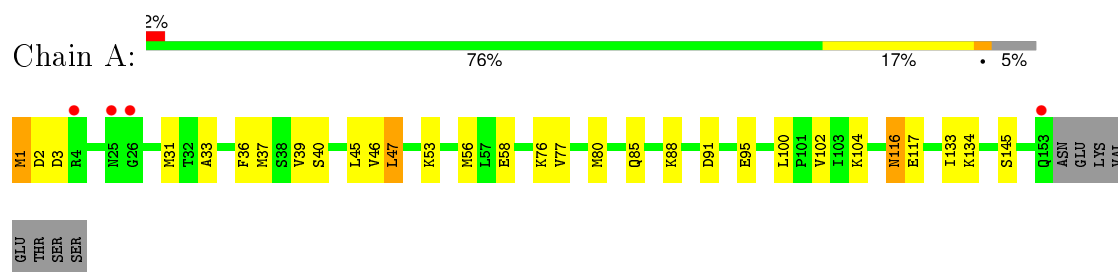
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	54	Total 54	O 54	0	0
3	F	47	Total 47	O 47	0	0
3	G	48	Total 48	O 48	0	0
3	H	39	Total 39	O 39	0	0

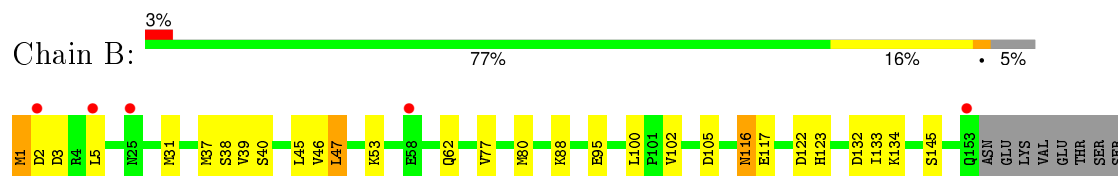
### 3 Residue-property plots [i](#)

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

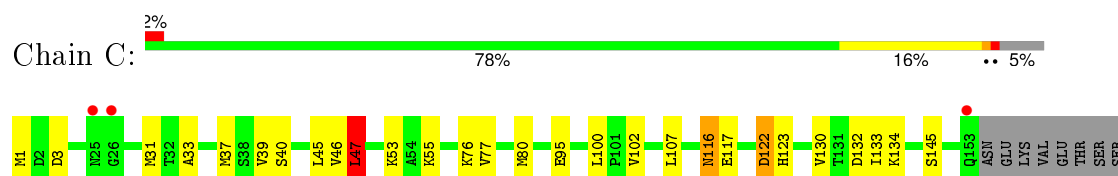
- Molecule 1: phenol 2-hydroxylase component B



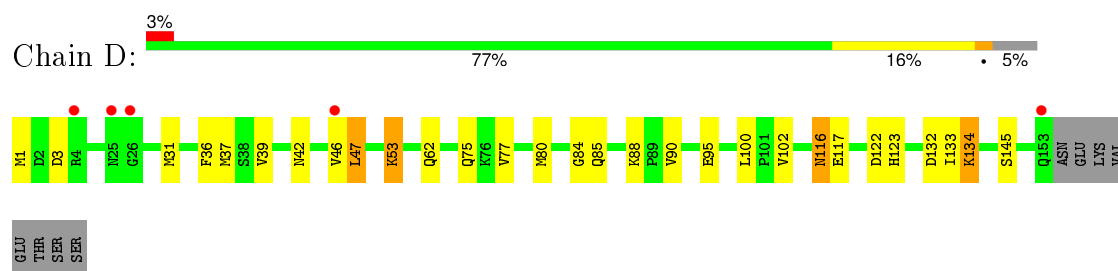
- Molecule 1: phenol 2-hydroxylase component B



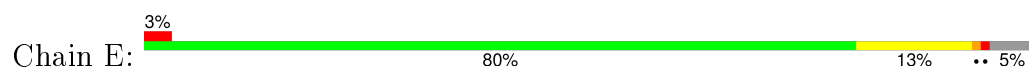
- Molecule 1: phenol 2-hydroxylase component B



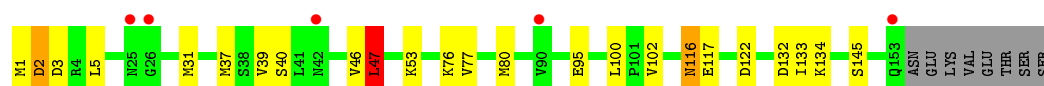
- Molecule 1: phenol 2-hydroxylase component B



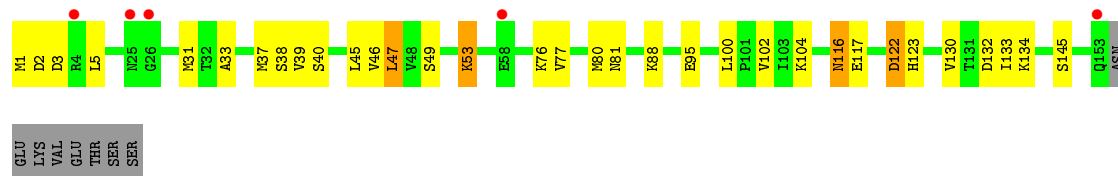
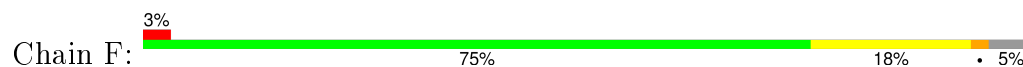
- Molecule 1: phenol 2-hydroxylase component B



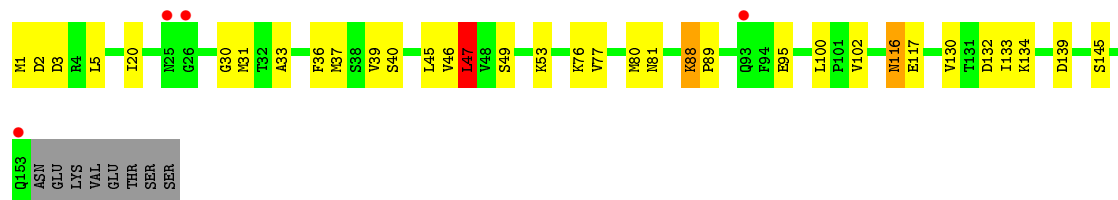
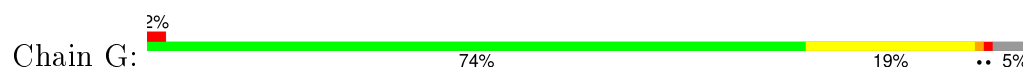




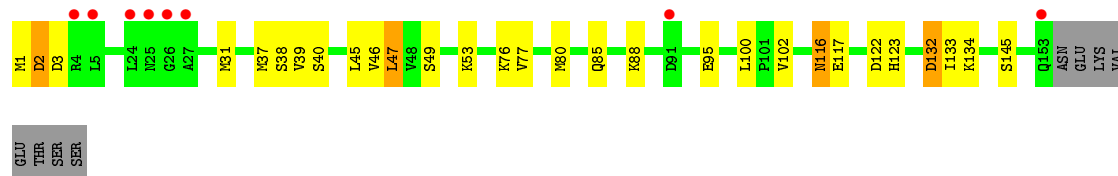
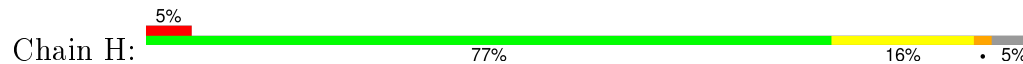
- Molecule 1: phenol 2-hydroxylase component B



- Molecule 1: phenol 2-hydroxylase component B



- Molecule 1: phenol 2-hydroxylase component B



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.54Å 154.27Å 83.87Å 90.00° 91.27° 90.00°	Depositor
Resolution (Å)	15.00 – 2.20 38.66 – 2.19	Depositor EDS
% Data completeness (in resolution range)	95.4 (15.00-2.20) 95.1 (38.66-2.19)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.1.27	Depositor
R, $R_{free}$	0.222 , 0.253 0.218 , 0.252	Depositor DCC
$R_{free}$ test set	1322 reflections (2.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.4	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 44.5	EDS
Estimated twinning fraction	0.145 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 66579 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10239	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	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 24.16 % 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 4.0457e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.67	0/1187	0.80	4/1592 (0.3%)
1	B	0.65	0/1187	0.81	5/1592 (0.3%)
1	C	0.64	0/1187	0.78	4/1592 (0.3%)
1	D	0.64	0/1187	0.80	3/1592 (0.2%)
1	E	0.62	0/1187	0.80	4/1592 (0.3%)
1	F	0.64	0/1187	0.81	5/1592 (0.3%)
1	G	0.66	0/1187	0.79	5/1592 (0.3%)
1	H	0.64	0/1187	0.78	3/1592 (0.2%)
All	All	0.64	0/9496	0.80	33/12736 (0.3%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	2	ASP	CB-CG-OD2	7.96	125.46	118.30
1	C	3	ASP	CB-CG-OD2	7.34	124.90	118.30
1	D	3	ASP	CB-CG-OD2	7.14	124.72	118.30
1	E	3	ASP	CB-CG-OD2	7.12	124.71	118.30
1	G	3	ASP	CB-CG-OD2	6.72	124.35	118.30
1	F	3	ASP	CB-CG-OD2	6.64	124.27	118.30
1	A	3	ASP	CB-CG-OD2	6.62	124.26	118.30
1	E	132	ASP	CB-CG-OD2	6.46	124.12	118.30
1	H	3	ASP	CB-CG-OD2	6.42	124.08	118.30
1	B	3	ASP	CB-CG-OD2	6.32	123.99	118.30
1	B	47	LEU	CA-CB-CG	6.12	129.38	115.30
1	A	2	ASP	CB-CG-OD2	6.03	123.73	118.30
1	G	47	LEU	CA-CB-CG	5.84	128.74	115.30
1	C	122	ASP	CB-CG-OD2	5.71	123.44	118.30
1	E	2	ASP	CB-CG-OD2	5.70	123.43	118.30
1	B	132	ASP	CB-CG-OD2	5.66	123.40	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	139	ASP	CB-CG-OD2	5.61	123.35	118.30
1	E	47	LEU	CA-CB-CG	5.57	128.11	115.30
1	A	47	LEU	CA-CB-CG	5.57	128.10	115.30
1	G	132	ASP	CB-CG-OD2	5.55	123.30	118.30
1	H	132	ASP	CB-CG-OD2	5.55	123.30	118.30
1	G	2	ASP	CB-CG-OD2	5.51	123.26	118.30
1	F	122	ASP	CB-CG-OD2	5.49	123.24	118.30
1	H	47	LEU	CA-CB-CG	5.45	127.84	115.30
1	B	2	ASP	CB-CG-OD2	5.39	123.16	118.30
1	C	132	ASP	CB-CG-OD2	5.28	123.05	118.30
1	F	47	LEU	CA-CB-CG	5.25	127.36	115.30
1	A	91	ASP	CB-CG-OD2	5.23	123.01	118.30
1	F	132	ASP	CB-CG-OD2	5.13	122.92	118.30
1	C	47	LEU	CA-CB-CG	5.13	127.09	115.30
1	D	47	LEU	CA-CB-CG	5.06	126.94	115.30
1	B	105	ASP	CB-CG-OD2	5.05	122.84	118.30
1	D	132	ASP	CB-CG-OD2	5.04	122.84	118.30

There are no chirality outliers.

There are no planarity outliers.

## 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	1176	0	1205	22	0
1	B	1176	0	1205	18	4
1	C	1176	0	1205	18	1
1	D	1176	0	1205	24	4
1	E	1176	0	1205	23	1
1	F	1176	0	1205	28	0
1	G	1176	0	1205	24	0
1	H	1176	0	1205	25	0
2	A	53	0	31	5	0
2	B	53	0	31	5	0
2	C	53	0	31	4	0
2	D	53	0	31	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	53	0	31	5	0
2	F	53	0	31	6	0
2	G	53	0	31	6	0
2	H	53	0	31	4	0
3	A	60	0	0	6	0
3	B	55	0	0	0	0
3	C	48	0	0	0	0
3	D	56	0	0	6	0
3	E	54	0	0	0	0
3	F	47	0	0	0	0
3	G	48	0	0	0	0
3	H	39	0	0	2	0
All	All	10239	0	9888	164	5

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 8.

All (164) 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:C:31:MSE:HE3	2:C:3200:FAD:H5'2	1.38	1.06
1:B:31:MSE:HE3	2:B:2200:FAD:H5'2	1.34	1.06
1:H:31:MSE:HE3	2:H:8200:FAD:H5'2	1.38	1.03
1:E:31:MSE:HE3	2:E:5200:FAD:H5'2	1.40	1.02
1:D:31:MSE:HE3	2:D:4200:FAD:H5'2	1.40	1.01
1:A:31:MSE:HE3	2:A:1200:FAD:H5'2	1.41	1.00
1:G:31:MSE:HE3	2:G:7200:FAD:H5'2	1.42	0.99
1:F:31:MSE:HE3	2:F:6200:FAD:H5'2	1.45	0.99
1:D:85:GLN:OE1	3:D:4255:HOH:O	1.85	0.94
1:F:31:MSE:HE2	2:F:6200:FAD:H2'	1.51	0.93
1:E:31:MSE:HE2	2:E:5200:FAD:H2'	1.48	0.92
1:A:31:MSE:SE	3:A:1211:HOH:O	2.37	0.90
1:G:31:MSE:HE2	2:G:7200:FAD:H2'	1.54	0.87
1:D:31:MSE:HE2	2:D:4200:FAD:H2'	1.57	0.87
1:B:31:MSE:HE2	2:B:2200:FAD:H2'	1.56	0.86
1:F:37:MSE:HE2	1:F:39:VAL:HG22	1.55	0.86
1:A:31:MSE:HE2	2:A:1200:FAD:H2'	1.57	0.86
1:H:31:MSE:HE2	2:H:8200:FAD:H2'	1.58	0.85
1:B:1:MSE:HG3	1:B:5:LEU:HD23	1.57	0.83
1:D:37:MSE:HE2	1:D:39:VAL:HG22	1.61	0.83
1:E:37:MSE:HE2	1:E:39:VAL:HG22	1.59	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:37:MSE:HE2	1:H:39:VAL:HG22	1.60	0.81
1:B:37:MSE:HE2	1:B:39:VAL:HG22	1.62	0.81
1:A:37:MSE:HE2	1:A:39:VAL:HG22	1.64	0.80
1:C:31:MSE:HE2	2:C:3200:FAD:H2'	1.63	0.79
1:C:37:MSE:HE2	1:C:39:VAL:HG22	1.65	0.78
1:H:31:MSE:HE1	3:H:8228:HOH:O	1.84	0.76
1:E:1:MSE:HG3	1:E:5:LEU:HD23	1.70	0.72
1:G:37:MSE:HE2	1:G:39:VAL:HG22	1.72	0.71
1:E:1:MSE:CG	1:E:5:LEU:HD23	2.19	0.71
1:A:104:LYS:HE2	3:A:1239:HOH:O	1.89	0.71
1:G:77:VAL:HA	1:G:80:MSE:HE3	1.71	0.70
1:A:77:VAL:HA	1:A:80:MSE:HE3	1.76	0.67
1:D:42:ASN:OD1	3:D:4233:HOH:O	2.14	0.66
1:F:37:MSE:CE	1:F:39:VAL:HG22	2.26	0.65
1:C:77:VAL:HA	1:C:80:MSE:HE3	1.79	0.64
1:A:37:MSE:CE	1:A:39:VAL:HG22	2.28	0.64
1:F:77:VAL:HA	1:F:80:MSE:HE3	1.80	0.63
1:A:58:GLU:HB3	3:A:1232:HOH:O	2.00	0.62
1:G:133:ILE:HD12	1:H:1:MSE:SE	2.49	0.62
1:A:104:LYS:CE	3:A:1239:HOH:O	2.46	0.61
1:A:31:MSE:CE	2:A:1200:FAD:H5'2	2.25	0.61
1:D:37:MSE:CE	1:D:39:VAL:HG22	2.30	0.61
1:G:37:MSE:CE	1:G:39:VAL:HG22	2.30	0.61
1:A:1:MSE:SE	1:B:133:ILE:HD12	2.50	0.61
1:E:77:VAL:HA	1:E:80:MSE:HE3	1.82	0.61
1:H:37:MSE:CE	1:H:39:VAL:HG22	2.30	0.61
1:F:37:MSE:HE2	1:F:39:VAL:CG2	2.30	0.61
1:F:31:MSE:CE	2:F:6200:FAD:H5'2	2.27	0.60
1:C:37:MSE:CE	1:C:39:VAL:HG22	2.32	0.59
1:H:77:VAL:HA	1:H:80:MSE:HE3	1.84	0.59
1:H:31:MSE:CE	3:H:8228:HOH:O	2.46	0.59
1:G:130:VAL:HG12	1:H:1:MSE:HE1	1.83	0.59
1:F:116:ASN:HD22	1:F:117:GLU:H	1.51	0.59
1:A:116:ASN:HD22	1:A:117:GLU:H	1.51	0.59
1:D:116:ASN:HD22	1:D:117:GLU:H	1.53	0.56
1:E:31:MSE:CE	2:E:5200:FAD:H2'	2.30	0.56
1:E:1:MSE:SE	1:F:133:ILE:HD12	2.56	0.56
1:B:31:MSE:CE	2:B:2200:FAD:H5'2	2.24	0.55
1:E:95:GLU:HG3	1:E:102:VAL:HG23	1.88	0.54
1:E:133:ILE:HD12	1:F:1:MSE:SE	2.57	0.54
1:D:37:MSE:HE2	1:D:39:VAL:CG2	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:LYS:NZ	3:D:4205:HOH:O	2.41	0.53
1:H:31:MSE:CE	2:H:8200:FAD:H2'	2.35	0.52
1:E:37:MSE:HE1	1:F:49:SER:HB2	1.90	0.52
1:A:95:GLU:HG3	1:A:102:VAL:HG23	1.91	0.52
1:E:31:MSE:CE	2:E:5200:FAD:H5'2	2.28	0.52
1:H:37:MSE:HE2	1:H:39:VAL:CG2	2.36	0.52
1:D:31:MSE:CE	2:D:4200:FAD:H2'	2.37	0.52
1:H:95:GLU:HG3	1:H:102:VAL:HG23	1.91	0.51
1:G:1:MSE:HE1	1:H:132:ASP:HA	1.92	0.51
1:C:1:MSE:SE	1:D:133:ILE:HD12	2.59	0.51
1:E:31:MSE:HE3	2:E:5200:FAD:C5'	2.27	0.51
1:A:31:MSE:HE3	2:A:1200:FAD:C5'	2.29	0.51
1:C:95:GLU:HG3	1:C:102:VAL:HG23	1.93	0.50
1:H:31:MSE:HE3	2:H:8200:FAD:C5'	2.27	0.50
1:B:95:GLU:HG3	1:B:102:VAL:HG23	1.92	0.50
1:D:75:GLN:HA	3:D:4226:HOH:O	2.10	0.50
1:D:77:VAL:HA	1:D:80:MSE:HE3	1.92	0.50
1:F:95:GLU:HG3	1:F:102:VAL:HG23	1.94	0.50
1:E:37:MSE:CE	1:E:39:VAL:HG22	2.37	0.50
1:H:76:LYS:HG2	1:H:80:MSE:HE2	1.94	0.49
1:B:37:MSE:CE	1:B:39:VAL:HG22	2.36	0.49
1:G:76:LYS:HG2	1:G:80:MSE:HE2	1.94	0.49
1:C:133:ILE:HD12	1:D:1:MSE:SE	2.62	0.49
1:A:133:ILE:HD12	1:B:1:MSE:SE	2.63	0.49
1:F:37:MSE:HG2	1:F:38:SER:O	2.13	0.48
1:E:1:MSE:HE1	1:F:130:VAL:HG12	1.96	0.48
1:G:95:GLU:HG3	1:G:102:VAL:HG23	1.96	0.48
1:E:122:ASP:HB2	1:F:40:SER:OG	2.15	0.47
1:C:76:LYS:HG2	1:C:80:MSE:HE2	1.97	0.47
1:E:116:ASN:HD22	1:E:117:GLU:H	1.62	0.47
1:D:31:MSE:CE	2:D:4200:FAD:H5'2	2.28	0.47
1:D:84:GLY:HA2	3:D:4206:HOH:O	2.15	0.47
1:A:76:LYS:HG2	1:A:80:MSE:HE2	1.96	0.47
1:E:1:MSE:HG2	1:E:5:LEU:HD23	1.97	0.47
1:G:31:MSE:CE	2:G:7200:FAD:H2'	2.37	0.46
1:G:116:ASN:HD22	1:G:117:GLU:H	1.62	0.46
1:C:40:SER:OG	1:D:122:ASP:HB2	2.16	0.46
1:F:1:MSE:HB2	1:F:5:LEU:HD23	1.98	0.46
1:D:116:ASN:ND2	1:D:117:GLU:H	2.12	0.46
1:G:1:MSE:SE	1:H:133:ILE:HD12	2.66	0.46
1:B:116:ASN:HD22	1:B:117:GLU:H	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:GLU:HG3	1:D:102:VAL:HG23	1.97	0.46
1:E:37:MSE:CE	1:F:49:SER:HB2	2.46	0.45
1:A:116:ASN:HD22	1:A:117:GLU:N	2.13	0.45
1:G:47:LEU:HD23	1:G:47:LEU:C	2.37	0.45
1:B:31:MSE:CE	2:B:2200:FAD:H2'	2.38	0.45
1:F:81:ASN:O	2:F:6200:FAD:H4B	2.16	0.45
1:B:77:VAL:HA	1:B:80:MSE:HE3	1.98	0.45
1:B:1:MSE:CG	1:B:5:LEU:HD23	2.40	0.45
1:F:31:MSE:HE3	2:F:6200:FAD:C5'	2.33	0.45
1:F:40:SER:HB3	1:F:45:LEU:HB2	1.99	0.45
1:G:1:MSE:HE1	1:H:132:ASP:CA	2.47	0.45
1:G:20:ILE:O	1:G:30:GLY:HA2	2.16	0.45
1:A:85:GLN:OE1	3:A:1230:HOH:O	2.21	0.45
1:G:40:SER:HB3	1:G:45:LEU:HB2	2.00	0.44
1:E:37:MSE:HE2	1:E:39:VAL:CG2	2.40	0.44
1:F:76:LYS:HG2	1:F:80:MSE:HE2	1.98	0.44
1:C:116:ASN:HD22	1:C:117:GLU:H	1.64	0.44
1:H:1:MSE:HG2	1:H:2:ASP:H	1.83	0.44
1:G:1:MSE:HG3	1:G:5:LEU:HD23	2.00	0.44
1:H:1:MSE:HG2	1:H:2:ASP:N	2.33	0.43
1:F:122:ASP:HB3	1:F:123:HIS:ND1	2.33	0.43
1:B:37:MSE:HG2	1:B:38:SER:O	2.18	0.43
1:C:122:ASP:HB3	1:C:123:HIS:ND1	2.32	0.43
1:C:130:VAL:HG12	1:D:1:MSE:HE1	2.01	0.43
1:D:122:ASP:HB3	1:D:123:HIS:ND1	2.34	0.42
1:C:31:MSE:CE	2:C:3200:FAD:H5'2	2.29	0.42
1:F:116:ASN:ND2	1:F:117:GLU:H	2.16	0.42
1:F:33:ALA:HA	2:F:6200:FAD:N5	2.35	0.42
1:E:76:LYS:HG2	1:E:80:MSE:HE2	2.02	0.42
1:E:40:SER:OG	1:F:122:ASP:HB2	2.19	0.42
1:F:53:LYS:HB2	1:F:53:LYS:HE3	1.76	0.41
1:F:1:MSE:HE2	1:F:1:MSE:HB3	1.84	0.41
1:H:116:ASN:HD22	1:H:117:GLU:H	1.66	0.41
1:C:47:LEU:HD23	1:C:47:LEU:C	2.41	0.41
2:G:7200:FAD:H9	2:G:7200:FAD:H1'1	1.87	0.41
1:G:81:ASN:O	2:G:7200:FAD:H4B	2.19	0.41
1:A:36:PHE:CG	1:A:37:MSE:N	2.88	0.41
1:H:122:ASP:HB3	1:H:123:HIS:ND1	2.36	0.41
1:C:33:ALA:HA	2:C:3200:FAD:N5	2.35	0.41
1:G:33:ALA:HA	2:G:7200:FAD:N5	2.35	0.41
1:A:56:MSE:HE2	3:A:1217:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:MSE:HE3	2:B:2200:FAD:C5'	2.25	0.41
1:C:40:SER:HB3	1:C:45:LEU:HB2	2.03	0.41
1:D:53:LYS:HB2	1:D:53:LYS:HE3	1.78	0.41
1:H:40:SER:HB3	1:H:45:LEU:HB2	2.02	0.41
1:G:36:PHE:CG	1:G:37:MSE:N	2.88	0.41
1:G:49:SER:HB2	1:H:37:MSE:HE1	2.02	0.41
1:B:37:MSE:HE2	1:B:39:VAL:CG2	2.44	0.41
1:G:37:MSE:HE1	1:H:49:SER:HB2	2.02	0.41
1:B:122:ASP:HB3	1:B:123:HIS:ND1	2.36	0.41
1:D:36:PHE:CG	1:D:37:MSE:N	2.89	0.41
1:H:37:MSE:HG2	1:H:38:SER:O	2.21	0.41
1:F:116:ASN:HD22	1:F:117:GLU:N	2.16	0.41
1:B:40:SER:HB3	1:B:45:LEU:HB2	2.03	0.41
1:A:33:ALA:HA	2:A:1200:FAD:N5	2.36	0.40
1:C:107:LEU:HD12	1:C:107:LEU:O	2.21	0.40
1:D:53:LYS:HB2	3:D:4212:HOH:O	2.21	0.40
2:D:4200:FAD:H9	2:D:4200:FAD:H1'1	1.89	0.40
1:A:40:SER:HB3	1:A:45:LEU:HB2	2.03	0.40
1:G:88:LYS:HA	1:G:89:PRO:HD3	1.89	0.40
1:E:47:LEU:C	1:E:47:LEU:HD23	2.41	0.40

All (5) 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:62:GLN:NE2	1:D:62:GLN:CG[1_455]	1.18	1.02
1:C:55:LYS:NZ	1:E:2:ASP:OD1[2_556]	2.02	0.18
1:B:62:GLN:NE2	1:D:62:GLN:CD[1_455]	2.11	0.09
1:B:62:GLN:NE2	1:D:62:GLN:CB[1_455]	2.18	0.02
1:B:62:GLN:CD	1:D:62:GLN:CG[1_455]	2.18	0.02

## 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	151/161 (94%)	148 (98%)	3 (2%)	0	100	100
1	B	151/161 (94%)	149 (99%)	2 (1%)	0	100	100
1	C	151/161 (94%)	148 (98%)	3 (2%)	0	100	100
1	D	151/161 (94%)	148 (98%)	3 (2%)	0	100	100
1	E	151/161 (94%)	147 (97%)	4 (3%)	0	100	100
1	F	151/161 (94%)	149 (99%)	2 (1%)	0	100	100
1	G	151/161 (94%)	148 (98%)	3 (2%)	0	100	100
1	H	151/161 (94%)	148 (98%)	3 (2%)	0	100	100
All	All	1208/1288 (94%)	1185 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	130/132 (98%)	121 (93%)	9 (7%)	19	20
1	B	130/132 (98%)	121 (93%)	9 (7%)	19	20
1	C	130/132 (98%)	123 (95%)	7 (5%)	27	31
1	D	130/132 (98%)	121 (93%)	9 (7%)	19	20
1	E	130/132 (98%)	123 (95%)	7 (5%)	27	31
1	F	130/132 (98%)	121 (93%)	9 (7%)	19	20
1	G	130/132 (98%)	122 (94%)	8 (6%)	23	25
1	H	130/132 (98%)	120 (92%)	10 (8%)	16	16
All	All	1040/1056 (98%)	972 (94%)	68 (6%)	21	23

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	46	VAL
1	A	47	LEU
1	A	53	LYS
1	A	88	LYS
1	A	100	LEU
1	A	116	ASN
1	A	134	LYS
1	A	145	SER
1	B	1	MSE
1	B	46	VAL
1	B	47	LEU
1	B	53	LYS
1	B	88	LYS
1	B	100	LEU
1	B	116	ASN
1	B	134	LYS
1	B	145	SER
1	C	46	VAL
1	C	47	LEU
1	C	53	LYS
1	C	100	LEU
1	C	116	ASN
1	C	134	LYS
1	C	145	SER
1	D	46	VAL
1	D	47	LEU
1	D	53	LYS
1	D	88	LYS
1	D	90	VAL
1	D	100	LEU
1	D	116	ASN
1	D	134	LYS
1	D	145	SER
1	E	46	VAL
1	E	47	LEU
1	E	53	LYS
1	E	100	LEU
1	E	116	ASN
1	E	134	LYS
1	E	145	SER
1	F	46	VAL
1	F	47	LEU

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Mol	Chain	Res	Type
1	F	53	LYS
1	F	88	LYS
1	F	100	LEU
1	F	104	LYS
1	F	116	ASN
1	F	134	LYS
1	F	145	SER
1	G	46	VAL
1	G	47	LEU
1	G	53	LYS
1	G	88	LYS
1	G	100	LEU
1	G	116	ASN
1	G	134	LYS
1	G	145	SER
1	H	2	ASP
1	H	46	VAL
1	H	47	LEU
1	H	53	LYS
1	H	85	GLN
1	H	88	LYS
1	H	100	LEU
1	H	116	ASN
1	H	134	LYS
1	H	145	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	116	ASN
1	B	116	ASN
1	C	116	ASN
1	D	42	ASN
1	D	85	GLN
1	D	116	ASN
1	E	116	ASN
1	F	116	ASN
1	G	116	ASN
1	H	116	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	FAD	A	1200	-	48,58,58	1.36	7 (14%)	54,89,89	2.19	10 (18%)
2	FAD	B	2200	-	48,58,58	1.40	6 (12%)	54,89,89	2.05	6 (11%)
2	FAD	C	3200	-	48,58,58	1.33	6 (12%)	54,89,89	2.11	12 (22%)
2	FAD	D	4200	-	48,58,58	1.41	6 (12%)	54,89,89	2.06	7 (12%)
2	FAD	E	5200	-	48,58,58	1.34	6 (12%)	54,89,89	2.10	9 (16%)
2	FAD	F	6200	-	48,58,58	1.35	7 (14%)	54,89,89	2.07	7 (12%)
2	FAD	G	7200	-	48,58,58	1.32	5 (10%)	54,89,89	2.10	9 (16%)
2	FAD	H	8200	-	48,58,58	1.41	8 (16%)	54,89,89	2.26	8 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	1200	-	-	0/30/50/50	0/6/6/6
2	FAD	B	2200	-	-	0/30/50/50	0/6/6/6
2	FAD	C	3200	-	-	0/30/50/50	0/6/6/6
2	FAD	D	4200	-	-	0/30/50/50	0/6/6/6
2	FAD	E	5200	-	-	0/30/50/50	0/6/6/6
2	FAD	F	6200	-	-	0/30/50/50	0/6/6/6
2	FAD	G	7200	-	-	0/30/50/50	0/6/6/6
2	FAD	H	8200	-	-	0/30/50/50	0/6/6/6

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1200	FAD	C5X-N5	2.01	1.38	1.35
2	A	1200	FAD	C10-N1	2.06	1.39	1.35
2	H	8200	FAD	C5X-N5	2.17	1.38	1.35
2	F	6200	FAD	C9A-N10	2.21	1.41	1.38
2	D	4200	FAD	C2A-N1A	2.28	1.38	1.33
2	G	7200	FAD	C2A-N1A	2.31	1.38	1.33
2	C	3200	FAD	C5X-N5	2.36	1.39	1.35
2	H	8200	FAD	C9A-N10	2.38	1.42	1.38
2	D	4200	FAD	C5X-N5	2.45	1.39	1.35
2	A	1200	FAD	C2A-N1A	2.45	1.38	1.33
2	F	6200	FAD	C2A-N1A	2.48	1.38	1.33
2	H	8200	FAD	C10-N1	2.49	1.39	1.35
2	E	5200	FAD	C5X-N5	2.50	1.39	1.35
2	B	2200	FAD	C5X-N5	2.50	1.39	1.35
2	E	5200	FAD	C2A-N1A	2.51	1.38	1.33
2	F	6200	FAD	C5X-N5	2.57	1.39	1.35
2	E	5200	FAD	C1'-N10	2.58	1.51	1.48
2	C	3200	FAD	C1'-N10	2.68	1.51	1.48
2	B	2200	FAD	C2A-N1A	2.75	1.39	1.33
2	H	8200	FAD	C1'-N10	2.84	1.51	1.48
2	H	8200	FAD	C2A-N1A	2.95	1.39	1.33
2	C	3200	FAD	C2A-N1A	2.97	1.39	1.33
2	C	3200	FAD	C4X-N5	2.97	1.38	1.33
2	F	6200	FAD	C1'-N10	3.03	1.51	1.48
2	F	6200	FAD	C4X-N5	3.09	1.38	1.33
2	A	1200	FAD	C4-N3	3.28	1.39	1.33
2	D	4200	FAD	C4-N3	3.28	1.39	1.33
2	F	6200	FAD	C4-N3	3.30	1.39	1.33
2	D	4200	FAD	C1'-N10	3.40	1.52	1.48
2	E	5200	FAD	C2A-N3A	3.51	1.38	1.32
2	B	2200	FAD	C1'-N10	3.52	1.52	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	7200	FAD	C1'-N10	3.53	1.52	1.48
2	B	2200	FAD	C4-N3	3.54	1.39	1.33
2	G	7200	FAD	C4-N3	3.55	1.39	1.33
2	G	7200	FAD	C4X-N5	3.58	1.38	1.33
2	C	3200	FAD	C4-N3	3.64	1.39	1.33
2	H	8200	FAD	C4X-N5	3.66	1.39	1.33
2	H	8200	FAD	C2A-N3A	3.71	1.38	1.32
2	A	1200	FAD	C1'-N10	3.72	1.52	1.48
2	G	7200	FAD	C2A-N3A	3.72	1.38	1.32
2	B	2200	FAD	C4X-N5	3.75	1.39	1.33
2	H	8200	FAD	C4-N3	3.79	1.40	1.33
2	C	3200	FAD	C2A-N3A	3.81	1.38	1.32
2	A	1200	FAD	C4X-N5	3.82	1.39	1.33
2	E	5200	FAD	C4X-N5	3.87	1.39	1.33
2	B	2200	FAD	C2A-N3A	3.96	1.39	1.32
2	A	1200	FAD	C2A-N3A	4.00	1.39	1.32
2	F	6200	FAD	C2A-N3A	4.03	1.39	1.32
2	D	4200	FAD	C2A-N3A	4.07	1.39	1.32
2	E	5200	FAD	C4-N3	4.07	1.40	1.33
2	D	4200	FAD	C4X-N5	4.25	1.40	1.33

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	8200	FAD	N3A-C2A-N1A	-12.37	119.42	128.89
2	E	5200	FAD	N3A-C2A-N1A	-11.79	119.87	128.89
2	A	1200	FAD	N3A-C2A-N1A	-11.55	120.05	128.89
2	B	2200	FAD	N3A-C2A-N1A	-11.41	120.16	128.89
2	F	6200	FAD	N3A-C2A-N1A	-11.35	120.20	128.89
2	D	4200	FAD	N3A-C2A-N1A	-11.35	120.20	128.89
2	G	7200	FAD	N3A-C2A-N1A	-11.31	120.24	128.89
2	C	3200	FAD	N3A-C2A-N1A	-10.71	120.69	128.89
2	A	1200	FAD	P-O3P-PA	-3.82	122.00	132.73
2	D	4200	FAD	P-O3P-PA	-3.77	122.14	132.73
2	B	2200	FAD	P-O3P-PA	-3.64	122.49	132.73
2	C	3200	FAD	P-O3P-PA	-3.57	122.71	132.73
2	C	3200	FAD	C4B-O4B-C1B	-3.55	105.82	109.72
2	G	7200	FAD	P-O3P-PA	-3.47	122.97	132.73
2	E	5200	FAD	P-O3P-PA	-3.41	123.16	132.73
2	H	8200	FAD	P-O3P-PA	-3.30	123.47	132.73
2	F	6200	FAD	P-O3P-PA	-2.90	124.60	132.73
2	A	1200	FAD	C4X-C4-N3	-2.72	119.87	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	7200	FAD	C4B-O4B-C1B	-2.71	106.74	109.72
2	C	3200	FAD	C4X-C4-N3	-2.69	119.91	123.59
2	E	5200	FAD	C4B-O4B-C1B	-2.69	106.77	109.72
2	C	3200	FAD	O3P-PA-O5B	-2.49	96.32	102.94
2	G	7200	FAD	C4X-C4-N3	-2.38	120.33	123.59
2	H	8200	FAD	C4X-C4-N3	-2.36	120.36	123.59
2	F	6200	FAD	C4X-C4-N3	-2.30	120.44	123.59
2	G	7200	FAD	O3P-PA-O5B	-2.29	96.86	102.94
2	F	6200	FAD	C4B-O4B-C1B	-2.28	107.21	109.72
2	D	4200	FAD	C4A-C5A-N7A	-2.24	107.42	109.48
2	H	8200	FAD	C4B-O4B-C1B	-2.20	107.31	109.72
2	A	1200	FAD	C4A-C5A-N7A	-2.15	107.50	109.48
2	E	5200	FAD	C4X-C4-N3	-2.15	120.65	123.59
2	A	1200	FAD	O3P-PA-O5B	-2.08	97.43	102.94
2	C	3200	FAD	C4A-C5A-N7A	-2.03	107.61	109.48
2	E	5200	FAD	C5X-C9A-N10	2.01	119.15	117.62
2	G	7200	FAD	O4B-C1B-N9A	2.07	112.43	108.10
2	C	3200	FAD	C1'-N10-C9A	2.12	121.24	118.86
2	H	8200	FAD	O4B-C1B-N9A	2.22	112.74	108.10
2	F	6200	FAD	O4B-C1B-N9A	2.27	112.84	108.10
2	A	1200	FAD	O4B-C1B-N9A	2.32	112.96	108.10
2	E	5200	FAD	O4B-C1B-N9A	2.36	113.04	108.10
2	D	4200	FAD	C5X-C9A-N10	2.37	119.42	117.62
2	C	3200	FAD	O2A-PA-O5B	2.38	120.49	108.46
2	C	3200	FAD	O4B-C1B-N9A	2.40	113.12	108.10
2	A	1200	FAD	O3P-P-O5'	2.41	109.34	102.94
2	C	3200	FAD	C5X-C9A-N10	2.48	119.50	117.62
2	E	5200	FAD	C4X-N5-C5X	2.48	119.61	116.76
2	D	4200	FAD	O4B-C1B-N9A	2.49	113.31	108.10
2	E	5200	FAD	C1'-N10-C9A	2.65	121.83	118.86
2	B	2200	FAD	C5X-C9A-N10	2.68	119.66	117.62
2	H	8200	FAD	C5X-C9A-N10	2.71	119.68	117.62
2	G	7200	FAD	C5X-C9A-N10	2.81	119.75	117.62
2	D	4200	FAD	C4X-N5-C5X	2.84	120.03	116.76
2	G	7200	FAD	C4X-N5-C5X	2.95	120.16	116.76
2	A	1200	FAD	C5X-C9A-N10	3.04	119.93	117.62
2	B	2200	FAD	O4B-C1B-N9A	3.06	114.51	108.10
2	A	1200	FAD	C4X-N5-C5X	3.14	120.37	116.76
2	C	3200	FAD	C4X-N5-C5X	3.37	120.64	116.76
2	B	2200	FAD	C4X-N5-C5X	3.63	120.94	116.76
2	B	2200	FAD	C4-N3-C2	3.76	118.49	115.25
2	E	5200	FAD	C4-N3-C2	4.00	118.71	115.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	6200	FAD	C4X-N5-C5X	4.01	121.37	116.76
2	H	8200	FAD	C4X-N5-C5X	4.30	121.71	116.76
2	D	4200	FAD	C4-N3-C2	4.36	119.01	115.25
2	C	3200	FAD	C4-N3-C2	4.49	119.13	115.25
2	F	6200	FAD	C4-N3-C2	4.52	119.15	115.25
2	G	7200	FAD	C4-N3-C2	4.83	119.42	115.25
2	H	8200	FAD	C4-N3-C2	5.03	119.60	115.25
2	A	1200	FAD	C4-N3-C2	5.37	119.89	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1200	FAD	5	0
2	B	2200	FAD	5	0
2	C	3200	FAD	4	0
2	D	4200	FAD	5	0
2	E	5200	FAD	5	0
2	F	6200	FAD	6	0
2	G	7200	FAD	6	0
2	H	8200	FAD	4	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	147/161 (91%)	0.17	4 (2%) 58 57	17, 28, 42, 52	0
1	B	147/161 (91%)	0.34	5 (3%) 49 47	17, 28, 44, 54	0
1	C	147/161 (91%)	0.11	3 (2%) 68 67	17, 28, 42, 52	0
1	D	147/161 (91%)	0.41	5 (3%) 49 47	17, 28, 44, 55	0
1	E	147/161 (91%)	0.09	5 (3%) 49 47	17, 28, 44, 53	0
1	F	147/161 (91%)	0.25	5 (3%) 49 47	17, 28, 42, 54	0
1	G	147/161 (91%)	0.11	4 (2%) 58 57	17, 28, 42, 55	0
1	H	147/161 (91%)	0.22	8 (5%) 29 29	17, 28, 42, 54	0
All	All	1176/1288 (91%)	0.21	39 (3%) 50 49	17, 28, 44, 55	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	26	GLY	8.3
1	D	25	ASN	8.3
1	D	26	GLY	8.2
1	G	26	GLY	5.6
1	F	25	ASN	3.9
1	G	153	GLN	3.9
1	E	153	GLN	3.9
1	H	5	LEU	3.6
1	F	153	GLN	3.6
1	E	25	ASN	3.6
1	H	27	ALA	3.5
1	D	153	GLN	3.3
1	H	26	GLY	3.3
1	A	4	ARG	3.0
1	A	25	ASN	2.8
1	H	153	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	4	ARG	2.8
1	G	25	ASN	2.8
1	E	26	GLY	2.7
1	A	26	GLY	2.7
1	B	2	ASP	2.5
1	H	25	ASN	2.5
1	F	58	GLU	2.4
1	H	4	ARG	2.4
1	E	90	VAL	2.4
1	H	24	LEU	2.4
1	G	93	GLN	2.4
1	H	91	ASP	2.3
1	C	153	GLN	2.3
1	B	5	LEU	2.3
1	B	25	ASN	2.3
1	A	153	GLN	2.3
1	C	26	GLY	2.2
1	C	25	ASN	2.2
1	B	58	GLU	2.2
1	E	42	ASN	2.1
1	F	4	ARG	2.1
1	B	153	GLN	2.1
1	D	46	VAL	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FAD	F	6200	53/53	0.90	0.16	0.34	29,36,42,43	0
2	FAD	D	4200	53/53	0.88	0.17	0.23	29,36,42,43	0
2	FAD	H	8200	53/53	0.88	0.16	0.20	29,36,42,43	0
2	FAD	G	7200	53/53	0.90	0.14	0.09	29,36,42,43	0
2	FAD	A	1200	53/53	0.91	0.15	-0.08	29,36,42,43	0
2	FAD	C	3200	53/53	0.91	0.13	-0.10	29,36,42,43	0
2	FAD	B	2200	53/53	0.86	0.16	-0.15	29,36,42,43	0
2	FAD	E	5200	53/53	0.90	0.13	-0.27	29,36,42,43	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.