



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:01 AM GMT

PDB ID : 3GWC  
Title : Crystal structure of Mycobacterium tuberculosis thymidylate synthase X bound to FdUMP and FAD  
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2009-03-31  
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 (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

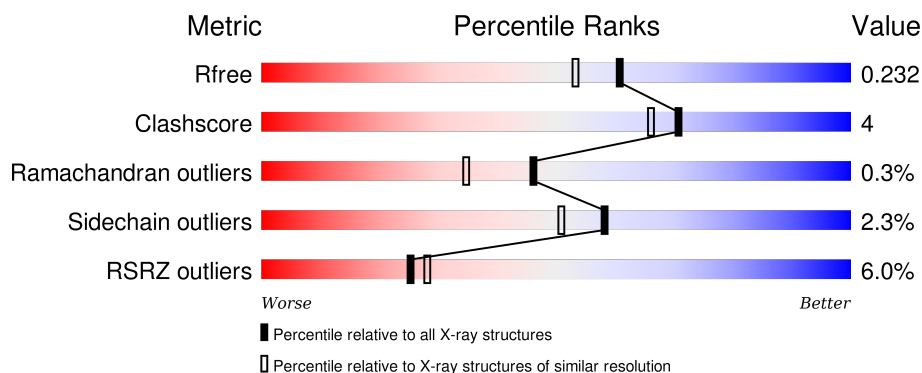
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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.



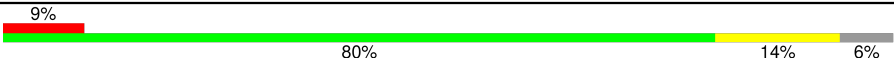

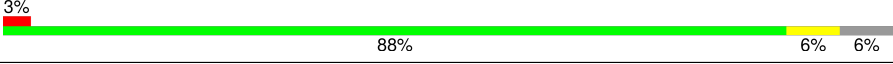
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	258	<div> <div>3%</div> <div>84%</div> <div>10%</div> <div>5%</div> </div>
1	B	258	<div> <div>4%</div> <div>82%</div> <div>9%</div> <div>7%</div> </div>
1	C	258	<div> <div>6%</div> <div>85%</div> <div>9%</div> <div>6%</div> </div>
1	D	258	<div> <div>6%</div> <div>89%</div> <div>5%</div> <div>6%</div> </div>
1	E	258	<div> <div>6%</div> <div>84%</div> <div>10%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	258	
1	G	258	
1	H	258	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	UFP	D	260	X	-	-	-
3	UFP	F	260	X	-	-	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16612 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 Thymidylate synthase thyX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	0	0
			1912	1203	349	355	5			
1	B	239	Total	C	N	O	S	0	0	0
			1855	1166	339	345	5			
1	C	243	Total	C	N	O	S	0	0	0
			1882	1183	342	352	5			
1	D	242	Total	C	N	O	S	0	0	0
			1877	1180	341	351	5			
1	E	244	Total	C	N	O	S	0	0	0
			1887	1186	343	353	5			
1	F	242	Total	C	N	O	S	0	0	0
			1884	1183	345	351	5			
1	G	245	Total	C	N	O	S	0	0	0
			1897	1194	344	354	5			
1	H	243	Total	C	N	O	S	0	0	0
			1883	1185	341	352	5			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	251	LEU	-	EXPRESSION TAG	UNP P66930
A	252	GLU	-	EXPRESSION TAG	UNP P66930
A	253	HIS	-	EXPRESSION TAG	UNP P66930
A	254	HIS	-	EXPRESSION TAG	UNP P66930
A	255	HIS	-	EXPRESSION TAG	UNP P66930
A	256	HIS	-	EXPRESSION TAG	UNP P66930
A	257	HIS	-	EXPRESSION TAG	UNP P66930
A	258	HIS	-	EXPRESSION TAG	UNP P66930
B	251	LEU	-	EXPRESSION TAG	UNP P66930
B	252	GLU	-	EXPRESSION TAG	UNP P66930
B	253	HIS	-	EXPRESSION TAG	UNP P66930
B	254	HIS	-	EXPRESSION TAG	UNP P66930
B	255	HIS	-	EXPRESSION TAG	UNP P66930

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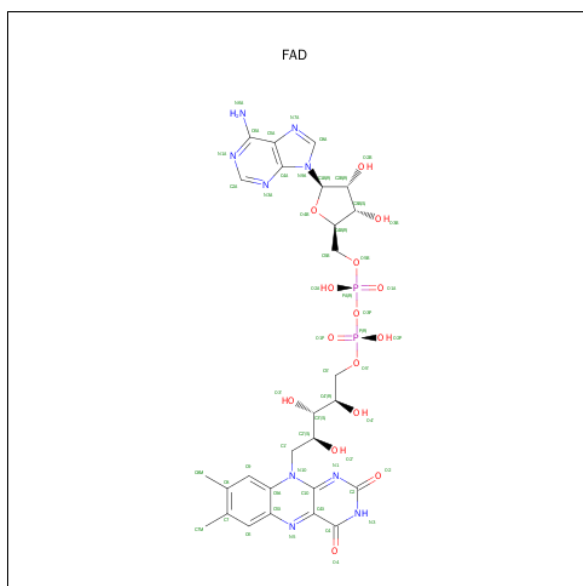
Chain	Residue	Modelled	Actual	Comment	Reference
B	256	HIS	-	EXPRESSION TAG	UNP P66930
B	257	HIS	-	EXPRESSION TAG	UNP P66930
B	258	HIS	-	EXPRESSION TAG	UNP P66930
C	251	LEU	-	EXPRESSION TAG	UNP P66930
C	252	GLU	-	EXPRESSION TAG	UNP P66930
C	253	HIS	-	EXPRESSION TAG	UNP P66930
C	254	HIS	-	EXPRESSION TAG	UNP P66930
C	255	HIS	-	EXPRESSION TAG	UNP P66930
C	256	HIS	-	EXPRESSION TAG	UNP P66930
C	257	HIS	-	EXPRESSION TAG	UNP P66930
C	258	HIS	-	EXPRESSION TAG	UNP P66930
D	251	LEU	-	EXPRESSION TAG	UNP P66930
D	252	GLU	-	EXPRESSION TAG	UNP P66930
D	253	HIS	-	EXPRESSION TAG	UNP P66930
D	254	HIS	-	EXPRESSION TAG	UNP P66930
D	255	HIS	-	EXPRESSION TAG	UNP P66930
D	256	HIS	-	EXPRESSION TAG	UNP P66930
D	257	HIS	-	EXPRESSION TAG	UNP P66930
D	258	HIS	-	EXPRESSION TAG	UNP P66930
E	251	LEU	-	EXPRESSION TAG	UNP P66930
E	252	GLU	-	EXPRESSION TAG	UNP P66930
E	253	HIS	-	EXPRESSION TAG	UNP P66930
E	254	HIS	-	EXPRESSION TAG	UNP P66930
E	255	HIS	-	EXPRESSION TAG	UNP P66930
E	256	HIS	-	EXPRESSION TAG	UNP P66930
E	257	HIS	-	EXPRESSION TAG	UNP P66930
E	258	HIS	-	EXPRESSION TAG	UNP P66930
F	251	LEU	-	EXPRESSION TAG	UNP P66930
F	252	GLU	-	EXPRESSION TAG	UNP P66930
F	253	HIS	-	EXPRESSION TAG	UNP P66930
F	254	HIS	-	EXPRESSION TAG	UNP P66930
F	255	HIS	-	EXPRESSION TAG	UNP P66930
F	256	HIS	-	EXPRESSION TAG	UNP P66930
F	257	HIS	-	EXPRESSION TAG	UNP P66930
F	258	HIS	-	EXPRESSION TAG	UNP P66930
G	251	LEU	-	EXPRESSION TAG	UNP P66930
G	252	GLU	-	EXPRESSION TAG	UNP P66930
G	253	HIS	-	EXPRESSION TAG	UNP P66930
G	254	HIS	-	EXPRESSION TAG	UNP P66930
G	255	HIS	-	EXPRESSION TAG	UNP P66930
G	256	HIS	-	EXPRESSION TAG	UNP P66930
G	257	HIS	-	EXPRESSION TAG	UNP P66930

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Chain	Residue	Modelled	Actual	Comment	Reference
G	258	HIS	-	EXPRESSION TAG	UNP P66930
H	251	LEU	-	EXPRESSION TAG	UNP P66930
H	252	GLU	-	EXPRESSION TAG	UNP P66930
H	253	HIS	-	EXPRESSION TAG	UNP P66930
H	254	HIS	-	EXPRESSION TAG	UNP P66930
H	255	HIS	-	EXPRESSION TAG	UNP P66930
H	256	HIS	-	EXPRESSION TAG	UNP P66930
H	257	HIS	-	EXPRESSION TAG	UNP P66930
H	258	HIS	-	EXPRESSION TAG	UNP P66930

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



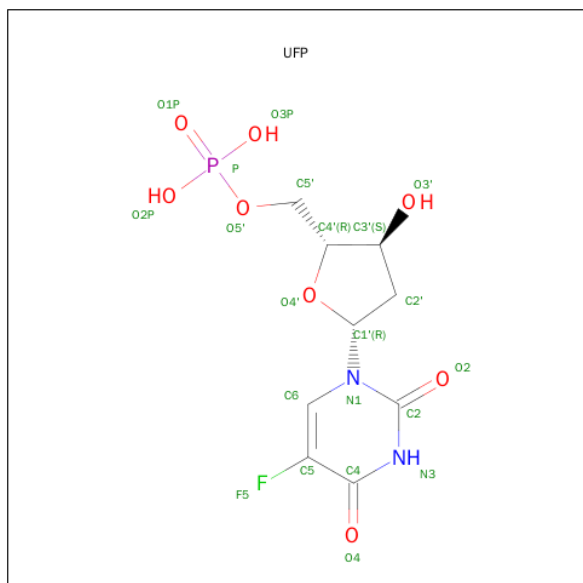
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	C	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	D	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	E	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	F	1	Total 53	C 27	N 9	O 15	P 2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 5-FLUORO-2'-DEOXYURIDINE-5'-MONOPHOSPHATE (three-letter code: UFP) (formula:  $C_9H_{12}FN_2O_8P$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	B	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	C	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	D	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	E	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	F	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	G	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0
3	H	1	Total 21	C 9	F 1	N 2	O 8	P 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

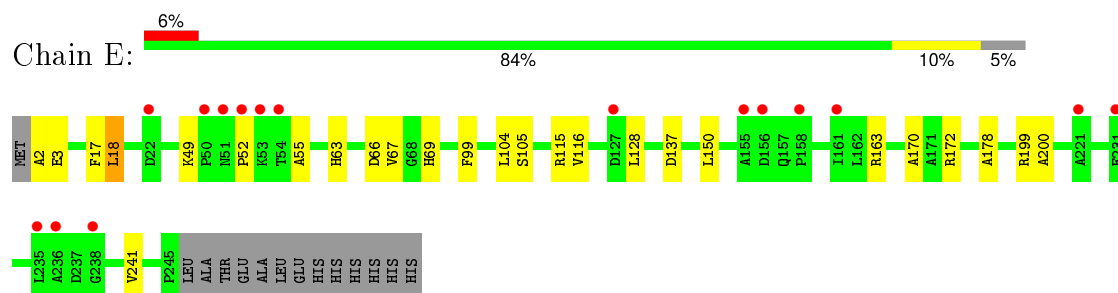
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	135	Total	O	0	0
			135	135		
5	B	145	Total	O	0	0
			145	145		
5	C	116	Total	O	0	0
			116	116		
5	D	119	Total	O	0	0
			119	119		
5	E	116	Total	O	0	0
			116	116		
5	F	94	Total	O	0	0
			94	94		
5	G	85	Total	O	0	0
			85	85		
5	H	127	Total	O	0	0
			127	127		



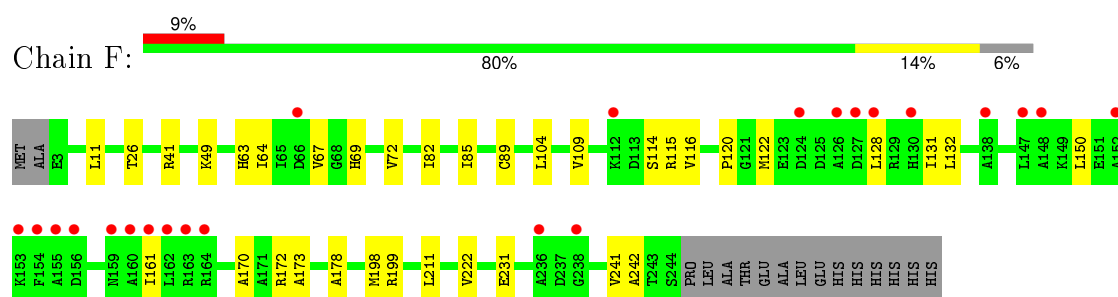


HIS  
HIS  
HIS  
HIS

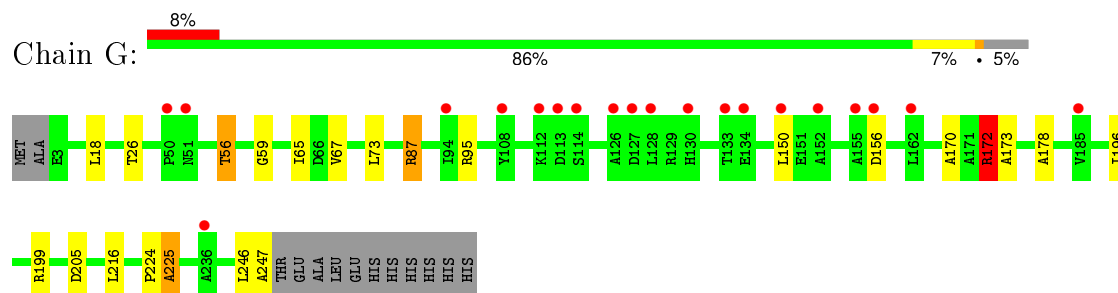
• Molecule 1: Thymidylate synthase thyX



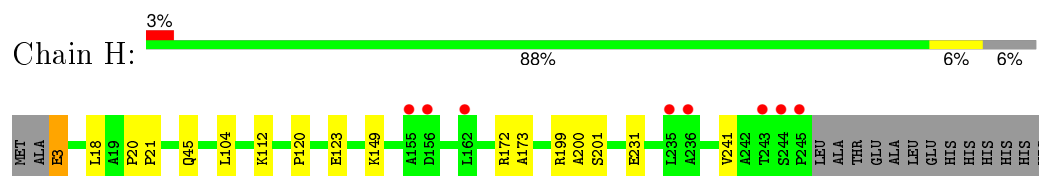
• Molecule 1: Thymidylate synthase thyX



• Molecule 1: Thymidylate synthase thyX



• Molecule 1: Thymidylate synthase thyX



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.04Å 78.45Å 168.96Å 90.00° 96.80° 90.00°	Depositor
Resolution (Å)	48.70 – 1.90 48.71 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (48.70-1.90) 91.6 (48.71-1.90)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, $R_{free}$	0.187 , 0.229 0.192 , 0.232	Depositor DCC
$R_{free}$ test set	7619 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.2	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 55.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 151876 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	16612	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.16% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UFP, GOL, 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	0.62	0/1956	0.71	1/2667 (0.0%)
1	B	0.65	0/1896	0.71	2/2584 (0.1%)
1	C	0.60	0/1925	0.70	1/2626 (0.0%)
1	D	0.62	0/1920	0.68	1/2619 (0.0%)
1	E	0.56	0/1930	0.67	0/2633
1	F	0.55	0/1927	0.66	0/2626
1	G	0.55	0/1941	0.68	3/2649 (0.1%)
1	H	0.59	0/1926	0.68	0/2627
All	All	0.59	0/15421	0.69	8/21031 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	ARG	NE-CZ-NH2	-8.51	116.04	120.30
1	B	87	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	G	172	ARG	NE-CZ-NH2	-7.45	116.58	120.30
1	G	172	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	C	168	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	G	87	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	D	163	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	B	87	ARG	NE-CZ-NH1	5.25	122.92	120.30

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	1912	0	1885	20	0
1	B	1855	0	1815	25	0
1	C	1882	0	1840	17	0
1	D	1877	0	1835	7	0
1	E	1887	0	1841	20	0
1	F	1884	0	1848	27	0
1	G	1897	0	1858	19	0
1	H	1883	0	1848	12	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
2	C	53	0	31	0	0
2	D	53	0	31	0	0
2	E	53	0	31	0	0
2	F	53	0	31	0	0
2	G	53	0	31	0	0
2	H	53	0	31	0	0
3	A	21	0	10	2	0
3	B	21	0	9	2	0
3	C	21	0	10	1	0
3	D	21	0	9	3	0
3	E	21	0	9	2	0
3	F	21	0	9	2	0
3	G	21	0	9	4	0
3	H	21	0	10	1	0
4	C	6	0	8	0	0
5	A	135	0	0	5	0
5	B	145	0	0	2	0
5	C	116	0	0	1	0
5	D	119	0	0	0	0
5	E	116	0	0	4	0
5	F	94	0	0	4	0
5	G	85	0	0	1	0
5	H	127	0	0	1	0
All	All	16612	0	15101	134	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 4.

All (134) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:ILE:HG23	1:B:162:LEU:HD13	1.42	1.02
1:A:199:ARG:HH12	3:D:260:UFP:HN3	1.14	0.95
1:C:161:ILE:HG22	1:C:162:LEU:HD23	1.50	0.93
3:A:260:UFP:HN3	1:D:199:ARG:HH12	1.11	0.93
1:F:199:ARG:HH12	3:G:260:UFP:HN3	1.15	0.89
3:F:260:UFP:HN3	1:G:199:ARG:HH12	1.18	0.88
3:E:260:UFP:HN3	1:H:199:ARG:HH12	1.21	0.88
1:C:123:GLU:O	1:C:129:ARG:NH1	2.07	0.87
3:B:260:UFP:HN3	1:C:199:ARG:HH12	1.23	0.84
1:B:199:ARG:HH12	3:C:260:UFP:HN3	1.22	0.84
1:E:199:ARG:HH12	3:H:260:UFP:HN3	1.25	0.84
1:F:69:HIS:O	1:F:72:VAL:HG12	1.78	0.83
1:E:67:VAL:HG13	1:E:69:HIS:CD2	2.14	0.82
1:F:41:ARG:CZ	5:F:898:HOH:O	2.26	0.81
1:F:41:ARG:NH1	5:F:898:HOH:O	2.17	0.78
1:C:69:HIS:O	1:C:72:VAL:HG12	1.85	0.76
1:A:168:ARG:CZ	5:A:645:HOH:O	2.35	0.73
1:C:67:VAL:HG12	1:C:69:HIS:NE2	2.04	0.73
1:G:56:THR:HG23	1:G:59:GLY:H	1.53	0.73
1:E:2:ALA:HB2	1:E:137:ASP:OD1	1.90	0.71
1:G:87:ARG:NH2	3:G:260:UFP:O3P	2.25	0.68
1:B:134:GLU:OE1	5:B:905:HOH:O	2.11	0.68
1:E:52:PRO:HA	1:E:55:ALA:HB2	1.76	0.67
1:B:49:LYS:CB	5:B:708:HOH:O	2.43	0.66
1:B:161:ILE:CG2	1:B:162:LEU:HD13	2.22	0.66
1:A:95:ARG:HG3	3:D:260:UFP:H2'2	1.77	0.66
1:B:104:LEU:HD13	1:D:45:GLN:HG2	1.76	0.65
1:A:2:ALA:HB2	1:A:137:ASP:OD1	1.95	0.65
1:G:224:PRO:O	1:G:225:ALA:HB3	1.98	0.64
1:A:87:ARG:NH2	3:A:260:UFP:O3P	2.31	0.64
1:F:104:LEU:CD1	1:F:109:VAL:HG21	2.29	0.62
1:C:63:HIS:CE1	1:C:67:VAL:HG21	2.36	0.61
1:E:99:PHE:CZ	5:E:284:HOH:O	2.52	0.59
1:F:173:ALA:HB1	1:G:178:ALA:HB2	1.83	0.58
1:B:69:HIS:O	1:B:72:VAL:HG22	2.03	0.58
1:A:205:ASP:OD2	5:A:835:HOH:O	2.17	0.58
1:A:65:ILE:HG22	1:A:246:LEU:HD13	1.86	0.57
1:C:162:LEU:HD22	1:C:165:LYS:HE3	1.86	0.57
1:F:199:ARG:NH1	3:G:260:UFP:HN3	1.96	0.56
1:D:18:LEU:HD22	1:H:112:LYS:HE2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:82:ILE:HD13	1:F:211:LEU:HD11	1.89	0.55
1:B:161:ILE:HG23	1:B:162:LEU:CD1	2.28	0.55
1:B:104:LEU:CD1	1:B:109:VAL:HG21	2.36	0.54
1:B:159:ASN:OD1	1:B:161:ILE:HG22	2.07	0.54
1:A:36:VAL:HG13	1:A:72:VAL:HG12	1.89	0.54
1:F:122:MET:HE2	1:G:150:LEU:HD11	1.90	0.54
1:C:162:LEU:HD22	1:C:165:LYS:CE	2.38	0.53
1:B:87:ARG:NH2	3:B:260:UFP:O3P	2.42	0.53
1:F:104:LEU:HD13	1:H:45:GLN:HG2	1.91	0.53
1:A:178:ALA:HB2	1:D:173:ALA:HB1	1.90	0.53
1:C:104:LEU:HD13	1:C:109:VAL:HG21	1.90	0.53
1:E:2:ALA:HB3	5:E:272:HOH:O	2.08	0.53
1:H:200:ALA:O	1:H:241:VAL:HG13	2.09	0.53
1:F:64:ILE:HD13	1:F:72:VAL:HG11	1.92	0.52
1:B:104:LEU:HD12	1:B:109:VAL:HG21	1.92	0.52
1:B:120:PRO:HA	1:B:123:GLU:HG3	1.92	0.51
1:G:205:ASP:OD2	5:G:581:HOH:O	2.19	0.51
1:G:67:VAL:O	1:G:67:VAL:HG22	2.11	0.51
3:E:260:UFP:HN3	1:H:199:ARG:NH1	2.00	0.50
1:C:67:VAL:CG1	1:C:69:HIS:NE2	2.73	0.50
1:B:119:PRO:HG2	1:B:122:MET:HE3	1.93	0.50
1:B:60:TYR:CE2	1:B:64:ILE:HD11	2.46	0.50
1:H:104:LEU:C	1:H:104:LEU:HD23	2.31	0.50
1:C:63:HIS:CE1	1:C:67:VAL:CG2	2.95	0.50
1:A:160:ALA:HB1	1:A:164:ARG:NH2	2.27	0.49
1:G:65:ILE:HG22	1:G:246:LEU:HD13	1.94	0.49
1:E:3:GLU:HB3	1:E:115:ARG:HD3	1.95	0.49
1:E:52:PRO:HA	1:E:55:ALA:CB	2.42	0.48
1:G:56:THR:HG23	1:G:59:GLY:N	2.25	0.48
1:B:48:SER:O	1:B:50:PRO:HD3	2.13	0.48
1:F:104:LEU:HD12	1:F:109:VAL:HG21	1.95	0.48
1:B:17:PHE:C	1:B:18:LEU:HD13	2.34	0.48
1:H:120:PRO:HA	1:H:123:GLU:HG3	1.95	0.48
1:C:205:ASP:OD2	5:C:881:HOH:O	2.20	0.47
1:F:161:ILE:HG22	5:F:847:HOH:O	2.13	0.47
1:E:99:PHE:CE2	5:E:284:HOH:O	2.68	0.47
1:B:60:TYR:HE2	1:B:64:ILE:HD11	1.79	0.46
1:B:17:PHE:O	1:B:18:LEU:HD13	2.16	0.46
1:E:104:LEU:HD23	1:E:104:LEU:C	2.35	0.46
1:G:224:PRO:O	1:G:225:ALA:CB	2.62	0.46
1:H:3:GLU:N	5:H:575:HOH:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:THR:O	1:B:94:ILE:HG12	2.16	0.46
1:D:116:VAL:HG13	1:D:178:ALA:HB1	1.98	0.46
1:G:172:ARG:NH2	3:G:260:UFP:O3P	2.49	0.45
1:E:200:ALA:O	1:E:241:VAL:HG13	2.16	0.45
1:B:119:PRO:HG2	1:B:122:MET:CE	2.46	0.45
1:F:67:VAL:HG22	1:F:67:VAL:O	2.17	0.45
1:A:200:ALA:O	1:A:241:VAL:HG13	2.17	0.45
1:F:11:LEU:HD11	1:F:222:VAL:HG21	1.99	0.45
1:F:128:LEU:HA	1:F:131:ILE:HD12	1.98	0.45
1:A:247:ALA:HB2	5:A:539:HOH:O	2.17	0.45
1:C:13:ALA:HB3	1:C:79:SER:HB2	1.99	0.45
1:F:122:MET:HE3	1:G:170:ALA:HB1	1.99	0.45
1:F:122:MET:CE	1:G:170:ALA:HB1	2.47	0.45
3:F:260:UFP:H2'2	1:G:95:ARG:HG3	1.99	0.44
1:B:161:ILE:HG23	1:B:162:LEU:N	2.31	0.44
1:A:160:ALA:HB1	1:A:164:ARG:HH21	1.82	0.44
1:G:65:ILE:HG22	1:G:246:LEU:CD1	2.47	0.44
1:B:161:ILE:CG2	1:B:162:LEU:N	2.80	0.44
1:C:120:PRO:HA	1:C:123:GLU:HG3	2.00	0.44
1:D:234:THR:HG22	1:D:235:LEU:O	2.18	0.44
1:H:18:LEU:N	1:H:18:LEU:HD12	2.32	0.44
1:E:128:LEU:HD21	1:H:149:LYS:HB3	2.00	0.44
1:C:104:LEU:HD12	1:C:104:LEU:C	2.38	0.43
1:A:116:VAL:HG13	5:A:264:HOH:O	2.18	0.43
1:F:115:ARG:NE	5:F:611:HOH:O	2.52	0.43
1:B:178:ALA:HB2	1:C:173:ALA:HB1	2.00	0.43
1:F:122:MET:HE3	1:F:122:MET:HB2	1.82	0.43
1:A:173:ALA:HB1	1:D:178:ALA:HB2	2.00	0.43
1:A:116:VAL:HG11	1:A:136:ALA:CB	2.48	0.43
1:F:26:THR:O	1:F:49:LYS:NZ	2.44	0.42
1:G:196:ILE:HD13	1:G:216:LEU:HD13	2.02	0.42
1:F:231:GLU:O	1:F:242:ALA:HA	2.20	0.42
1:G:246:LEU:O	1:G:247:ALA:C	2.57	0.42
1:B:150:LEU:HD13	1:B:170:ALA:HB3	2.01	0.41
1:A:236:ALA:HB3	5:A:850:HOH:O	2.20	0.41
1:E:163:ARG:HD2	5:E:845:HOH:O	2.21	0.41
1:A:36:VAL:HG11	1:A:73:LEU:HD23	2.02	0.41
1:F:63:HIS:O	1:F:67:VAL:HG12	2.19	0.41
1:E:104:LEU:HD23	1:E:105:SER:N	2.36	0.41
1:F:120:PRO:C	1:F:122:MET:H	2.24	0.41
1:A:95:ARG:CG	3:D:260:UFP:H2'2	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:THR:HG22	1:C:234:THR:N	2.36	0.41
1:H:20:PRO:HA	1:H:21:PRO:HD3	1.90	0.41
1:E:150:LEU:HD13	1:E:170:ALA:HB3	2.01	0.41
1:F:178:ALA:HB2	1:G:173:ALA:HB1	2.02	0.41
1:E:17:PHE:C	1:E:18:LEU:HD13	2.41	0.41
1:E:67:VAL:CG1	1:E:69:HIS:CD2	2.94	0.41
1:F:85:ILE:HG12	1:F:89:CYS:HB3	2.03	0.41
1:E:178:ALA:HB2	1:H:173:ALA:HB1	2.03	0.40
1:A:224:PRO:O	1:A:225:ALA:HB3	2.21	0.40
1:F:150:LEU:HD13	1:F:170:ALA:HB3	2.03	0.40
1:E:63:HIS:O	1:E:67:VAL:HG12	2.21	0.40
1:E:116:VAL:HG23	1:E:178:ALA:CB	2.52	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	244/258 (95%)	241 (99%)	2 (1%)	1 (0%)	39	27
1	B	235/258 (91%)	232 (99%)	2 (1%)	1 (0%)	39	27
1	C	241/258 (93%)	234 (97%)	7 (3%)	0	100	100
1	D	240/258 (93%)	236 (98%)	3 (1%)	1 (0%)	39	27
1	E	242/258 (94%)	237 (98%)	4 (2%)	1 (0%)	39	27
1	F	240/258 (93%)	232 (97%)	8 (3%)	0	100	100
1	G	243/258 (94%)	232 (96%)	10 (4%)	1 (0%)	39	27
1	H	241/258 (93%)	238 (99%)	3 (1%)	0	100	100
All	All	1926/2064 (93%)	1882 (98%)	39 (2%)	5 (0%)	46	35

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	ASP
1	D	155	ALA
1	G	225	ALA
1	E	49	LYS
1	B	49	LYS

### 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	197/209 (94%)	194 (98%)	3 (2%)	72	69
1	B	190/209 (91%)	185 (97%)	5 (3%)	54	45
1	C	193/209 (92%)	189 (98%)	4 (2%)	61	55
1	D	193/209 (92%)	189 (98%)	4 (2%)	61	55
1	E	193/209 (92%)	190 (98%)	3 (2%)	70	66
1	F	194/209 (93%)	188 (97%)	6 (3%)	47	37
1	G	195/209 (93%)	189 (97%)	6 (3%)	47	37
1	H	194/209 (93%)	190 (98%)	4 (2%)	61	55
All	All	1549/1672 (93%)	1514 (98%)	35 (2%)	58	51

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	ARG
1	A	172	ARG
1	A	201	SER
1	B	18	LEU
1	B	87	ARG
1	B	162	LEU
1	B	172	ARG
1	B	201	SER
1	C	8	ARG
1	C	104	LEU
1	C	172	ARG

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Mol	Chain	Res	Type
1	C	201	SER
1	D	14	LYS
1	D	163	ARG
1	D	172	ARG
1	D	201	SER
1	E	18	LEU
1	E	66	ASP
1	E	172	ARG
1	F	114	SER
1	F	116	VAL
1	F	132	LEU
1	F	172	ARG
1	F	198	MET
1	F	241	VAL
1	G	18	LEU
1	G	26	THR
1	G	56	THR
1	G	73	LEU
1	G	156	ASP
1	G	172	ARG
1	H	3	GLU
1	H	172	ARG
1	H	201	SER
1	H	231	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

17 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	259	-	48,58,58	1.00	3 (6%)	54,89,89	2.06	8 (14%)
3	UFP	A	260	-	18,22,22	1.34	2 (11%)	21,33,33	3.17	4 (19%)
2	FAD	B	259	-	48,58,58	1.01	3 (6%)	54,89,89	2.09	9 (16%)
3	UFP	B	260	-	18,22,22	1.19	1 (5%)	21,33,33	3.03	7 (33%)
2	FAD	C	259	-	48,58,58	1.03	4 (8%)	54,89,89	1.84	8 (14%)
3	UFP	C	260	-	18,22,22	1.03	1 (5%)	21,33,33	2.97	5 (23%)
4	GOL	C	261	-	5,5,5	0.68	0	5,5,5	0.37	0
2	FAD	D	259	-	48,58,58	0.98	2 (4%)	54,89,89	2.09	11 (20%)
3	UFP	D	260	-	18,22,22	1.12	1 (5%)	21,33,33	3.11	9 (42%)
2	FAD	E	259	-	48,58,58	1.05	4 (8%)	54,89,89	2.07	11 (20%)
3	UFP	E	260	-	18,22,22	1.24	2 (11%)	21,33,33	2.95	5 (23%)
2	FAD	F	259	-	48,58,58	0.90	2 (4%)	54,89,89	2.06	6 (11%)
3	UFP	F	260	-	18,22,22	1.08	1 (5%)	21,33,33	2.81	6 (28%)
2	FAD	G	259	-	48,58,58	0.89	2 (4%)	54,89,89	2.13	8 (14%)
3	UFP	G	260	-	18,22,22	1.28	2 (11%)	21,33,33	3.02	7 (33%)
2	FAD	H	259	-	48,58,58	1.00	3 (6%)	54,89,89	2.23	11 (20%)
3	UFP	H	260	-	18,22,22	1.28	2 (11%)	21,33,33	2.72	4 (19%)

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	259	-	-	0/30/50/50	0/6/6/6
3	UFP	A	260	-	-	0/6/22/22	0/2/2/2
2	FAD	B	259	-	-	0/30/50/50	0/6/6/6
3	UFP	B	260	-	-	0/6/22/22	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	C	259	-	-	0/30/50/50	0/6/6/6
3	UFP	C	260	-	-	0/6/22/22	0/2/2/2
4	GOL	C	261	-	-	0/4/4/4	0/0/0/0
2	FAD	D	259	-	-	0/30/50/50	0/6/6/6
3	UFP	D	260	-	1/1/4/4	0/6/22/22	0/2/2/2
2	FAD	E	259	-	-	0/30/50/50	0/6/6/6
3	UFP	E	260	-	-	0/6/22/22	0/2/2/2
2	FAD	F	259	-	-	0/30/50/50	0/6/6/6
3	UFP	F	260	-	1/1/4/4	0/6/22/22	0/2/2/2
2	FAD	G	259	-	-	0/30/50/50	0/6/6/6
3	UFP	G	260	-	-	0/6/22/22	0/2/2/2
2	FAD	H	259	-	-	0/30/50/50	0/6/6/6
3	UFP	H	260	-	-	0/6/22/22	0/2/2/2

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	259	FAD	C10-N10	-3.41	1.35	1.39
2	E	259	FAD	C10-N10	-3.18	1.35	1.39
2	H	259	FAD	C10-N10	-3.01	1.35	1.39
2	C	259	FAD	C10-N10	-2.69	1.36	1.39
2	B	259	FAD	C10-N10	-2.62	1.36	1.39
2	A	259	FAD	C10-N10	-2.51	1.36	1.39
3	H	260	UFP	O4'-C1'	-2.41	1.36	1.42
3	A	260	UFP	O4'-C1'	-2.33	1.37	1.42
3	G	260	UFP	P-O3P	-2.32	1.46	1.54
2	F	259	FAD	C10-N10	-2.29	1.36	1.39
2	A	259	FAD	C9A-N10	-2.06	1.35	1.38
2	A	259	FAD	O4B-C1B	2.07	1.43	1.41
2	G	259	FAD	O4B-C1B	2.09	1.43	1.41
2	C	259	FAD	C4X-N5	2.13	1.36	1.33
2	G	259	FAD	C4X-N5	2.18	1.36	1.33
2	B	259	FAD	C4X-N5	2.28	1.36	1.33
3	E	260	UFP	C6-N1	2.33	1.38	1.35
2	F	259	FAD	C4-N3	2.36	1.37	1.33
3	F	260	UFP	C4-N3	2.38	1.37	1.33
2	H	259	FAD	O4B-C1B	2.41	1.44	1.41
2	C	259	FAD	C4-N3	2.52	1.37	1.33
2	E	259	FAD	O4B-C1B	2.58	1.44	1.41
3	C	260	UFP	C4-N3	2.77	1.38	1.33
3	E	260	UFP	C4-N3	2.86	1.38	1.33
3	H	260	UFP	C4-N3	2.91	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	260	UFP	C4-N3	2.95	1.38	1.33
2	E	259	FAD	C4X-N5	2.95	1.38	1.33
2	D	259	FAD	C4X-N5	2.98	1.38	1.33
3	G	260	UFP	C4-N3	2.98	1.38	1.33
3	B	260	UFP	C4-N3	2.98	1.38	1.33
2	C	259	FAD	O4B-C1B	2.99	1.45	1.41
2	B	259	FAD	O4B-C1B	3.05	1.45	1.41
2	E	259	FAD	C4-N3	3.16	1.39	1.33
3	A	260	UFP	C4-N3	3.25	1.39	1.33
2	H	259	FAD	C4X-N5	3.32	1.38	1.33

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	259	FAD	N3A-C2A-N1A	-11.28	120.25	128.89
2	H	259	FAD	N3A-C2A-N1A	-11.02	120.45	128.89
2	A	259	FAD	N3A-C2A-N1A	-10.85	120.58	128.89
2	G	259	FAD	N3A-C2A-N1A	-10.69	120.71	128.89
2	E	259	FAD	N3A-C2A-N1A	-10.44	120.90	128.89
2	B	259	FAD	N3A-C2A-N1A	-9.81	121.39	128.89
2	D	259	FAD	N3A-C2A-N1A	-9.44	121.67	128.89
2	C	259	FAD	N3A-C2A-N1A	-9.00	122.00	128.89
3	D	260	UFP	C4'-O4'-C1'	-5.22	96.28	109.47
3	G	260	UFP	C5-C4-N3	-3.60	118.33	122.34
3	C	260	UFP	C5-C4-N3	-3.59	118.33	122.34
3	G	260	UFP	C4'-O4'-C1'	-3.43	100.80	109.47
3	D	260	UFP	C3'-C2'-C1'	-3.38	94.25	102.40
3	B	260	UFP	C4'-O4'-C1'	-3.36	100.97	109.47
3	A	260	UFP	C5-C4-N3	-3.23	118.74	122.34
2	F	259	FAD	C4X-C4-N3	-3.02	119.46	123.59
2	H	259	FAD	C4-C4X-C10	-2.96	118.05	119.94
2	B	259	FAD	C4-C4X-C10	-2.90	118.08	119.94
2	E	259	FAD	C4-C4X-C10	-2.79	118.15	119.94
2	H	259	FAD	C4X-C4-N3	-2.74	119.84	123.59
3	C	260	UFP	O5'-P-O1P	-2.73	100.19	107.14
2	G	259	FAD	C4X-C4-N3	-2.70	119.90	123.59
2	A	259	FAD	C1B-N9A-C4A	-2.67	122.91	126.94
2	B	259	FAD	C4X-C4-N3	-2.62	120.01	123.59
3	E	260	UFP	C4'-O4'-C1'	-2.58	102.95	109.47
2	D	259	FAD	C9A-C5X-N5	-2.57	118.56	122.36
3	F	260	UFP	C4'-O4'-C1'	-2.54	103.04	109.47
3	B	260	UFP	C5-C4-N3	-2.52	119.53	122.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	259	FAD	C4A-C5A-N7A	-2.45	107.22	109.48
2	F	259	FAD	O2B-C2B-C3B	-2.30	104.36	111.83
2	D	259	FAD	C4X-C10-N10	-2.23	119.20	120.52
3	F	260	UFP	C5-C4-N3	-2.19	119.90	122.34
2	C	259	FAD	C4X-C4-N3	-2.18	120.60	123.59
2	E	259	FAD	C9A-C5X-N5	-2.13	119.20	122.36
3	D	260	UFP	C5-C4-N3	-2.13	119.97	122.34
2	A	259	FAD	C4X-C4-N3	-2.12	120.69	123.59
2	D	259	FAD	C4-C4X-C10	-2.10	118.60	119.94
2	D	259	FAD	C4X-C4-N3	-2.08	120.74	123.59
2	E	259	FAD	C4X-C4-N3	-2.04	120.80	123.59
3	H	260	UFP	C4'-O4'-C1'	-2.03	104.34	109.47
2	G	259	FAD	O2A-PA-O1A	2.00	123.38	112.53
3	G	260	UFP	F5-C5-C4	2.03	122.33	118.56
2	G	259	FAD	C2A-N1A-C6A	2.06	122.45	118.77
2	G	259	FAD	C4X-N5-C5X	2.08	119.15	116.76
2	F	259	FAD	O2A-PA-O3P	2.09	114.58	105.09
2	G	259	FAD	C1'-N10-C9A	2.13	121.26	118.86
3	E	260	UFP	O3P-P-O2P	2.16	115.60	107.38
3	B	260	UFP	C2'-C1'-N1	2.21	119.53	114.16
2	H	259	FAD	C2B-C1B-N9A	2.22	117.68	114.29
2	D	259	FAD	C1'-N10-C9A	2.22	121.35	118.86
2	B	259	FAD	O2A-PA-O1A	2.22	124.55	112.53
2	A	259	FAD	C1'-N10-C9A	2.28	121.42	118.86
2	C	259	FAD	O2A-PA-O1A	2.29	124.92	112.53
3	D	260	UFP	C2'-C3'-C4'	2.34	107.62	102.77
2	E	259	FAD	C5X-C9A-N10	2.38	119.42	117.62
2	E	259	FAD	O3P-P-O5'	2.42	109.37	102.94
2	H	259	FAD	O2A-PA-O1A	2.46	125.85	112.53
3	G	260	UFP	C2'-C1'-N1	2.47	120.16	114.16
3	F	260	UFP	C2'-C1'-N1	2.48	120.19	114.16
2	C	259	FAD	O3P-P-O5'	2.52	109.62	102.94
2	E	259	FAD	O2A-PA-O1A	2.53	126.22	112.53
2	E	259	FAD	C2B-C1B-N9A	2.55	118.19	114.29
2	A	259	FAD	C5X-C9A-N10	2.56	119.56	117.62
2	A	259	FAD	C2B-C1B-N9A	2.56	118.20	114.29
3	C	260	UFP	O4'-C1'-C2'	2.58	111.41	106.27
2	B	259	FAD	O3P-P-O5'	2.62	109.89	102.94
2	H	259	FAD	C4X-N5-C5X	2.65	119.81	116.76
2	C	259	FAD	C4X-N5-C5X	2.66	119.82	116.76
2	B	259	FAD	C4-C4X-N5	2.72	122.02	118.72
2	D	259	FAD	O2A-PA-O1A	2.79	127.66	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	259	FAD	O3P-P-O5'	2.86	110.51	102.94
2	H	259	FAD	C1'-N10-C9A	2.92	122.14	118.86
2	C	259	FAD	C4-C4X-N5	3.00	122.36	118.72
3	B	260	UFP	F5-C5-C4	3.06	124.24	118.56
3	E	260	UFP	O4'-C1'-C2'	3.10	112.44	106.27
2	H	259	FAD	C5X-C9A-N10	3.10	119.98	117.62
3	F	260	UFP	O4'-C1'-C2'	3.18	112.61	106.27
2	H	259	FAD	C4-C4X-N5	3.18	122.58	118.72
2	F	259	FAD	C4X-N5-C5X	3.26	120.52	116.76
2	E	259	FAD	C4-C4X-N5	3.35	122.79	118.72
2	D	259	FAD	C4X-N5-C5X	3.37	120.64	116.76
3	D	260	UFP	F5-C5-C4	3.39	124.85	118.56
3	A	260	UFP	F5-C5-C4	3.41	124.89	118.56
2	B	259	FAD	C1'-N10-C9A	3.45	122.74	118.86
2	D	259	FAD	C5X-C9A-N10	3.54	120.31	117.62
2	E	259	FAD	C4X-N5-C5X	3.54	120.83	116.76
3	B	260	UFP	O4'-C1'-C2'	3.60	113.45	106.27
3	H	260	UFP	O4'-C1'-C2'	3.74	113.73	106.27
2	G	259	FAD	C5X-C9A-N10	3.92	120.60	117.62
2	D	259	FAD	O3P-P-O5'	3.92	113.35	102.94
2	A	259	FAD	O3P-P-O5'	4.01	113.56	102.94
3	D	260	UFP	C2'-C1'-N1	4.04	123.97	114.16
2	B	259	FAD	C5X-C9A-N10	4.18	120.80	117.62
2	A	259	FAD	C4-N3-C2	4.30	118.97	115.25
3	G	260	UFP	O4'-C1'-C2'	4.34	114.93	106.27
3	D	260	UFP	O4'-C1'-C2'	4.34	114.94	106.27
2	E	259	FAD	C4-N3-C2	4.80	119.39	115.25
2	F	259	FAD	C4-N3-C2	5.25	119.78	115.25
3	F	260	UFP	C4-N3-C2	5.50	120.00	115.25
2	D	259	FAD	C4-N3-C2	5.73	120.20	115.25
2	C	259	FAD	C4-N3-C2	5.89	120.34	115.25
2	B	259	FAD	C4-N3-C2	5.94	120.38	115.25
3	H	260	UFP	C4-N3-C2	6.55	120.91	115.25
2	H	259	FAD	C4-N3-C2	6.56	120.92	115.25
3	E	260	UFP	C4-N3-C2	6.68	121.02	115.25
2	G	259	FAD	C4-N3-C2	6.74	121.07	115.25
3	D	260	UFP	C4-N3-C2	6.89	121.20	115.25
3	D	260	UFP	O4'-C1'-N1	7.31	120.38	107.72
3	A	260	UFP	C4-N3-C2	7.66	121.86	115.25
3	C	260	UFP	C4-N3-C2	7.68	121.89	115.25
3	G	260	UFP	C4-N3-C2	7.73	121.93	115.25
3	B	260	UFP	C4-N3-C2	7.80	121.98	115.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	260	UFP	O4'-C1'-N1	8.37	122.21	107.72
3	H	260	UFP	O4'-C1'-N1	8.70	122.79	107.72
3	B	260	UFP	O4'-C1'-N1	8.89	123.12	107.72
3	C	260	UFP	O4'-C1'-N1	9.14	123.55	107.72
3	F	260	UFP	O4'-C1'-N1	9.82	124.72	107.72
3	E	260	UFP	O4'-C1'-N1	10.13	125.26	107.72
3	A	260	UFP	O4'-C1'-N1	10.86	126.52	107.72

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	260	UFP	C1'
3	F	260	UFP	C1'

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	260	UFP	2	0
3	B	260	UFP	2	0
3	C	260	UFP	1	0
3	D	260	UFP	3	0
3	E	260	UFP	2	0
3	F	260	UFP	2	0
3	G	260	UFP	4	0
3	H	260	UFP	1	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	246/258 (95%)	0.12	9 (3%) 45 49	9, 21, 36, 49	0
1	B	239/258 (92%)	0.20	11 (4%) 36 39	9, 19, 38, 49	1 (0%)
1	C	243/258 (94%)	0.17	15 (6%) 24 27	10, 23, 43, 51	0
1	D	242/258 (93%)	0.31	15 (6%) 24 27	10, 22, 41, 48	1 (0%)
1	E	244/258 (94%)	0.20	16 (6%) 22 24	12, 24, 44, 54	0
1	F	242/258 (93%)	0.47	23 (9%) 10 12	11, 26, 54, 63	1 (0%)
1	G	245/258 (94%)	0.45	20 (8%) 14 16	13, 27, 48, 53	1 (0%)
1	H	243/258 (94%)	0.03	8 (3%) 50 53	10, 20, 40, 48	0
All	All	1944/2064 (94%)	0.24	117 (6%) 25 28	9, 23, 44, 63	4 (0%)

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	155	ALA	5.2
1	F	154	PHE	5.2
1	E	52	PRO	5.1
1	D	53	LYS	5.0
1	D	124	ASP	4.8
1	D	236	ALA	4.7
1	E	155	ALA	4.6
1	A	52	PRO	4.6
1	H	245	PRO	4.5
1	D	54	THR	4.4
1	A	247	ALA	4.2
1	D	155	ALA	4.2
1	C	235	LEU	4.0
1	C	238	GLY	3.7
1	F	161	ILE	3.6
1	G	236	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	50	PRO	3.5
1	G	134	GLU	3.5
1	D	51	ASN	3.5
1	F	138	ALA	3.4
1	F	127	ASP	3.4
1	G	51	ASN	3.4
1	D	52	PRO	3.3
1	A	236	ALA	3.3
1	H	155	ALA	3.3
1	F	148	ALA	3.2
1	G	127	ASP	3.2
1	G	156	ASP	3.2
1	C	2	ALA	3.2
1	C	156	ASP	3.1
1	F	159	ASN	3.1
1	G	50	PRO	3.1
1	E	53	LYS	3.1
1	D	161	ILE	3.1
1	D	228	ALA	3.1
1	B	160	ALA	3.0
1	G	130	HIS	3.0
1	C	236	ALA	3.0
1	C	158	PRO	3.0
1	F	163	ARG	3.0
1	G	128	LEU	3.0
1	F	130	HIS	2.9
1	E	236	ALA	2.9
1	C	162	LEU	2.9
1	E	156	ASP	2.9
1	E	231	GLU	2.8
1	H	236	ALA	2.8
1	C	124	ASP	2.8
1	A	50	PRO	2.8
1	A	55	ALA	2.7
1	F	112	LYS	2.7
1	D	50	PRO	2.7
1	E	51	ASN	2.7
1	F	160	ALA	2.7
1	E	158	PRO	2.7
1	F	153	LYS	2.7
1	D	156	ASP	2.7
1	F	236	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	22	ASP	2.7
1	G	113	ASP	2.7
1	F	164	ARG	2.7
1	F	156	ASP	2.6
1	B	153	LYS	2.6
1	G	150	LEU	2.6
1	B	161	ILE	2.6
1	B	50	PRO	2.6
1	F	152	ALA	2.6
1	B	159	ASN	2.5
1	B	21	PRO	2.5
1	C	161	ILE	2.5
1	C	231	GLU	2.5
1	C	65	ILE	2.5
1	C	155	ALA	2.5
1	F	147	LEU	2.4
1	H	162	LEU	2.4
1	E	127	ASP	2.4
1	G	112	LYS	2.4
1	C	50	PRO	2.4
1	E	54	THR	2.4
1	G	155	ALA	2.4
1	H	156	ASP	2.4
1	F	126	ALA	2.4
1	E	235	LEU	2.4
1	A	2	ALA	2.4
1	B	124	ASP	2.4
1	A	51	ASN	2.3
1	G	162	LEU	2.3
1	D	152	ALA	2.3
1	E	221	ALA	2.3
1	G	152	ALA	2.3
1	D	67	VAL	2.3
1	H	235	LEU	2.3
1	D	164	ARG	2.3
1	C	239	THR	2.3
1	G	126	ALA	2.3
1	G	108	TYR	2.3
1	G	114	SER	2.2
1	B	164	ARG	2.2
1	E	22	ASP	2.2
1	H	243	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	154	PHE	2.2
1	H	244	SER	2.2
1	F	124	ASP	2.2
1	F	128	LEU	2.2
1	G	185	VAL	2.2
1	D	22	ASP	2.2
1	F	66	ASP	2.2
1	E	161	ILE	2.1
1	G	94	ILE	2.1
1	G	133	THR	2.1
1	F	162	LEU	2.1
1	B	163	ARG	2.1
1	A	53	LYS	2.0
1	A	155	ALA	2.0
1	B	162	LEU	2.0
1	E	238	GLY	2.0
1	F	238	GLY	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	C	261	6/6	0.81	0.17	0.56	32,34,35,35	0
2	FAD	G	259	53/53	0.95	0.13	-0.29	18,25,28,30	0
2	FAD	F	259	53/53	0.94	0.13	-0.31	21,27,31,32	0
2	FAD	D	259	53/53	0.95	0.11	-0.40	14,22,25,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	UFP	A	260	21/21	0.97	0.09	-0.43	11,15,19,20	0
3	UFP	H	260	21/21	0.97	0.09	-0.44	11,15,19,24	0
3	UFP	C	260	21/21	0.98	0.09	-0.49	10,12,15,15	0
2	FAD	A	259	53/53	0.96	0.11	-0.60	14,19,25,27	0
3	UFP	B	260	21/21	0.98	0.08	-0.66	11,16,17,17	0
2	FAD	H	259	53/53	0.96	0.10	-0.68	16,20,26,28	0
2	FAD	C	259	53/53	0.96	0.10	-0.68	14,20,25,27	0
2	FAD	E	259	53/53	0.96	0.09	-0.71	14,22,26,29	0
2	FAD	B	259	53/53	0.96	0.10	-0.72	14,18,24,26	0
3	UFP	D	260	21/21	0.98	0.08	-1.02	11,13,14,16	0
3	UFP	G	260	21/21	0.97	0.09	-1.20	17,21,24,27	0
3	UFP	F	260	21/21	0.98	0.08	-1.33	17,20,21,26	0
3	UFP	E	260	21/21	0.98	0.07	-1.38	11,16,20,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.