Full wwPDB X-ray Structure Validation Report (i)

Sep 8, 2016 – 11:23 AM EDT

PDB ID	:	5K3I
Title	:	Crystal structure of Acyl-CoA oxidase-1 in Caenorhabditis elegans complexed with FAD and ATP
Authors	:	Zhang, X.; Li, K.; Jones, R.A.; Bruner, S.D.; Butcher, R.A.
Deposited on	:	2016-05-19
Resolution	:	2.68 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

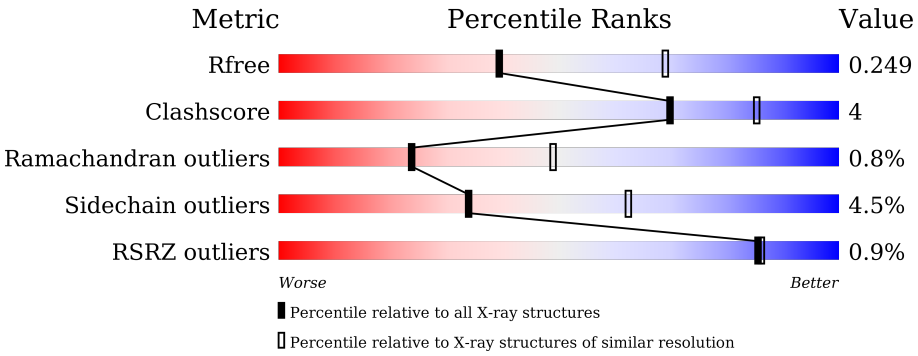
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 2.68 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	2780 (2.70-2.66)
Clashscore	102246	3138 (2.70-2.66)
Ramachandran outliers	100387	3089 (2.70-2.66)
Sidechain outliers	100360	3089 (2.70-2.66)
RSRZ outliers	91569	2789 (2.70-2.66)

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. 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	684	84% 11% • •
1	B	684	2% 85% 11% • •
1	C	684	85% 9% • 5%
1	D	684	84% 10% • 5%
1	E	684	84% 11% • •
1	F	684	83% 10% • 5%

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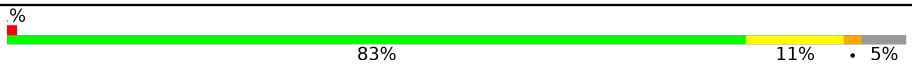
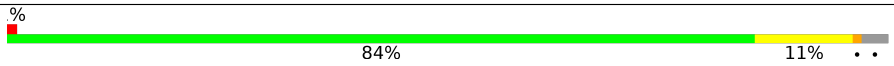
Mol	Chain	Length	Quality of chain
1	G	684	
1	H	684	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 42900 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 Acyl-coenzyme A oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	661	Total	C	N	O	S	0	0	0
			5236	3321	921	966	28			
1	B	657	Total	C	N	O	S	0	0	0
			5211	3307	916	960	28			
1	C	650	Total	C	N	O	S	0	0	0
			5166	3281	907	950	28			
1	D	653	Total	C	N	O	S	0	0	0
			5188	3294	911	955	28			
1	E	661	Total	C	N	O	S	0	0	0
			5236	3321	921	966	28			
1	F	651	Total	C	N	O	S	0	0	0
			5164	3275	906	955	28			
1	G	653	Total	C	N	O	S	0	0	0
			5182	3288	911	955	28			
1	H	661	Total	C	N	O	S	0	0	0
			5236	3321	921	966	28			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	434	ALA	GLU	engineered mutation	UNP O62140
A	675	HIS	-	expression tag	UNP O62140
A	676	HIS	-	expression tag	UNP O62140
A	677	HIS	-	expression tag	UNP O62140
A	678	HIS	-	expression tag	UNP O62140
A	679	HIS	-	expression tag	UNP O62140
A	680	HIS	-	expression tag	UNP O62140
A	681	HIS	-	expression tag	UNP O62140
A	682	HIS	-	expression tag	UNP O62140
A	683	HIS	-	expression tag	UNP O62140
A	684	HIS	-	expression tag	UNP O62140
B	434	ALA	GLU	engineered mutation	UNP O62140
B	675	HIS	-	expression tag	UNP O62140

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Chain	Residue	Modelled	Actual	Comment	Reference
B	676	HIS	-	expression tag	UNP O62140
B	677	HIS	-	expression tag	UNP O62140
B	678	HIS	-	expression tag	UNP O62140
B	679	HIS	-	expression tag	UNP O62140
B	680	HIS	-	expression tag	UNP O62140
B	681	HIS	-	expression tag	UNP O62140
B	682	HIS	-	expression tag	UNP O62140
B	683	HIS	-	expression tag	UNP O62140
B	684	HIS	-	expression tag	UNP O62140
C	434	ALA	GLU	engineered mutation	UNP O62140
C	675	HIS	-	expression tag	UNP O62140
C	676	HIS	-	expression tag	UNP O62140
C	677	HIS	-	expression tag	UNP O62140
C	678	HIS	-	expression tag	UNP O62140
C	679	HIS	-	expression tag	UNP O62140
C	680	HIS	-	expression tag	UNP O62140
C	681	HIS	-	expression tag	UNP O62140
C	682	HIS	-	expression tag	UNP O62140
C	683	HIS	-	expression tag	UNP O62140
C	684	HIS	-	expression tag	UNP O62140
D	434	ALA	GLU	engineered mutation	UNP O62140
D	675	HIS	-	expression tag	UNP O62140
D	676	HIS	-	expression tag	UNP O62140
D	677	HIS	-	expression tag	UNP O62140
D	678	HIS	-	expression tag	UNP O62140
D	679	HIS	-	expression tag	UNP O62140
D	680	HIS	-	expression tag	UNP O62140
D	681	HIS	-	expression tag	UNP O62140
D	682	HIS	-	expression tag	UNP O62140
D	683	HIS	-	expression tag	UNP O62140
D	684	HIS	-	expression tag	UNP O62140
E	434	ALA	GLU	engineered mutation	UNP O62140
E	675	HIS	-	expression tag	UNP O62140
E	676	HIS	-	expression tag	UNP O62140
E	677	HIS	-	expression tag	UNP O62140
E	678	HIS	-	expression tag	UNP O62140
E	679	HIS	-	expression tag	UNP O62140
E	680	HIS	-	expression tag	UNP O62140
E	681	HIS	-	expression tag	UNP O62140
E	682	HIS	-	expression tag	UNP O62140
E	683	HIS	-	expression tag	UNP O62140
E	684	HIS	-	expression tag	UNP O62140

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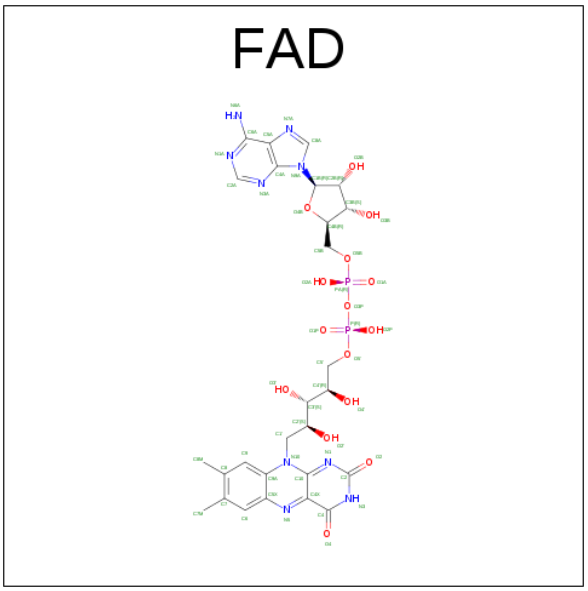
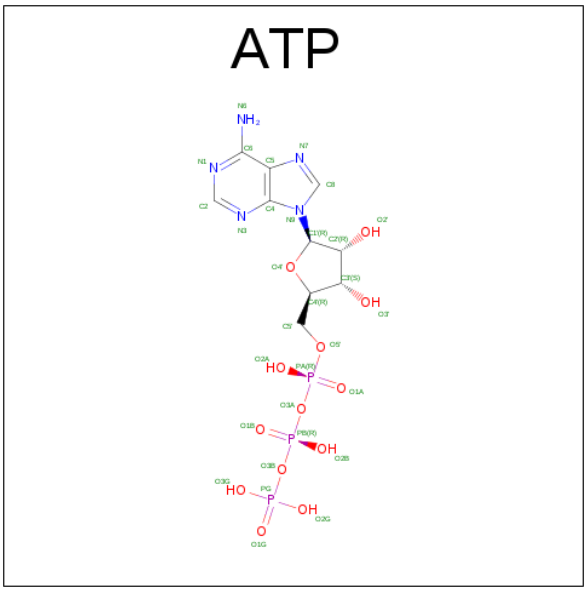
Chain	Residue	Modelled	Actual	Comment	Reference
F	434	ALA	GLU	engineered mutation	UNP O62140
F	675	HIS	-	expression tag	UNP O62140
F	676	HIS	-	expression tag	UNP O62140
F	677	HIS	-	expression tag	UNP O62140
F	678	HIS	-	expression tag	UNP O62140
F	679	HIS	-	expression tag	UNP O62140
F	680	HIS	-	expression tag	UNP O62140
F	681	HIS	-	expression tag	UNP O62140
F	682	HIS	-	expression tag	UNP O62140
F	683	HIS	-	expression tag	UNP O62140
F	684	HIS	-	expression tag	UNP O62140
G	434	ALA	GLU	engineered mutation	UNP O62140
G	675	HIS	-	expression tag	UNP O62140
G	676	HIS	-	expression tag	UNP O62140
G	677	HIS	-	expression tag	UNP O62140
G	678	HIS	-	expression tag	UNP O62140
G	679	HIS	-	expression tag	UNP O62140
G	680	HIS	-	expression tag	UNP O62140
G	681	HIS	-	expression tag	UNP O62140
G	682	HIS	-	expression tag	UNP O62140
G	683	HIS	-	expression tag	UNP O62140
G	684	HIS	-	expression tag	UNP O62140
H	434	ALA	GLU	engineered mutation	UNP O62140
H	675	HIS	-	expression tag	UNP O62140
H	676	HIS	-	expression tag	UNP O62140
H	677	HIS	-	expression tag	UNP O62140
H	678	HIS	-	expression tag	UNP O62140
H	679	HIS	-	expression tag	UNP O62140
H	680	HIS	-	expression tag	UNP O62140
H	681	HIS	-	expression tag	UNP O62140
H	682	HIS	-	expression tag	UNP O62140
H	683	HIS	-	expression tag	UNP O62140
H	684	HIS	-	expression tag	UNP O62140

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



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

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	H	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

- Molecule 5 is water.

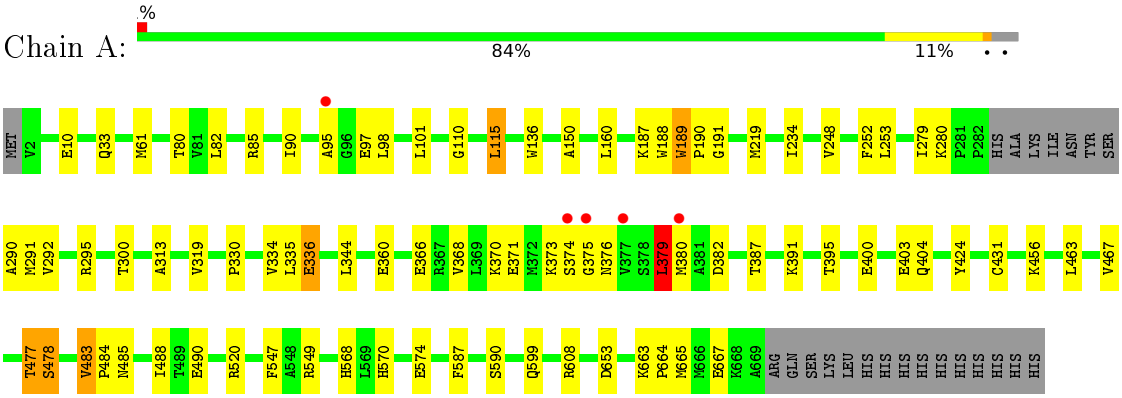
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	102	Total O 102 102	0	0
5	B	69	Total O 69 69	0	0
5	C	58	Total O 58 58	0	0
5	D	76	Total O 76 76	0	0
5	E	82	Total O 82 82	0	0
5	F	58	Total O 58 58	0	0
5	G	71	Total O 71 71	0	0
5	H	85	Total O 85 85	0	0

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.

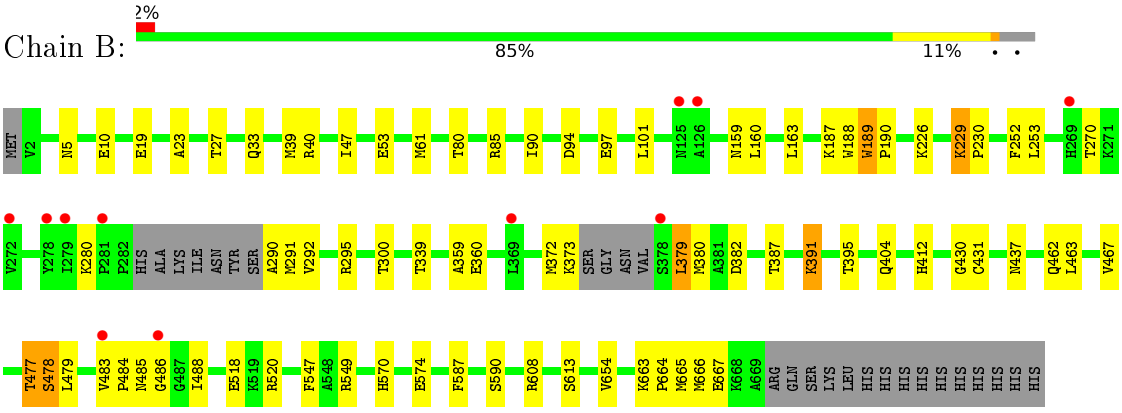
- Molecule 1: Acyl-coenzyme A oxidase

Chain A:



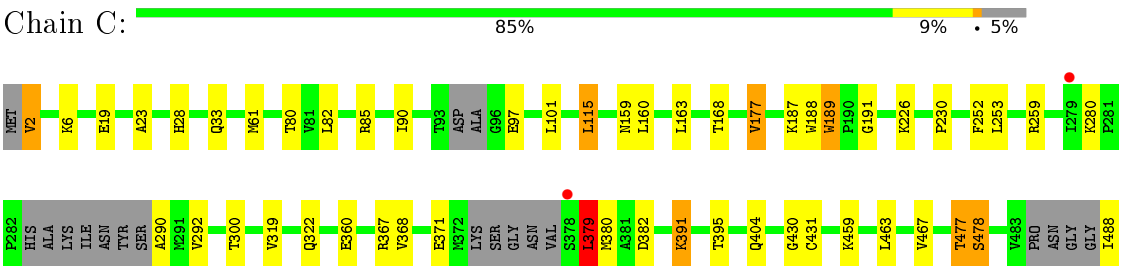
- Molecule 1: Acyl-coenzyme A oxidase

Chain B:



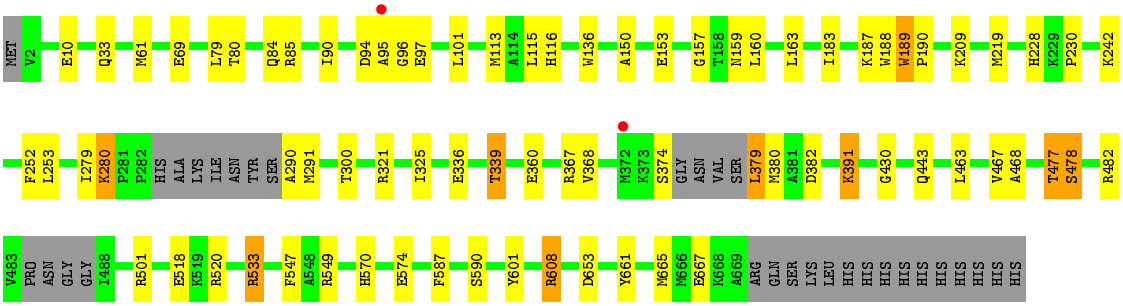
- Molecule 1: Acyl-coenzyme A oxidase

Chain C:



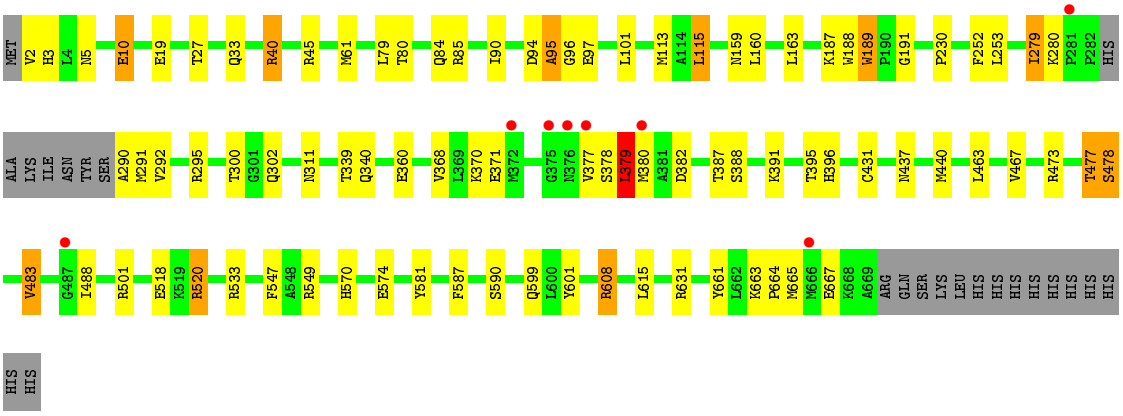
• Molecule 1: Acyl-coenzyme A oxidase

Chain D:



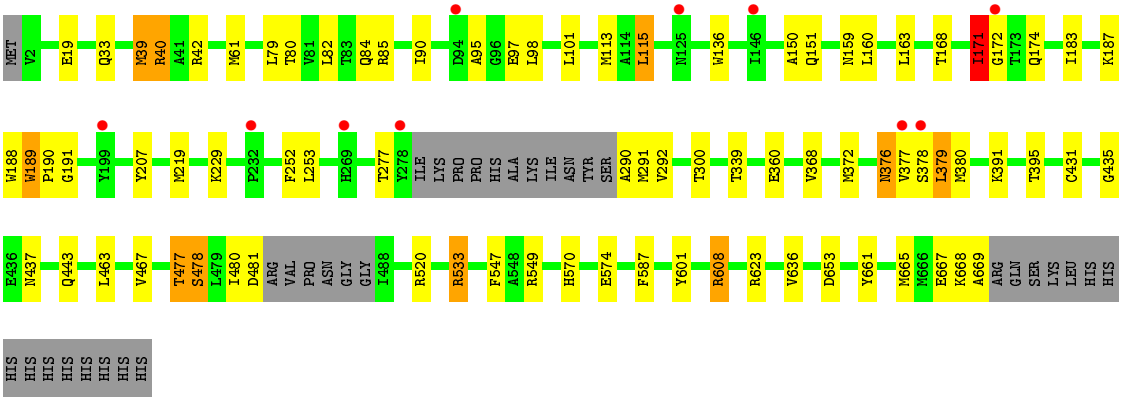
• Molecule 1: Acyl-coenzyme A oxidase

Chain E:



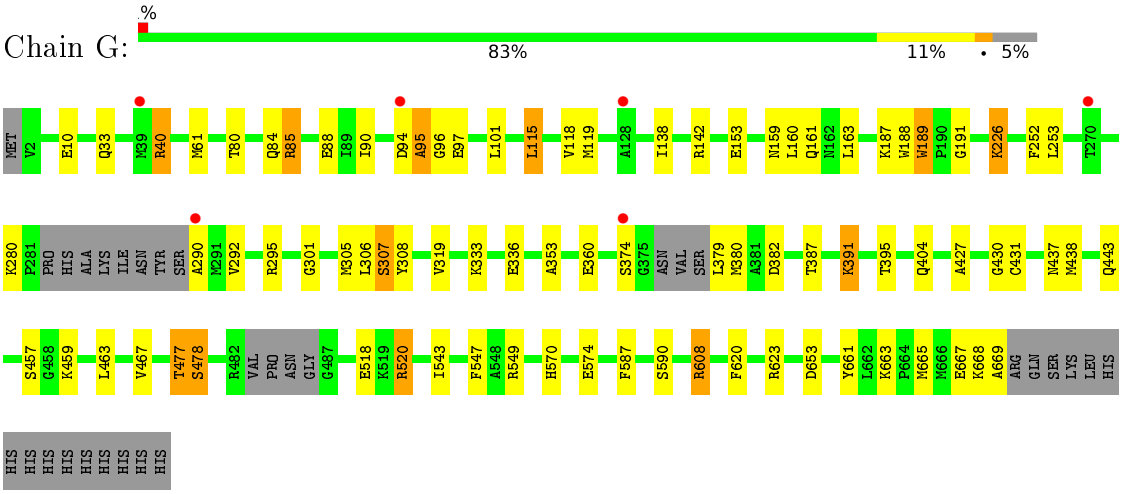
• Molecule 1: Acyl-coenzyme A oxidase

Chain F:



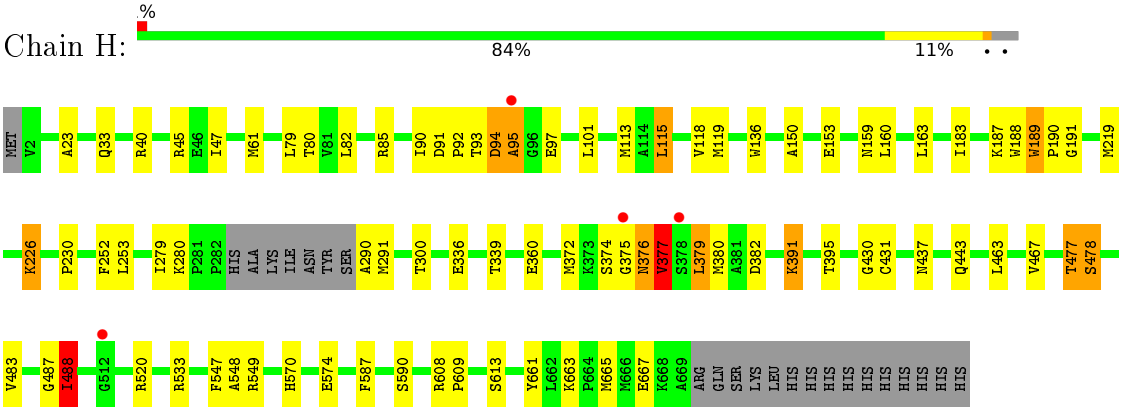
• Molecule 1: Acyl-coenzyme A oxidase

Chain G:



- Molecule 1: Acyl-coenzyme A oxidase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	152.34Å 141.50Å 154.97Å 90.00° 116.76° 90.00°	Depositor
Resolution (Å)	38.74 – 2.68 38.74 – 2.68	Depositor EDS
% Data completeness (in resolution range)	99.6 (38.74-2.68) 94.1 (38.74-2.68)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	2.50 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.217 , 0.232 0.234 , 0.249	Depositor DCC
R_{free} test set	8012 reflections (4.91%)	DCC
Wilson B-factor (Å^2)	30.2	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 2.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.176 for l,-k,h	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	42900	wwPDB-VP
Average B, all atoms (Å^2)	34.0	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 52.22 % 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 5.0142e-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, FAD, ATP

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	0.32	0/5343	0.58	0/7224
1	B	0.32	0/5317	0.56	0/7187
1	C	0.31	0/5269	0.57	0/7119
1	D	0.31	0/5292	0.52	0/7151
1	E	0.31	0/5343	0.54	0/7224
1	F	0.31	0/5267	0.54	0/7118
1	G	0.30	0/5285	0.55	0/7139
1	H	0.31	0/5343	0.54	0/7224
All	All	0.31	0/42459	0.55	0/57386

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	95	ALA	Peptide

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	5236	0	5260	49	0
1	B	5211	0	5236	43	0
1	C	5166	0	5193	55	0
1	D	5188	0	5216	47	0
1	E	5236	0	5260	56	0
1	F	5164	0	5180	55	0
1	G	5182	0	5206	52	0
1	H	5236	0	5260	53	0
2	A	53	0	29	1	0
2	B	53	0	30	1	0
2	C	53	0	30	1	0
2	D	53	0	30	1	0
2	E	53	0	30	0	0
2	F	53	0	30	4	0
2	G	53	0	30	0	0
2	H	53	0	30	2	0
3	A	31	0	12	2	0
3	B	31	0	12	0	0
3	C	31	0	12	0	0
3	D	31	0	12	1	0
3	E	31	0	12	0	0
3	F	31	0	12	0	0
3	G	31	0	12	2	0
3	H	31	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	102	0	0	4	0
5	B	69	0	0	3	0
5	C	58	0	0	7	0
5	D	76	0	0	5	0
5	E	82	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	58	0	0	4	0
5	G	71	0	0	5	0
5	H	85	0	0	1	0
All	All	42900	0	42146	378	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 (378) 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:520:ARG:NH2	1:E:483:VAL:HG13	1.48	1.26
1:C:520:ARG:HH21	1:E:483:VAL:HG13	1.05	1.00
1:B:47:ILE:HD11	1:B:97:GLU:HG2	1.43	0.99
1:F:171:ILE:HG23	1:F:172:GLY:H	1.23	0.99
1:C:520:ARG:NH2	1:E:483:VAL:CG1	2.33	0.91
1:H:336:GLU:OE1	1:H:608:ARG:NH2	2.07	0.86
1:D:95:ALA:N	1:D:96:GLY:HA3	1.94	0.81
1:H:47:ILE:HD11	1:H:97:GLU:HG2	1.61	0.81
1:B:90:ILE:HD12	1:B:97:GLU:HB3	1.68	0.76
1:F:478:SER:HB2	1:F:587:PHE:CE2	2.22	0.74
1:A:478:SER:HB2	1:A:587:PHE:CE2	2.23	0.73
1:G:478:SER:HB2	1:G:587:PHE:CE2	2.23	0.73
1:E:478:SER:HB2	1:E:587:PHE:CE2	2.24	0.73
1:C:478:SER:HB2	1:C:587:PHE:CE2	2.24	0.72
1:B:478:SER:HB2	1:B:587:PHE:CE2	2.25	0.72
1:F:171:ILE:HG23	1:F:172:GLY:N	2.02	0.72
1:D:478:SER:HB2	1:D:587:PHE:CE2	2.25	0.71
1:G:438:MET:SD	5:G:867:HOH:O	2.48	0.71
1:H:478:SER:HB2	1:H:587:PHE:CE2	2.26	0.71
5:A:837:HOH:O	1:B:666:MET:SD	2.49	0.70
1:D:90:ILE:HG13	1:D:101:LEU:HD22	1.74	0.69
1:D:90:ILE:HD12	1:D:97:GLU:HB3	1.74	0.68
1:G:115:LEU:HD13	1:G:191:GLY:HA3	1.75	0.67
1:B:90:ILE:HG13	1:B:101:LEU:HD22	1.75	0.67
1:E:295:ARG:HB3	1:E:387:THR:HG23	1.75	0.67
1:H:90:ILE:HG13	1:H:101:LEU:HD22	1.76	0.67
1:A:400:GLU:O	1:A:404:GLN:HG2	1.95	0.66
1:B:295:ARG:HB3	1:B:387:THR:HG23	1.77	0.66
1:B:479:LEU:HB3	1:B:483:VAL:HG23	1.77	0.66
1:F:95:ALA:HB1	1:F:98:LEU:H	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:LEU:HG	1:A:335:LEU:O	1.94	0.66
1:B:290:ALA:HA	1:B:292:VAL:H	1.60	0.66
1:E:90:ILE:HG13	1:E:101:LEU:HD22	1.78	0.66
1:A:295:ARG:HB3	1:A:387:THR:HG23	1.78	0.65
1:G:90:ILE:HG13	1:G:101:LEU:HD22	1.77	0.65
1:F:623:ARG:NH1	5:F:801:HOH:O	2.30	0.64
1:C:520:ARG:HB2	1:C:520:ARG:HH11	1.63	0.64
1:F:90:ILE:HG13	1:F:101:LEU:HD22	1.77	0.64
1:G:301:GLY:O	1:G:305:MET:HG3	1.97	0.63
1:A:290:ALA:HA	1:A:292:VAL:H	1.63	0.63
1:B:477:THR:O	1:B:478:SER:HB3	1.99	0.63
1:F:19:GLU:OE1	1:F:608:ARG:NH1	2.32	0.63
1:C:115:LEU:HD13	1:C:191:GLY:HA3	1.81	0.63
1:C:19:GLU:OE1	1:C:608:ARG:NH1	2.32	0.63
1:G:336:GLU:OE2	1:G:608:ARG:NH1	2.32	0.62
1:G:85:ARG:NH1	1:G:88:GLU:OE2	2.31	0.62
1:E:2:VAL:HG13	1:E:3:HIS:H	1.63	0.62
2:F:701:FAD:H8A	2:F:701:FAD:O1A	1.99	0.62
1:A:477:THR:O	1:A:478:SER:HB3	2.00	0.62
1:E:19:GLU:OE1	1:E:608:ARG:NH1	2.32	0.62
3:A:702:ATP:H1'	1:B:404:GLN:NE2	2.14	0.62
1:C:477:THR:O	1:C:478:SER:HB3	2.00	0.62
1:C:90:ILE:HG13	1:C:101:LEU:HD22	1.81	0.62
1:C:90:ILE:HD12	1:C:97:GLU:HB3	1.81	0.61
1:C:488:ILE:N	5:C:803:HOH:O	2.33	0.61
1:H:90:ILE:HG23	1:H:97:GLU:HB3	1.83	0.61
1:G:295:ARG:HB3	1:G:387:THR:HG23	1.81	0.61
1:A:403:GLU:HG2	1:A:424:TYR:CD1	2.35	0.61
1:B:19:GLU:OE1	1:B:608:ARG:NH1	2.33	0.61
1:E:10:GLU:N	1:E:10:GLU:OE2	2.33	0.61
1:A:290:ALA:N	5:A:807:HOH:O	2.34	0.60
1:A:90:ILE:HD12	1:A:97:GLU:HB3	1.82	0.60
1:E:40:ARG:NH2	1:E:94:ASP:OD1	2.34	0.60
1:A:90:ILE:HG13	1:A:101:LEU:HD22	1.82	0.60
1:C:259:ARG:HG3	5:C:805:HOH:O	2.01	0.60
1:F:95:ALA:HA	1:F:97:GLU:H	1.66	0.60
1:B:40:ARG:NH2	1:B:94:ASP:OD1	2.34	0.60
1:A:115:LEU:HD13	1:A:191:GLY:HA3	1.84	0.59
1:E:302:GLN:HG2	5:E:809:HOH:O	2.02	0.59
1:H:608:ARG:HB3	1:H:609:PRO:HD3	1.84	0.59
1:A:80:THR:HG22	1:B:665:MET:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:115:LEU:HD13	1:E:191:GLY:HA3	1.84	0.58
1:E:520:ARG:NH2	5:E:803:HOH:O	2.36	0.58
1:D:336:GLU:OE2	1:D:608:ARG:NH1	2.36	0.58
1:A:95:ALA:HB1	1:A:98:LEU:HB3	1.84	0.58
1:C:80:THR:HG22	1:D:665:MET:HB2	1.86	0.58
1:D:501:ARG:NH2	5:D:907:HOH:O	2.37	0.58
1:D:90:ILE:CD1	1:D:97:GLU:HB3	2.33	0.58
1:H:94:ASP:HB3	1:H:97:GLU:H	1.68	0.58
1:D:468:ALA:N	5:D:905:HOH:O	2.35	0.58
1:G:138:ILE:HB	5:G:803:HOH:O	2.03	0.58
3:A:702:ATP:H1'	1:B:404:GLN:HE22	1.69	0.57
1:C:521:GLU:HG2	1:D:325:ILE:O	2.04	0.57
1:E:396:HIS:NE2	5:E:801:HOH:O	2.33	0.57
1:A:665:MET:HB2	1:B:80:THR:HG22	1.86	0.57
1:B:47:ILE:HD11	1:B:97:GLU:CG	2.28	0.57
2:C:701:FAD:H8A	2:C:701:FAD:O1A	2.04	0.57
1:F:160:LEU:HA	1:F:163:LEU:HG	1.88	0.56
1:G:623:ARG:NH1	5:G:805:HOH:O	2.38	0.56
1:H:90:ILE:HD12	1:H:97:GLU:HB3	1.85	0.56
1:C:501:ARG:NE	5:C:809:HOH:O	2.38	0.56
1:C:459:LYS:HE3	1:E:599:GLN:OE1	2.06	0.56
1:C:160:LEU:HA	1:C:163:LEU:HG	1.87	0.55
1:G:160:LEU:HA	1:G:163:LEU:HG	1.89	0.55
1:G:95:ALA:HB3	1:G:96:GLY:HA3	1.88	0.55
1:B:463:LEU:HD22	1:B:467:VAL:HG13	1.88	0.55
1:G:90:ILE:HD12	1:G:97:GLU:HB3	1.89	0.55
1:H:160:LEU:HA	1:H:163:LEU:HG	1.88	0.55
1:F:188:TRP:O	1:F:189:TRP:HB2	2.07	0.54
1:G:187:LYS:HB2	1:G:253:LEU:HB3	1.89	0.54
1:E:360:GLU:OE1	1:E:549:ARG:NH1	2.41	0.54
1:E:665:MET:HB2	1:F:80:THR:HG22	1.89	0.54
1:A:485:ASN:ND2	1:A:490:GLU:HG2	2.21	0.54
1:E:160:LEU:HA	1:E:163:LEU:HG	1.89	0.54
1:F:368:VAL:HB	1:F:376:ASN:OD1	2.07	0.54
1:D:209:LYS:N	5:D:910:HOH:O	2.40	0.54
1:E:90:ILE:HD12	1:E:97:GLU:HB3	1.90	0.53
1:C:520:ARG:CZ	1:E:483:VAL:HG13	2.30	0.53
1:F:90:ILE:HD12	1:F:97:GLU:HB3	1.90	0.53
1:F:95:ALA:HA	1:F:97:GLU:N	2.24	0.53
1:H:159:ASN:O	1:H:160:LEU:HB2	2.08	0.53
1:F:187:LYS:HB2	1:F:253:LEU:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:LEU:HA	1:B:163:LEU:HG	1.90	0.53
1:E:19:GLU:CD	1:E:608:ARG:HH12	2.12	0.53
1:H:188:TRP:O	1:H:189:TRP:HB2	2.08	0.53
1:D:367:ARG:NH2	5:D:913:HOH:O	2.42	0.52
1:E:95:ALA:HB3	1:E:96:GLY:HA3	1.90	0.52
2:B:702:FAD:H8A	2:B:702:FAD:O1A	2.08	0.52
1:F:39:MET:HA	1:F:42:ARG:HG2	1.90	0.52
1:B:159:ASN:O	1:B:160:LEU:HB2	2.09	0.52
1:B:484:PRO:O	1:B:485:ASN:HB2	2.09	0.52
1:C:159:ASN:O	1:C:160:LEU:HB2	2.09	0.52
1:F:171:ILE:CG2	1:F:172:GLY:H	2.06	0.52
1:H:115:LEU:HD13	1:H:191:GLY:HA3	1.90	0.52
1:E:601:TYR:OH	1:F:533:ARG:NH1	2.42	0.52
1:E:188:TRP:O	1:E:189:TRP:HB2	2.10	0.52
1:C:19:GLU:CD	1:C:608:ARG:HH12	2.13	0.52
1:H:360:GLU:OE1	1:H:549:ARG:NH1	2.43	0.52
1:F:95:ALA:HB1	1:F:98:LEU:CB	2.40	0.52
1:B:19:GLU:CD	1:B:608:ARG:HH12	2.14	0.51
1:D:160:LEU:HA	1:D:163:LEU:HG	1.92	0.51
1:A:360:GLU:OE1	1:A:549:ARG:NH1	2.44	0.51
1:E:533:ARG:NH1	1:F:601:TYR:OH	2.43	0.51
1:G:188:TRP:O	1:G:189:TRP:HB2	2.09	0.51
1:G:290:ALA:HA	1:G:292:VAL:H	1.76	0.51
1:D:188:TRP:O	1:D:189:TRP:HB2	2.10	0.51
1:B:488:ILE:O	1:B:488:ILE:HG22	2.10	0.51
1:G:463:LEU:HD22	1:G:467:VAL:HG13	1.91	0.51
1:C:463:LEU:HD22	1:C:467:VAL:HG13	1.93	0.51
1:A:463:LEU:HD22	1:A:467:VAL:HG13	1.93	0.50
1:C:2:VAL:N	5:C:818:HOH:O	2.44	0.50
1:D:90:ILE:HD12	1:D:97:GLU:CB	2.39	0.50
1:F:19:GLU:CD	1:F:608:ARG:HH12	2.14	0.50
1:G:159:ASN:O	1:G:160:LEU:HB2	2.10	0.50
1:C:367:ARG:HG2	1:C:367:ARG:HH11	1.77	0.50
1:C:360:GLU:OE1	1:C:549:ARG:NH1	2.45	0.50
1:G:360:GLU:OE1	1:G:549:ARG:NH1	2.45	0.50
1:B:391:LYS:NZ	1:B:430:GLY:O	2.44	0.49
1:D:463:LEU:HD22	1:D:467:VAL:HG13	1.94	0.49
1:H:608:ARG:HB3	1:H:609:PRO:CD	2.42	0.49
1:C:187:LYS:O	1:C:252:PHE:HA	2.13	0.49
1:D:391:LYS:NZ	1:D:430:GLY:O	2.46	0.49
1:G:477:THR:O	1:G:478:SER:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:360:GLU:OE1	1:F:549:ARG:NH1	2.45	0.49
1:E:159:ASN:O	1:E:160:LEU:HB2	2.11	0.49
1:E:290:ALA:HA	1:E:292:VAL:H	1.78	0.49
1:B:360:GLU:OE1	1:B:549:ARG:NH1	2.46	0.49
1:F:463:LEU:HD22	1:F:467:VAL:HG13	1.93	0.49
1:H:477:THR:O	1:H:477:THR:HG23	2.13	0.49
1:E:187:LYS:HB2	1:E:253:LEU:HB3	1.94	0.49
1:F:115:LEU:HD13	1:F:191:GLY:HA3	1.94	0.49
1:B:188:TRP:O	1:B:189:TRP:HB2	2.13	0.49
1:D:95:ALA:N	1:D:96:GLY:CA	2.73	0.48
1:F:159:ASN:O	1:F:160:LEU:HB2	2.12	0.48
1:D:360:GLU:OE1	1:D:549:ARG:NH1	2.46	0.48
1:F:477:THR:O	1:F:478:SER:HB3	2.14	0.48
1:D:159:ASN:O	1:D:160:LEU:HB2	2.12	0.48
1:H:187:LYS:HB2	1:H:253:LEU:HB3	1.94	0.48
1:D:187:LYS:HB2	1:D:253:LEU:HB3	1.96	0.48
1:A:188:TRP:O	1:A:189:TRP:HB2	2.14	0.48
1:F:95:ALA:HB1	1:F:98:LEU:HB3	1.95	0.48
1:D:477:THR:O	1:D:478:SER:HB3	2.13	0.48
1:B:90:ILE:HG23	1:B:97:GLU:HB3	1.96	0.48
1:A:234:ILE:N	5:A:802:HOH:O	2.43	0.48
1:B:654:VAL:HA	5:B:838:HOH:O	2.14	0.48
1:A:568:HIS:NE2	1:G:457:SER:HB2	2.28	0.48
1:H:90:ILE:O	1:H:92:PRO:HD3	2.13	0.48
1:C:521:GLU:OE1	1:C:521:GLU:N	2.41	0.47
1:G:142:ARG:NH2	5:G:811:HOH:O	2.47	0.47
1:A:403:GLU:HG2	1:A:424:TYR:CE1	2.49	0.47
1:G:665:MET:HB2	1:H:80:THR:HG22	1.94	0.47
1:H:372:MET:HG3	1:H:377:VAL:HG23	1.96	0.47
1:E:370:LYS:HD3	1:E:371:GLU:OE1	2.14	0.47
1:E:230:PRO:HD3	1:F:653:ASP:OD1	2.15	0.47
1:B:187:LYS:O	1:B:252:PHE:HA	2.14	0.47
1:E:477:THR:O	1:E:478:SER:HB3	2.14	0.47
1:G:353:ALA:HB1	1:G:543:ILE:CG2	2.45	0.47
1:C:168:THR:HB	1:C:177:VAL:HG12	1.96	0.47
1:C:80:THR:CG2	1:D:661:TYR:HB3	2.45	0.47
1:G:404:GLN:NE2	3:H:702:ATP:H1'	2.29	0.47
1:A:599:GLN:OE1	1:G:459:LYS:HE3	2.15	0.47
1:F:372:MET:HA	1:F:376:ASN:HB2	1.96	0.47
1:C:187:LYS:HB2	1:C:253:LEU:HB3	1.96	0.47
1:E:45:ARG:NH1	5:E:804:HOH:O	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:ALA:HA	1:C:292:VAL:H	1.80	0.47
1:C:665:MET:HB2	1:D:80:THR:HG22	1.97	0.47
1:A:136:TRP:CE2	1:A:219:MET:HG2	2.50	0.46
1:E:311:ASN:OD1	1:E:615:LEU:HB3	2.14	0.46
1:A:290:ALA:CA	1:A:291:MET:HB2	2.46	0.46
1:C:322:GLN:HG2	2:D:803:FAD:O1A	2.15	0.46
1:H:487:GLY:C	1:H:488:ILE:HG23	2.36	0.46
1:A:187:LYS:O	1:A:252:PHE:HA	2.15	0.46
1:A:188:TRP:CD1	1:B:412:HIS:HE1	2.33	0.46
3:G:703:ATP:O1A	3:G:703:ATP:O1B	2.33	0.46
1:H:477:THR:O	1:H:478:SER:HB3	2.16	0.46
1:A:477:THR:O	1:A:587:PHE:O	2.34	0.46
1:A:371:GLU:O	1:A:376:ASN:HB3	2.15	0.46
1:B:229:LYS:HE3	1:B:229:LYS:HB3	1.87	0.46
1:F:290:ALA:HA	1:F:292:VAL:H	1.80	0.46
1:C:188:TRP:O	1:C:189:TRP:HB2	2.15	0.46
1:E:395:THR:HG21	1:E:431:CYS:HA	1.98	0.46
1:A:403:GLU:CG	1:A:424:TYR:CE1	2.99	0.46
1:C:395:THR:HG23	1:C:431:CYS:SG	2.56	0.46
1:H:94:ASP:CB	1:H:97:GLU:HB2	2.46	0.46
1:E:80:THR:HG21	1:F:661:TYR:HB3	1.99	0.45
1:G:95:ALA:H	1:G:97:GLU:N	2.14	0.45
1:A:187:LYS:HB2	1:A:253:LEU:HB3	1.98	0.45
1:C:19:GLU:HA	5:C:808:HOH:O	2.16	0.45
1:C:658:VAL:HG11	1:D:228:HIS:CD2	2.51	0.45
1:C:80:THR:HG21	1:D:661:TYR:HB3	1.97	0.45
1:A:366:GLU:O	1:A:370:LYS:HB2	2.16	0.45
1:D:150:ALA:HA	1:D:190:PRO:HG3	1.98	0.45
1:G:187:LYS:O	1:G:252:PHE:HA	2.16	0.45
1:H:153:GLU:HG2	1:H:187:LYS:HD3	1.97	0.45
1:H:190:PRO:HA	2:H:701:FAD:C4	2.47	0.45
1:A:485:ASN:HD21	1:A:490:GLU:HG2	1.81	0.45
1:G:395:THR:HG21	1:G:431:CYS:HA	1.98	0.45
1:C:477:THR:O	1:C:587:PHE:O	2.34	0.45
1:D:280:LYS:H	1:D:280:LYS:HG2	1.62	0.45
1:G:661:TYR:HB3	1:H:80:THR:HG21	1.99	0.45
1:A:663:LYS:HB3	1:A:664:PRO:HD3	1.99	0.45
1:A:653:ASP:OD1	1:B:230:PRO:HD3	2.16	0.45
1:F:480:ILE:O	1:F:481:ASP:HB3	2.16	0.45
1:H:136:TRP:CE2	1:H:219:MET:HG2	2.52	0.45
1:E:463:LEU:HD22	1:E:467:VAL:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ALA:HB1	1:A:344:LEU:HD21	1.99	0.44
1:A:334:VAL:C	1:A:336:GLU:H	2.21	0.44
1:D:136:TRP:CE2	1:D:219:MET:HG2	2.52	0.44
1:F:395:THR:HG21	1:F:431:CYS:HA	1.98	0.44
1:A:484:PRO:O	1:G:520:ARG:NH2	2.49	0.44
1:H:187:LYS:O	1:H:252:PHE:HA	2.17	0.44
1:C:605:GLN:HG2	5:C:837:HOH:O	2.17	0.44
1:D:477:THR:O	1:D:477:THR:HG23	2.18	0.44
1:F:168:THR:HG22	1:F:207:TYR:HB2	1.98	0.44
1:H:395:THR:HG23	1:H:431:CYS:SG	2.57	0.44
1:B:477:THR:O	1:B:587:PHE:O	2.35	0.44
1:C:391:LYS:NZ	1:C:430:GLY:O	2.48	0.44
1:E:279:ILE:HG13	1:E:279:ILE:O	2.17	0.44
1:G:118:VAL:HG12	1:G:119:MET:HG3	1.99	0.44
1:G:391:LYS:NZ	1:G:430:GLY:O	2.45	0.44
1:H:463:LEU:HD22	1:H:467:VAL:HG13	1.98	0.44
1:D:570:HIS:O	1:D:574:GLU:HG2	2.17	0.44
1:E:570:HIS:O	1:E:574:GLU:HG2	2.17	0.44
1:F:115:LEU:HD21	2:F:701:FAD:O4	2.18	0.44
1:B:188:TRP:C	1:B:190:PRO:HD3	2.38	0.44
1:B:663:LYS:HB3	1:B:664:PRO:HD3	2.00	0.44
1:G:94:ASP:HA	1:G:95:ALA:HB2	1.99	0.44
1:B:187:LYS:HB2	1:B:253:LEU:HB3	2.00	0.44
1:D:116:HIS:CD2	1:D:116:HIS:O	2.71	0.44
1:G:80:THR:HG22	1:H:665:MET:HB2	1.98	0.44
1:C:230:PRO:HD3	1:D:653:ASP:OD1	2.17	0.44
1:C:519:LYS:HE2	1:C:519:LYS:HB3	1.65	0.44
1:D:290:ALA:HA	1:D:291:MET:HB2	1.99	0.44
1:E:80:THR:HG22	1:F:665:MET:HB2	2.00	0.44
1:G:653:ASP:OD1	1:H:230:PRO:HD3	2.18	0.44
1:G:95:ALA:H	1:G:97:GLU:H	1.66	0.44
1:C:367:ARG:NH1	1:C:379:LEU:HD22	2.33	0.43
1:C:663:LYS:HB3	1:C:664:PRO:HD3	1.99	0.43
1:E:501:ARG:NH2	1:E:581:TYR:O	2.43	0.43
3:G:703:ATP:O3G	3:G:703:ATP:O1B	2.36	0.43
1:H:79:LEU:HD21	1:H:113:MET:HG3	2.00	0.43
1:H:91:ASP:C	1:H:93:THR:H	2.20	0.43
1:A:190:PRO:HA	2:A:701:FAD:C4	2.48	0.43
1:F:636:VAL:N	5:F:805:HOH:O	2.34	0.43
1:F:39:MET:H	1:F:39:MET:CE	2.31	0.43
1:H:82:LEU:HD11	1:H:101:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:47:ILE:HD11	1:H:97:GLU:CG	2.41	0.43
1:A:82:LEU:HD11	1:A:101:LEU:HD21	2.01	0.43
1:C:367:ARG:NH1	1:C:371:GLU:OE2	2.52	0.43
1:E:661:TYR:HB3	1:F:80:THR:HG21	1.99	0.43
1:F:378:SER:N	5:F:820:HOH:O	2.52	0.43
1:G:226:LYS:O	1:H:663:LYS:HD2	2.18	0.43
1:H:570:HIS:O	1:H:574:GLU:HG2	2.19	0.43
1:B:5:ASN:HA	1:B:27:THR:HG23	2.00	0.43
1:C:520:ARG:CB	1:C:520:ARG:HH11	2.31	0.43
1:E:94:ASP:HA	1:E:95:ALA:HB2	2.00	0.43
1:B:462:GLN:HG3	5:B:817:HOH:O	2.18	0.43
1:A:395:THR:HG21	1:A:431:CYS:HA	2.00	0.43
1:B:53:GLU:HA	1:B:53:GLU:OE2	2.17	0.43
1:C:653:ASP:OD1	1:D:230:PRO:HD3	2.19	0.43
1:F:39:MET:HG2	1:F:40:ARG:N	2.34	0.43
1:G:668:LYS:O	1:G:669:ALA:HB2	2.19	0.43
1:H:45:ARG:NH1	5:H:801:HOH:O	2.31	0.43
2:H:701:FAD:O1A	2:H:701:FAD:H8A	2.18	0.43
1:C:395:THR:HG21	1:C:431:CYS:HA	2.01	0.42
1:E:290:ALA:CA	1:E:291:MET:HB2	2.49	0.42
1:E:477:THR:HG23	1:E:477:THR:O	2.19	0.42
1:E:79:LEU:HD21	1:E:113:MET:HG3	2.00	0.42
1:F:477:THR:O	1:F:477:THR:HG23	2.19	0.42
1:D:153:GLU:HG2	1:D:187:LYS:HD3	2.00	0.42
1:D:187:LYS:O	1:D:252:PHE:HA	2.19	0.42
1:B:395:THR:HG21	1:B:431:CYS:HA	2.01	0.42
1:D:242:LYS:HE2	1:D:242:LYS:HB2	1.84	0.42
1:H:376:ASN:HD22	1:H:376:ASN:HA	1.61	0.42
1:B:570:HIS:O	1:B:574:GLU:HG2	2.19	0.42
1:D:150:ALA:HA	1:D:190:PRO:CG	2.49	0.42
1:F:82:LEU:HD11	1:F:101:LEU:HD21	2.02	0.42
1:G:305:MET:CE	1:G:427:ALA:HA	2.49	0.42
1:G:477:THR:HG23	1:G:477:THR:O	2.19	0.42
1:H:488:ILE:HD11	1:H:548:ALA:HB2	2.02	0.42
1:C:601:TYR:OH	1:D:533:ARG:NH1	2.53	0.42
1:D:290:ALA:CA	1:D:291:MET:HB2	2.49	0.42
1:C:404:GLN:NE2	3:D:801:ATP:H1'	2.34	0.42
1:F:480:ILE:O	1:F:481:ASP:CB	2.67	0.42
1:G:307:SER:O	1:G:308:TYR:C	2.58	0.42
1:B:359:ALA:HB3	5:B:804:HOH:O	2.19	0.42
1:F:668:LYS:O	1:F:669:ALA:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:395:THR:HG23	1:G:431:CYS:SG	2.59	0.42
1:G:570:HIS:O	1:G:574:GLU:HG2	2.19	0.42
1:H:118:VAL:HG12	1:H:119:MET:HG3	2.01	0.42
1:E:340:GLN:OE1	2:F:701:FAD:O3B	2.38	0.42
1:F:570:HIS:O	1:F:574:GLU:HG2	2.19	0.42
1:H:94:ASP:HB3	1:H:97:GLU:HB2	2.02	0.42
1:A:456:LYS:HB2	5:A:808:HOH:O	2.20	0.42
1:B:290:ALA:CA	1:B:291:MET:HB2	2.50	0.42
1:C:6:LYS:HG3	1:C:28:HIS:ND1	2.34	0.42
1:E:95:ALA:H	1:E:97:GLU:N	2.17	0.42
1:F:151:GLN:HB3	2:F:701:FAD:O2	2.20	0.42
1:E:5:ASN:HA	1:E:27:THR:HG23	2.02	0.41
1:E:371:GLU:N	1:E:371:GLU:OE1	2.53	0.41
1:E:395:THR:HG23	1:E:431:CYS:SG	2.60	0.41
1:E:663:LYS:HB3	1:E:664:PRO:HD3	2.01	0.41
1:G:307:SER:HB3	1:G:620:PHE:HE2	1.85	0.41
1:G:80:THR:HG21	1:H:661:TYR:HB3	2.01	0.41
1:H:23:ALA:HB2	1:H:613:SER:OG	2.19	0.41
5:C:806:HOH:O	1:D:339:THR:CG2	2.67	0.41
1:E:187:LYS:O	1:E:252:PHE:HA	2.19	0.41
1:E:368:VAL:HG12	1:E:379:LEU:HB3	2.02	0.41
1:H:391:LYS:NZ	1:H:430:GLY:O	2.52	0.41
1:A:368:VAL:HG12	1:A:379:LEU:HB3	2.02	0.41
1:A:295:ARG:CB	1:A:387:THR:HG23	2.48	0.41
1:C:82:LEU:HD11	1:C:101:LEU:HD21	2.01	0.41
1:D:368:VAL:HG12	1:D:379:LEU:HB3	2.03	0.41
1:F:150:ALA:HA	1:F:190:PRO:CG	2.51	0.41
1:H:376:ASN:HB3	1:H:377:VAL:H	1.67	0.41
1:C:533:ARG:NH1	1:D:601:TYR:OH	2.53	0.41
1:F:187:LYS:O	1:F:252:PHE:HA	2.20	0.41
1:F:435:GLY:HA2	5:F:803:HOH:O	2.21	0.41
1:A:483:VAL:HG13	1:G:520:ARG:NH2	2.36	0.41
1:H:290:ALA:HA	1:H:291:MET:HB2	2.01	0.41
1:C:368:VAL:HG12	1:C:379:LEU:HB3	2.03	0.41
1:H:290:ALA:CA	1:H:291:MET:HB2	2.50	0.41
1:A:570:HIS:O	1:A:574:GLU:HG2	2.21	0.41
1:H:150:ALA:HA	1:H:190:PRO:CG	2.51	0.41
1:G:333:LYS:O	1:G:336:GLU:HB2	2.21	0.41
1:D:79:LEU:HD21	1:D:113:MET:HG3	2.03	0.41
1:D:321:ARG:HD3	5:D:963:HOH:O	2.19	0.41
1:E:631:ARG:HD2	5:E:830:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:79:LEU:HD21	1:F:113:MET:HG3	2.02	0.41
1:F:395:THR:HG23	1:F:431:CYS:SG	2.61	0.41
1:G:153:GLU:HG2	1:G:187:LYS:HD3	2.01	0.41
1:H:377:VAL:HG13	1:H:377:VAL:O	2.20	0.41
1:H:40:ARG:HH11	1:H:40:ARG:HD2	1.72	0.41
1:A:483:VAL:HG13	1:G:520:ARG:CZ	2.51	0.41
1:E:477:THR:O	1:E:587:PHE:O	2.39	0.41
1:A:95:ALA:HB1	1:A:98:LEU:CB	2.48	0.41
1:F:187:LYS:HD3	1:F:187:LYS:HA	1.89	0.41
1:F:136:TRP:CE2	1:F:219:MET:HG2	2.56	0.41
1:A:110:GLY:HA3	1:A:248:VAL:HG23	2.02	0.40
1:G:663:LYS:HD2	1:H:226:LYS:O	2.20	0.40
1:C:23:ALA:HB2	1:C:613:SER:OG	2.20	0.40
1:E:388:SER:HB3	1:E:440:MET:O	2.21	0.40
1:H:150:ALA:HA	1:H:190:PRO:HG3	2.03	0.40
1:A:150:ALA:HA	1:A:190:PRO:CG	2.52	0.40
1:B:23:ALA:HB2	1:B:613:SER:OG	2.22	0.40
1:D:115:LEU:HD13	1:D:115:LEU:HA	1.97	0.40
1:F:290:ALA:CA	1:F:291:MET:HB2	2.52	0.40
1:G:138:ILE:N	5:G:803:HOH:O	2.54	0.40

There are no symmetry-related clashes.

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	657/684 (96%)	619 (94%)	30 (5%)	8 (1%)	16	37
1	B	651/684 (95%)	619 (95%)	27 (4%)	5 (1%)	24	49
1	C	640/684 (94%)	613 (96%)	23 (4%)	4 (1%)	30	56
1	D	645/684 (94%)	616 (96%)	25 (4%)	4 (1%)	30	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	657/684 (96%)	622 (95%)	29 (4%)	6 (1%)	21	46
1	F	645/684 (94%)	613 (95%)	28 (4%)	4 (1%)	30	56
1	G	645/684 (94%)	620 (96%)	21 (3%)	4 (1%)	30	56
1	H	657/684 (96%)	622 (95%)	27 (4%)	8 (1%)	16	37
All	All	5197/5472 (95%)	4944 (95%)	210 (4%)	43 (1%)	24	49

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	TRP
1	A	488	ILE
1	B	189	TRP
1	C	189	TRP
1	D	189	TRP
1	D	279	ILE
1	E	189	TRP
1	E	488	ILE
1	F	171	ILE
1	F	189	TRP
1	G	40	ARG
1	G	189	TRP
1	H	189	TRP
1	H	488	ILE
1	A	279	ILE
1	B	270	THR
1	C	379	LEU
1	H	279	ILE
1	H	375	GLY
1	H	377	VAL
1	A	374	SER
1	A	379	LEU
1	B	379	LEU
1	D	478	SER
1	E	95	ALA
1	E	379	LEU
1	E	478	SER
1	F	478	SER
1	G	95	ALA
1	G	478	SER
1	H	379	LEU
1	H	478	SER

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Mol	Chain	Res	Type
1	A	160	LEU
1	E	378	SER
1	H	95	ALA
1	A	375	GLY
1	A	478	SER
1	B	478	SER
1	C	478	SER
1	F	379	LEU
1	C	519	LYS
1	B	486	GLY
1	D	157	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	556/578 (96%)	534 (96%)	22 (4%)	38	67
1	B	553/578 (96%)	530 (96%)	23 (4%)	36	65
1	C	549/578 (95%)	529 (96%)	20 (4%)	42	71
1	D	551/578 (95%)	525 (95%)	26 (5%)	32	61
1	E	556/578 (96%)	530 (95%)	26 (5%)	32	61
1	F	548/578 (95%)	521 (95%)	27 (5%)	31	58
1	G	549/578 (95%)	522 (95%)	27 (5%)	31	58
1	H	556/578 (96%)	529 (95%)	27 (5%)	31	58
All	All	4418/4624 (96%)	4220 (96%)	198 (4%)	34	62

All (198) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLU
1	A	33	GLN
1	A	61	MET
1	A	85	ARG

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Mol	Chain	Res	Type
1	A	115	LEU
1	A	280	LYS
1	A	300	THR
1	A	319	VAL
1	A	330	PRO
1	A	336	GLU
1	A	373	LYS
1	A	379	LEU
1	A	380	MET
1	A	382	ASP
1	A	391	LYS
1	A	477	THR
1	A	483	VAL
1	A	520	ARG
1	A	547	PHE
1	A	590	SER
1	A	608	ARG
1	A	667	GLU
1	B	10	GLU
1	B	33	GLN
1	B	39	MET
1	B	61	MET
1	B	85	ARG
1	B	226	LYS
1	B	229	LYS
1	B	280	LYS
1	B	300	THR
1	B	339	THR
1	B	372	MET
1	B	373	LYS
1	B	379	LEU
1	B	380	MET
1	B	382	ASP
1	B	391	LYS
1	B	437	ASN
1	B	477	THR
1	B	518	GLU
1	B	520	ARG
1	B	547	PHE
1	B	590	SER
1	B	667	GLU
1	C	2	VAL

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Mol	Chain	Res	Type
1	C	33	GLN
1	C	61	MET
1	C	85	ARG
1	C	115	LEU
1	C	177	VAL
1	C	226	LYS
1	C	280	LYS
1	C	300	THR
1	C	319	VAL
1	C	379	LEU
1	C	380	MET
1	C	382	ASP
1	C	391	LYS
1	C	477	THR
1	C	519	LYS
1	C	520	ARG
1	C	547	PHE
1	C	590	SER
1	C	667	GLU
1	D	10	GLU
1	D	33	GLN
1	D	61	MET
1	D	69	GLU
1	D	84	GLN
1	D	85	ARG
1	D	94	ASP
1	D	183	ILE
1	D	280	LYS
1	D	300	THR
1	D	339	THR
1	D	374	SER
1	D	379	LEU
1	D	380	MET
1	D	382	ASP
1	D	391	LYS
1	D	443	GLN
1	D	477	THR
1	D	482	ARG
1	D	518	GLU
1	D	520	ARG
1	D	533	ARG
1	D	547	PHE

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Mol	Chain	Res	Type
1	D	590	SER
1	D	608	ARG
1	D	667	GLU
1	E	10	GLU
1	E	33	GLN
1	E	40	ARG
1	E	61	MET
1	E	84	GLN
1	E	85	ARG
1	E	115	LEU
1	E	279	ILE
1	E	280	LYS
1	E	300	THR
1	E	339	THR
1	E	377	VAL
1	E	379	LEU
1	E	380	MET
1	E	382	ASP
1	E	391	LYS
1	E	437	ASN
1	E	473	ARG
1	E	477	THR
1	E	483	VAL
1	E	518	GLU
1	E	520	ARG
1	E	547	PHE
1	E	590	SER
1	E	608	ARG
1	E	667	GLU
1	F	33	GLN
1	F	39	MET
1	F	40	ARG
1	F	61	MET
1	F	84	GLN
1	F	85	ARG
1	F	115	LEU
1	F	171	ILE
1	F	174	GLN
1	F	183	ILE
1	F	229	LYS
1	F	277	THR
1	F	300	THR

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Mol	Chain	Res	Type
1	F	339	THR
1	F	376	ASN
1	F	377	VAL
1	F	379	LEU
1	F	380	MET
1	F	391	LYS
1	F	437	ASN
1	F	443	GLN
1	F	477	THR
1	F	520	ARG
1	F	533	ARG
1	F	547	PHE
1	F	608	ARG
1	F	667	GLU
1	G	10	GLU
1	G	33	GLN
1	G	40	ARG
1	G	61	MET
1	G	84	GLN
1	G	85	ARG
1	G	115	LEU
1	G	161	GLN
1	G	226	LYS
1	G	280	LYS
1	G	306	LEU
1	G	307	SER
1	G	319	VAL
1	G	374	SER
1	G	379	LEU
1	G	380	MET
1	G	382	ASP
1	G	391	LYS
1	G	437	ASN
1	G	443	GLN
1	G	477	THR
1	G	518	GLU
1	G	520	ARG
1	G	547	PHE
1	G	590	SER
1	G	608	ARG
1	G	667	GLU
1	H	33	GLN

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Mol	Chain	Res	Type
1	H	61	MET
1	H	85	ARG
1	H	94	ASP
1	H	115	LEU
1	H	183	ILE
1	H	226	LYS
1	H	280	LYS
1	H	300	THR
1	H	339	THR
1	H	374	SER
1	H	376	ASN
1	H	377	VAL
1	H	379	LEU
1	H	380	MET
1	H	382	ASP
1	H	391	LYS
1	H	437	ASN
1	H	443	GLN
1	H	477	THR
1	H	483	VAL
1	H	488	ILE
1	H	520	ARG
1	H	533	ARG
1	H	547	PHE
1	H	590	SER
1	H	667	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	404	GLN
1	B	384	HIS
1	B	516	ASN
1	D	570	HIS
1	E	462	GLN
1	F	174	GLN
1	G	462	GLN

5.3.3 RNA

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 (i)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 for Mogul analysis.

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	701	-	52,58,58	4.28	18 (34%)	52,89,89	3.07	13 (25%)
3	ATP	A	702	4	26,33,33	1.04	2 (7%)	26,52,52	2.10	4 (15%)
2	FAD	B	702	-	52,58,58	4.26	17 (32%)	52,89,89	2.60	11 (21%)
3	ATP	B	703	4	26,33,33	0.96	1 (3%)	26,52,52	1.67	1 (3%)
2	FAD	C	701	-	52,58,58	4.26	18 (34%)	52,89,89	2.62	11 (21%)
3	ATP	C	703	4	26,33,33	1.01	1 (3%)	26,52,52	1.84	3 (11%)
3	ATP	D	801	4	26,33,33	0.92	1 (3%)	26,52,52	1.84	2 (7%)
2	FAD	D	803	-	52,58,58	4.31	19 (36%)	52,89,89	2.40	9 (17%)
2	FAD	E	701	-	52,58,58	4.31	20 (38%)	52,89,89	2.75	11 (21%)
3	ATP	E	703	4	26,33,33	0.97	1 (3%)	26,52,52	1.90	4 (15%)
2	FAD	F	701	-	52,58,58	4.27	18 (34%)	52,89,89	2.79	13 (25%)
3	ATP	F	702	4	26,33,33	1.02	1 (3%)	26,52,52	1.75	3 (11%)
2	FAD	G	701	-	52,58,58	4.24	21 (40%)	52,89,89	2.68	12 (23%)
3	ATP	G	703	4	26,33,33	1.01	2 (7%)	26,52,52	1.75	4 (15%)
2	FAD	H	701	-	52,58,58	4.28	19 (36%)	52,89,89	2.96	12 (23%)
3	ATP	H	702	4	26,33,33	0.99	2 (7%)	26,52,52	1.66	2 (7%)

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	701	-	-	0/30/50/50	0/6/6/6
3	ATP	A	702	4	-	0/18/38/38	0/3/3/3
2	FAD	B	702	-	-	0/30/50/50	0/6/6/6
3	ATP	B	703	4	-	0/18/38/38	0/3/3/3
2	FAD	C	701	-	-	0/30/50/50	0/6/6/6
3	ATP	C	703	4	-	0/18/38/38	0/3/3/3
3	ATP	D	801	4	-	0/18/38/38	0/3/3/3
2	FAD	D	803	-	-	0/30/50/50	0/6/6/6
2	FAD	E	701	-	-	0/30/50/50	0/6/6/6
3	ATP	E	703	4	-	0/18/38/38	0/3/3/3
2	FAD	F	701	-	-	0/30/50/50	0/6/6/6
3	ATP	F	702	4	-	0/18/38/38	0/3/3/3
2	FAD	G	701	-	-	0/30/50/50	0/6/6/6
3	ATP	G	703	4	-	0/18/38/38	0/3/3/3
2	FAD	H	701	-	-	0/30/50/50	0/6/6/6
3	ATP	H	702	4	-	0/18/38/38	0/3/3/3

All (161) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	701	FAD	C2B-C1B	-14.91	1.29	1.53
2	H	701	FAD	C2B-C1B	-14.81	1.30	1.53
2	E	701	FAD	C2B-C1B	-14.81	1.30	1.53
2	B	702	FAD	C2B-C1B	-14.71	1.30	1.53
2	C	701	FAD	C2B-C1B	-14.62	1.30	1.53
2	F	701	FAD	C2B-C1B	-14.56	1.30	1.53
2	D	803	FAD	C2B-C1B	-14.50	1.30	1.53
2	A	701	FAD	C2B-C1B	-14.42	1.30	1.53
2	A	701	FAD	O4B-C4B	-6.43	1.30	1.45
2	D	803	FAD	O4B-C4B	-6.05	1.31	1.45
2	H	701	FAD	O4B-C4B	-6.02	1.31	1.45
2	C	701	FAD	O4B-C4B	-6.00	1.31	1.45
2	E	701	FAD	O4B-C4B	-6.00	1.31	1.45
2	G	701	FAD	O4B-C4B	-5.95	1.31	1.45
2	B	702	FAD	O4B-C4B	-5.94	1.31	1.45
2	F	701	FAD	O4B-C4B	-5.66	1.32	1.45
2	B	702	FAD	O4-C4	-3.27	1.16	1.24
2	F	701	FAD	O4-C4	-3.21	1.16	1.24
2	H	701	FAD	O4-C4	-3.15	1.16	1.24
2	A	701	FAD	O4-C4	-3.13	1.16	1.24
2	F	701	FAD	O3B-C3B	-3.09	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	701	FAD	O4-C4	-3.03	1.16	1.24
2	H	701	FAD	O3B-C3B	-3.01	1.35	1.43
2	C	701	FAD	O4-C4	-2.98	1.17	1.24
2	D	803	FAD	O3B-C3B	-2.96	1.36	1.43
2	B	702	FAD	O3B-C3B	-2.91	1.36	1.43
2	C	701	FAD	O3B-C3B	-2.79	1.36	1.43
2	E	701	FAD	O4-C4	-2.75	1.17	1.24
2	E	701	FAD	O3B-C3B	-2.70	1.36	1.43
2	A	701	FAD	O3B-C3B	-2.68	1.36	1.43
2	G	701	FAD	O3B-C3B	-2.66	1.36	1.43
2	A	701	FAD	C5A-C4A	-2.66	1.34	1.40
2	D	803	FAD	C5A-C4A	-2.66	1.34	1.40
2	E	701	FAD	C5A-C4A	-2.64	1.34	1.40
2	A	701	FAD	C1'-N10	-2.62	1.45	1.48
2	F	701	FAD	C1'-N10	-2.43	1.45	1.48
2	B	702	FAD	C5A-C4A	-2.38	1.35	1.40
2	D	803	FAD	O4-C4	-2.34	1.18	1.24
2	H	701	FAD	C1'-N10	-2.34	1.45	1.48
2	G	701	FAD	C5A-C4A	-2.29	1.35	1.40
2	G	701	FAD	C1'-N10	-2.22	1.46	1.48
2	H	701	FAD	C5A-C4A	-2.20	1.35	1.40
2	F	701	FAD	C5A-C4A	-2.20	1.35	1.40
2	C	701	FAD	C5A-C4A	-2.14	1.35	1.40
2	E	701	FAD	C1'-N10	-2.04	1.46	1.48
2	G	701	FAD	O4'-C4'	-2.03	1.38	1.43
2	G	701	FAD	C7M-C7	2.01	1.55	1.51
3	H	702	ATP	O4'-C1'	2.01	1.44	1.41
2	G	701	FAD	C2A-N3A	2.05	1.35	1.32
2	H	701	FAD	C7M-C7	2.07	1.55	1.51
2	E	701	FAD	C2A-N3A	2.08	1.35	1.32
2	E	701	FAD	C7M-C7	2.12	1.55	1.51
2	C	701	FAD	C2A-N3A	2.22	1.36	1.32
3	A	702	ATP	O4'-C1'	2.25	1.44	1.41
3	G	703	ATP	C2-N3	2.25	1.36	1.32
2	D	803	FAD	C2A-N3A	2.35	1.36	1.32
2	G	701	FAD	C6A-N6A	2.44	1.44	1.34
2	B	702	FAD	C6A-N6A	2.48	1.44	1.34
2	A	701	FAD	C6A-N6A	2.50	1.44	1.34
2	C	701	FAD	C6A-N6A	2.51	1.44	1.34
2	F	701	FAD	C6A-N6A	2.54	1.44	1.34
2	D	803	FAD	C6A-N6A	2.62	1.44	1.34
2	H	701	FAD	C6A-N6A	2.64	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	701	FAD	C6A-N6A	2.64	1.44	1.34
2	D	803	FAD	C4X-C10	2.74	1.45	1.40
2	F	701	FAD	O2B-C2B	2.81	1.49	1.43
3	D	801	ATP	C5-C4	2.92	1.47	1.40
3	A	702	ATP	C5-C4	2.93	1.47	1.40
3	G	703	ATP	C5-C4	2.94	1.47	1.40
3	E	703	ATP	C5-C4	2.95	1.47	1.40
2	E	701	FAD	O2B-C2B	3.02	1.50	1.43
3	H	702	ATP	C5-C4	3.03	1.47	1.40
2	D	803	FAD	O2B-C2B	3.04	1.50	1.43
2	H	701	FAD	O2B-C2B	3.05	1.50	1.43
3	C	703	ATP	C5-C4	3.06	1.47	1.40
3	B	703	ATP	C5-C4	3.07	1.47	1.40
2	A	701	FAD	O2B-C2B	3.19	1.50	1.43
2	G	701	FAD	O2B-C2B	3.26	1.50	1.43
3	F	702	ATP	C5-C4	3.26	1.47	1.40
2	C	701	FAD	O2B-C2B	3.30	1.50	1.43
2	B	702	FAD	O2B-C2B	3.54	1.51	1.43
2	G	701	FAD	C4-C4X	3.90	1.49	1.41
2	B	702	FAD	C4-C4X	3.96	1.49	1.41
2	E	701	FAD	C4-C4X	4.22	1.49	1.41
2	C	701	FAD	C4-C4X	4.27	1.50	1.41
2	A	701	FAD	C2-N1	4.42	1.47	1.38
2	F	701	FAD	C4-C4X	4.52	1.50	1.41
2	H	701	FAD	C4-C4X	4.55	1.50	1.41
2	E	701	FAD	C2-N1	4.56	1.47	1.38
2	A	701	FAD	C4-C4X	4.60	1.50	1.41
2	H	701	FAD	C2-N1	4.63	1.47	1.38
2	F	701	FAD	C2-N1	4.74	1.48	1.38
2	F	701	FAD	C2-N3	4.90	1.48	1.38
2	A	701	FAD	C10-N10	4.91	1.44	1.39
2	H	701	FAD	C2-N3	4.99	1.48	1.38
2	A	701	FAD	C2-N3	5.00	1.48	1.38
2	D	803	FAD	C2-N1	5.01	1.48	1.38
2	C	701	FAD	C2-N1	5.03	1.48	1.38
2	C	701	FAD	C2-N3	5.04	1.48	1.38
2	D	803	FAD	C4-C4X	5.13	1.51	1.41
2	G	701	FAD	C2-N1	5.15	1.48	1.38
2	B	702	FAD	C2-N1	5.18	1.49	1.38
2	E	701	FAD	C2-N3	5.23	1.49	1.38
2	B	702	FAD	C2-N3	5.26	1.49	1.38
2	G	701	FAD	C2-N3	5.32	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	803	FAD	C10-N10	5.34	1.45	1.39
2	D	803	FAD	C2-N3	5.35	1.49	1.38
2	H	701	FAD	C10-N10	5.39	1.45	1.39
2	F	701	FAD	C10-N10	5.44	1.45	1.39
2	E	701	FAD	C10-N10	5.86	1.46	1.39
2	B	702	FAD	C10-N10	6.23	1.46	1.39
2	G	701	FAD	C10-N10	6.24	1.46	1.39
2	B	702	FAD	C4-N3	6.38	1.44	1.33
2	C	701	FAD	C10-N10	6.43	1.46	1.39
2	B	702	FAD	C4X-N5	6.46	1.43	1.33
2	A	701	FAD	C10-N1	6.48	1.46	1.35
2	D	803	FAD	C10-N1	6.52	1.46	1.35
2	E	701	FAD	C10-N1	6.53	1.46	1.35
2	B	702	FAD	C10-N1	6.59	1.46	1.35
2	H	701	FAD	C10-N1	6.61	1.46	1.35
2	F	701	FAD	C10-N1	6.82	1.47	1.35
2	C	701	FAD	C4-N3	6.83	1.45	1.33
2	F	701	FAD	C4-N3	6.85	1.45	1.33
2	C	701	FAD	C10-N1	6.85	1.47	1.35
2	G	701	FAD	C4-N3	6.92	1.45	1.33
2	G	701	FAD	C4X-N5	6.96	1.44	1.33
2	H	701	FAD	C4-N3	7.05	1.45	1.33
2	E	701	FAD	C4-N3	7.14	1.45	1.33
2	G	701	FAD	C10-N1	7.18	1.47	1.35
2	A	701	FAD	C4-N3	7.18	1.46	1.33
2	E	701	FAD	C4X-N5	7.20	1.44	1.33
2	G	701	FAD	C5X-N5	7.22	1.46	1.35
2	D	803	FAD	C4-N3	7.32	1.46	1.33
2	B	702	FAD	C5X-N5	7.32	1.46	1.35
2	C	701	FAD	C4X-N5	7.53	1.44	1.33
2	A	701	FAD	C4X-N5	7.62	1.45	1.33
2	H	701	FAD	C4X-N5	7.73	1.45	1.33
2	D	803	FAD	C9A-N10	7.86	1.50	1.38
2	F	701	FAD	C4X-N5	7.90	1.45	1.33
2	C	701	FAD	C5X-N5	7.94	1.47	1.35
2	E	701	FAD	C5X-N5	8.03	1.48	1.35
2	D	803	FAD	C4X-N5	8.07	1.45	1.33
2	H	701	FAD	C9A-N10	8.18	1.50	1.38
2	A	701	FAD	C9A-N10	8.29	1.50	1.38
2	A	701	FAD	C5X-N5	8.30	1.48	1.35
2	G	701	FAD	C9A-N10	8.49	1.50	1.38
2	F	701	FAD	C9A-N10	8.51	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	701	FAD	C5X-N5	8.56	1.48	1.35
2	H	701	FAD	C5X-N5	8.56	1.48	1.35
2	B	702	FAD	C9A-N10	8.74	1.51	1.38
2	E	701	FAD	C9A-N10	8.88	1.51	1.38
2	C	701	FAD	C9A-N10	8.88	1.51	1.38
2	D	803	FAD	C5X-N5	8.88	1.49	1.35
2	G	701	FAD	O4B-C1B	14.50	1.61	1.41
2	C	701	FAD	O4B-C1B	14.52	1.62	1.41
2	H	701	FAD	O4B-C1B	14.83	1.62	1.41
2	D	803	FAD	O4B-C1B	14.92	1.62	1.41
2	F	701	FAD	O4B-C1B	15.06	1.62	1.41
2	B	702	FAD	O4B-C1B	15.45	1.63	1.41
2	E	701	FAD	O4B-C1B	15.47	1.63	1.41
2	A	701	FAD	O4B-C1B	15.50	1.63	1.41

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	FAD	N3A-C2A-N1A	-12.07	119.39	128.87
2	H	701	FAD	N3A-C2A-N1A	-11.91	119.52	128.87
2	E	701	FAD	N3A-C2A-N1A	-10.96	120.26	128.87
2	G	701	FAD	N3A-C2A-N1A	-10.25	120.82	128.87
2	F	701	FAD	N3A-C2A-N1A	-10.13	120.92	128.87
2	E	701	FAD	N6A-C6A-N1A	-10.03	101.69	118.52
2	F	701	FAD	N6A-C6A-N1A	-9.86	101.98	118.52
2	A	701	FAD	N6A-C6A-N1A	-9.74	102.18	118.52
2	H	701	FAD	N6A-C6A-N1A	-9.72	102.21	118.52
2	C	701	FAD	N3A-C2A-N1A	-9.72	121.24	128.87
2	B	702	FAD	N6A-C6A-N1A	-9.49	102.59	118.52
2	D	803	FAD	N3A-C2A-N1A	-9.45	121.45	128.87
2	B	702	FAD	N3A-C2A-N1A	-9.41	121.48	128.87
2	C	701	FAD	N6A-C6A-N1A	-8.97	103.46	118.52
2	G	701	FAD	N6A-C6A-N1A	-8.81	103.73	118.52
2	D	803	FAD	N6A-C6A-N1A	-8.05	105.00	118.52
3	A	702	ATP	N3-C2-N1	-7.80	122.75	128.87
3	D	801	ATP	N3-C2-N1	-7.19	123.22	128.87
3	C	703	ATP	N3-C2-N1	-6.96	123.41	128.87
3	E	703	ATP	N3-C2-N1	-6.81	123.52	128.87
3	B	703	ATP	N3-C2-N1	-6.62	123.67	128.87
3	H	702	ATP	N3-C2-N1	-6.49	123.78	128.87
3	F	702	ATP	N3-C2-N1	-6.42	123.83	128.87
3	G	703	ATP	N3-C2-N1	-6.21	123.99	128.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	FAD	N3-C2-N1	-6.03	117.53	127.69
2	C	701	FAD	N3-C2-N1	-5.60	118.25	127.69
2	H	701	FAD	N3-C2-N1	-5.53	118.37	127.69
2	B	702	FAD	C7M-C7-C6	-5.49	104.83	120.33
2	G	701	FAD	N3-C2-N1	-5.47	118.48	127.69
2	F	701	FAD	N3-C2-N1	-5.46	118.49	127.69
2	H	701	FAD	C4B-O4B-C1B	-5.23	104.10	109.64
2	A	701	FAD	C7M-C7-C6	-5.19	105.66	120.33
2	G	701	FAD	C7M-C7-C6	-5.19	105.67	120.33
2	E	701	FAD	N3-C2-N1	-5.18	118.97	127.69
2	E	701	FAD	C7M-C7-C6	-4.87	106.58	120.33
2	C	701	FAD	C7M-C7-C6	-4.81	106.73	120.33
2	F	701	FAD	C7M-C7-C6	-4.72	107.00	120.33
2	D	803	FAD	N3-C2-N1	-4.69	119.79	127.69
2	H	701	FAD	C7M-C7-C6	-4.53	107.53	120.33
2	D	803	FAD	C7M-C7-C6	-4.41	107.87	120.33
2	H	701	FAD	C5B-C4B-C3B	-4.37	98.29	115.20
2	A	701	FAD	C4B-O4B-C1B	-4.34	105.04	109.64
2	F	701	FAD	C4B-O4B-C1B	-4.17	105.22	109.64
2	A	701	FAD	C1B-N9A-C4A	-4.09	122.24	126.81
2	B	702	FAD	N3-C2-N1	-4.00	120.96	127.69
2	F	701	FAD	C5B-C4B-C3B	-3.87	100.22	115.20
2	A	701	FAD	C4-C4X-C10	-3.58	117.65	119.94
2	C	701	FAD	C4B-O4B-C1B	-3.50	105.93	109.64
2	G	701	FAD	C4B-O4B-C1B	-3.40	106.03	109.64
2	A	701	FAD	C5B-C4B-C3B	-3.13	103.10	115.20
2	F	701	FAD	C4-C4X-C10	-3.10	117.96	119.94
2	D	803	FAD	C4X-C4-N3	-2.91	119.71	123.52
2	G	701	FAD	C4X-C10-N10	-2.59	118.64	120.52
2	E	701	FAD	C4X-C4-N3	-2.49	120.27	123.52
3	E	703	ATP	C2'-C1'-N9	-2.43	106.95	113.47
3	A	702	ATP	C2'-C1'-N9	-2.36	107.14	113.47
2	F	701	FAD	O5B-C5B-C4B	-2.34	100.65	109.09
3	G	703	ATP	C2'-C1'-N9	-2.26	107.41	113.47
2	E	701	FAD	C4B-O4B-C1B	-2.20	107.31	109.64
2	G	701	FAD	C5B-C4B-C3B	-2.18	106.75	115.20
2	H	701	FAD	C4-C4X-C10	-2.18	118.54	119.94
2	B	702	FAD	C4-C4X-N5	-2.17	116.05	118.70
2	C	701	FAD	C5B-C4B-C3B	-2.15	106.89	115.20
3	C	703	ATP	C2'-C1'-N9	-2.06	107.96	113.47
2	E	701	FAD	C5B-C4B-C3B	-2.02	107.38	115.20
2	B	702	FAD	C2B-C3B-C4B	2.00	106.73	102.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	703	ATP	N6-C6-N1	2.03	121.92	118.52
3	D	801	ATP	O3G-PG-O2G	2.04	114.92	107.44
3	E	703	ATP	C2'-C3'-C4'	2.14	107.02	102.64
2	G	701	FAD	C6-C5X-C9A	2.14	121.47	119.11
3	G	703	ATP	O3G-PG-O2G	2.15	115.32	107.44
2	H	701	FAD	C4-C4X-N5	2.15	121.31	118.70
2	B	702	FAD	C6-C5X-C9A	2.15	121.48	119.11
3	H	702	ATP	O4'-C1'-N9	2.24	112.33	108.11
2	A	701	FAD	C5X-C9A-N10	2.32	119.31	117.58
2	F	701	FAD	C4-C4X-N5	2.34	121.54	118.70
2	C	701	FAD	C6-C5X-C9A	2.38	121.73	119.11
3	F	702	ATP	O3G-PG-O2G	2.38	116.17	107.44
3	C	703	ATP	O4'-C1'-N9	2.40	112.63	108.11
2	B	702	FAD	C4-N3-C2	2.51	117.25	115.16
2	G	701	FAD	C4X-N5-C5X	2.69	119.89	116.72
2	C	701	FAD	C4X-N5-C5X	2.73	119.94	116.72
3	F	702	ATP	O4'-C1'-N9	2.82	113.42	108.11
2	D	803	FAD	C4X-N5-C5X	2.85	120.08	116.72
2	A	701	FAD	C4X-N5-C5X	2.90	120.14	116.72
2	A	701	FAD	C4-C4X-N5	2.96	122.29	118.70
2	E	701	FAD	C4X-N5-C5X	2.97	120.23	116.72
2	B	702	FAD	C5X-C9A-N10	3.06	119.87	117.58
3	A	702	ATP	O2G-PG-O1G	3.12	120.81	110.63
2	F	701	FAD	C4X-N5-C5X	3.26	120.57	116.72
2	D	803	FAD	C5X-C9A-N10	3.27	120.03	117.58
3	E	703	ATP	O4'-C1'-N9	3.32	114.38	108.11
2	H	701	FAD	C4X-N5-C5X	3.37	120.69	116.72
2	E	701	FAD	C5X-C9A-N10	3.43	120.15	117.58
3	A	702	ATP	O4'-C1'-N9	3.66	115.01	108.11
2	C	701	FAD	C5X-C9A-N10	3.73	120.38	117.58
2	B	702	FAD	C4-C4X-C10	3.74	122.33	119.94
2	H	701	FAD	C5X-C9A-N10	3.76	120.39	117.58
2	F	701	FAD	C5X-C9A-N10	3.78	120.41	117.58
2	G	701	FAD	C5X-C9A-N10	4.02	120.59	117.58
2	F	701	FAD	C4-N3-C2	4.34	118.78	115.16
2	C	701	FAD	C4-N3-C2	4.70	119.08	115.16
2	G	701	FAD	C4-N3-C2	4.78	119.15	115.16
2	H	701	FAD	C7M-C7-C8	5.15	131.81	120.73
2	E	701	FAD	C4-N3-C2	5.16	119.47	115.16
2	D	803	FAD	C7M-C7-C8	5.27	132.07	120.73
2	F	701	FAD	C7M-C7-C8	5.47	132.50	120.73
2	D	803	FAD	C4-N3-C2	5.51	119.75	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	701	FAD	C7M-C7-C8	5.58	132.73	120.73
2	H	701	FAD	C4-N3-C2	5.59	119.82	115.16
2	A	701	FAD	C7M-C7-C8	5.73	133.05	120.73
2	E	701	FAD	C7M-C7-C8	5.75	133.11	120.73
2	G	701	FAD	C7M-C7-C8	5.89	133.39	120.73
2	A	701	FAD	C4-N3-C2	5.95	120.12	115.16
2	B	702	FAD	C7M-C7-C8	6.46	134.63	120.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	FAD	1	0
3	A	702	ATP	2	0
2	B	702	FAD	1	0
2	C	701	FAD	1	0
3	D	801	ATP	1	0
2	D	803	FAD	1	0
2	F	701	FAD	4	0
3	G	703	ATP	2	0
2	H	701	FAD	2	0
3	H	702	ATP	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{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	661/684 (96%)	-0.39	5 (0%) 87 88	17, 27, 47, 73	0
1	B	657/684 (96%)	-0.26	11 (1%) 73 72	17, 32, 65, 80	0
1	C	650/684 (95%)	-0.26	2 (0%) 94 95	20, 34, 56, 72	0
1	D	653/684 (95%)	-0.38	2 (0%) 94 95	18, 30, 49, 66	0
1	E	661/684 (96%)	-0.25	8 (1%) 81 81	20, 33, 57, 77	0
1	F	651/684 (95%)	-0.16	10 (1%) 76 75	22, 36, 66, 84	0
1	G	653/684 (95%)	-0.25	6 (0%) 85 86	20, 33, 63, 74	0
1	H	661/684 (96%)	-0.38	4 (0%) 90 91	18, 27, 48, 67	0
All	All	5247/5472 (95%)	-0.29	48 (0%) 85 86	17, 31, 59, 84	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	377	VAL	7.2
1	F	378	SER	3.9
1	B	126	ALA	3.6
1	E	375	GLY	3.5
1	B	378	SER	3.4
1	H	375	GLY	3.4
1	A	375	GLY	3.3
1	B	272	VAL	2.9
1	B	483	VAL	2.8
1	G	290	ALA	2.8
1	F	199	TYR	2.8
1	F	232	PRO	2.8
1	D	95	ALA	2.8
1	H	95	ALA	2.7
1	B	486	GLY	2.7
1	C	378	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	374	SER	2.7
1	B	281	PRO	2.6
1	B	279	ILE	2.6
1	B	269	HIS	2.5
1	F	146	ILE	2.5
1	F	125	ASN	2.5
1	A	377	VAL	2.5
1	E	372	MET	2.5
1	F	278	TYR	2.5
1	E	666	MET	2.5
1	F	94	ASP	2.5
1	F	269	HIS	2.4
1	D	372	MET	2.4
1	G	270	THR	2.4
1	E	376	ASN	2.4
1	H	378	SER	2.4
1	G	128	ALA	2.4
1	E	380	MET	2.3
1	B	125	ASN	2.3
1	B	369	LEU	2.3
1	A	95	ALA	2.3
1	B	278	TYR	2.3
1	E	487	GLY	2.2
1	G	39	MET	2.2
1	E	281	PRO	2.2
1	E	377	VAL	2.1
1	G	94	ASP	2.1
1	A	380	MET	2.1
1	A	374	SER	2.1
1	C	279	ILE	2.0
1	F	172	GLY	2.0
1	H	512	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

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^{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	LLDF	B-factors(Å^2)	Q<0.9
2	FAD	H	701	53/53	0.95	0.16	0.33	19,23,25,26	0
2	FAD	F	701	53/53	0.94	0.14	0.25	21,25,27,28	0
2	FAD	D	803	53/53	0.95	0.14	0.15	21,22,23,23	0
2	FAD	A	701	53/53	0.95	0.14	-0.05	20,21,23,25	0
3	ATP	B	703	31/31	0.95	0.14	-0.05	16,18,19,19	0
2	FAD	G	701	53/53	0.96	0.14	-0.16	24,25,26,26	0
3	ATP	F	702	31/31	0.96	0.13	-0.19	21,22,23,23	0
3	ATP	A	702	31/31	0.97	0.13	-0.45	16,16,17,17	0
2	FAD	B	702	53/53	0.96	0.13	-0.47	21,24,25,26	0
2	FAD	C	701	53/53	0.96	0.13	-0.62	22,26,29,31	0
2	FAD	E	701	53/53	0.96	0.13	-0.64	22,25,28,28	0
3	ATP	D	801	31/31	0.96	0.13	-0.68	20,21,23,23	0
3	ATP	H	702	31/31	0.97	0.12	-0.99	19,22,24,26	0
3	ATP	G	703	31/31	0.97	0.12	-0.99	18,19,19,19	0
3	ATP	C	703	31/31	0.97	0.12	-1.00	19,21,22,22	0
3	ATP	E	703	31/31	0.97	0.13	-1.14	19,21,22,23	0
4	MG	B	701	1/1	0.97	0.21	-	14,14,14,14	0
4	MG	E	702	1/1	0.98	0.18	-	22,22,22,22	0
4	MG	H	703	1/1	0.94	0.16	-	14,14,14,14	0
4	MG	D	802	1/1	0.95	0.23	-	23,23,23,23	0
4	MG	F	703	1/1	0.95	0.16	-	23,23,23,23	0
4	MG	G	702	1/1	0.97	0.20	-	22,22,22,22	0
4	MG	A	703	1/1	0.96	0.17	-	18,18,18,18	0
4	MG	C	702	1/1	0.98	0.17	-	20,20,20,20	0

6.5 Other polymers

There are no such residues in this entry.