Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:40 AM GMT

PDB ID	:	3MPJ
Title	:	Structure of the glutaryl-coenzyme A dehydrogenase
Authors	:	Wischgoll, S.; Warkentin, E.; Boll, M.; Ermler, U.
Deposited on	:	2010-04-27
Resolution	:	2.10 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:

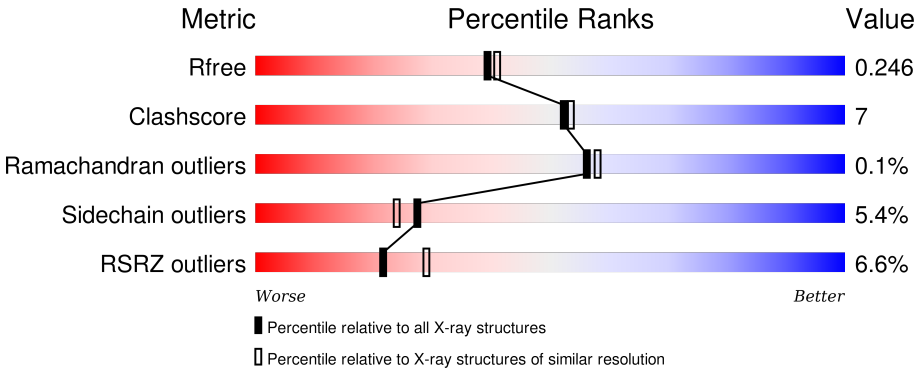
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	397	81% 15%
1	B	397	2% 82% 15%
1	D	397	11% 83% 14%
1	E	397	21% 77% 21%
1	F	397	% 86% 10%

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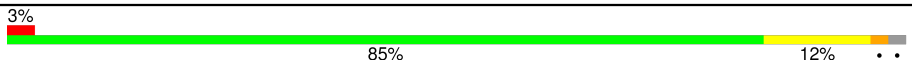
Mol	Chain	Length	Quality of chain
1	G	397	
2	Y	8	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19170 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 Glutaryl-CoA dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	2	0
			2992	1891	510	571	20			
1	B	393	Total	C	N	O	S	0	2	0
			3026	1913	520	573	20			
1	D	390	Total	C	N	O	S	0	2	0
			3004	1899	515	570	20			
1	E	391	Total	C	N	O	S	0	1	0
			2999	1896	515	568	20			
1	F	390	Total	C	N	O	S	0	2	0
			3001	1898	514	569	20			
1	G	389	Total	C	N	O	S	0	0	0
			2975	1882	508	565	20			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	390	LYS	-	EXPRESSION TAG	UNP C3UVB0
A	391	GLY	-	EXPRESSION TAG	UNP C3UVB0
A	392	HIS	-	EXPRESSION TAG	UNP C3UVB0
A	393	HIS	-	EXPRESSION TAG	UNP C3UVB0
A	394	HIS	-	EXPRESSION TAG	UNP C3UVB0
A	395	HIS	-	EXPRESSION TAG	UNP C3UVB0
A	396	HIS	-	EXPRESSION TAG	UNP C3UVB0
A	397	HIS	-	EXPRESSION TAG	UNP C3UVB0
B	390	LYS	-	EXPRESSION TAG	UNP C3UVB0
B	391	GLY	-	EXPRESSION TAG	UNP C3UVB0
B	392	HIS	-	EXPRESSION TAG	UNP C3UVB0
B	393	HIS	-	EXPRESSION TAG	UNP C3UVB0
B	394	HIS	-	EXPRESSION TAG	UNP C3UVB0
B	395	HIS	-	EXPRESSION TAG	UNP C3UVB0
B	396	HIS	-	EXPRESSION TAG	UNP C3UVB0
B	397	HIS	-	EXPRESSION TAG	UNP C3UVB0
D	390	LYS	-	EXPRESSION TAG	UNP C3UVB0

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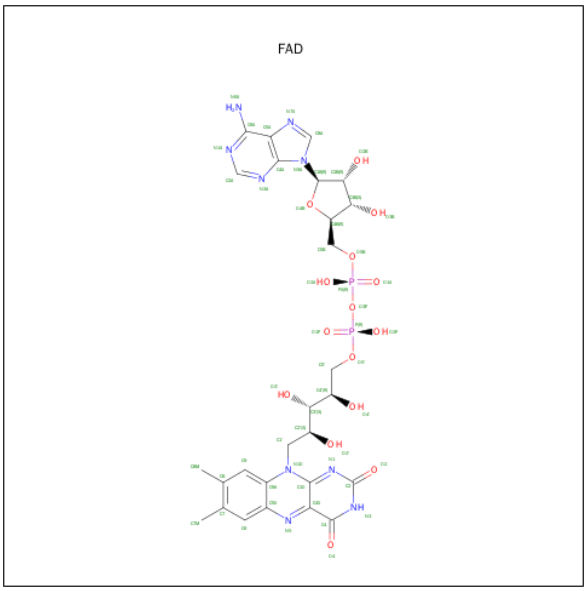
Chain	Residue	Modelled	Actual	Comment	Reference
D	391	GLY	-	EXPRESSION TAG	UNP C3UVB0
D	392	HIS	-	EXPRESSION TAG	UNP C3UVB0
D	393	HIS	-	EXPRESSION TAG	UNP C3UVB0
D	394	HIS	-	EXPRESSION TAG	UNP C3UVB0
D	395	HIS	-	EXPRESSION TAG	UNP C3UVB0
D	396	HIS	-	EXPRESSION TAG	UNP C3UVB0
D	397	HIS	-	EXPRESSION TAG	UNP C3UVB0
E	390	LYS	-	EXPRESSION TAG	UNP C3UVB0
E	391	GLY	-	EXPRESSION TAG	UNP C3UVB0
E	392	HIS	-	EXPRESSION TAG	UNP C3UVB0
E	393	HIS	-	EXPRESSION TAG	UNP C3UVB0
E	394	HIS	-	EXPRESSION TAG	UNP C3UVB0
E	395	HIS	-	EXPRESSION TAG	UNP C3UVB0
E	396	HIS	-	EXPRESSION TAG	UNP C3UVB0
E	397	HIS	-	EXPRESSION TAG	UNP C3UVB0
F	390	LYS	-	EXPRESSION TAG	UNP C3UVB0
F	391	GLY	-	EXPRESSION TAG	UNP C3UVB0
F	392	HIS	-	EXPRESSION TAG	UNP C3UVB0
F	393	HIS	-	EXPRESSION TAG	UNP C3UVB0
F	394	HIS	-	EXPRESSION TAG	UNP C3UVB0
F	395	HIS	-	EXPRESSION TAG	UNP C3UVB0
F	396	HIS	-	EXPRESSION TAG	UNP C3UVB0
F	397	HIS	-	EXPRESSION TAG	UNP C3UVB0
G	390	LYS	-	EXPRESSION TAG	UNP C3UVB0
G	391	GLY	-	EXPRESSION TAG	UNP C3UVB0
G	392	HIS	-	EXPRESSION TAG	UNP C3UVB0
G	393	HIS	-	EXPRESSION TAG	UNP C3UVB0
G	394	HIS	-	EXPRESSION TAG	UNP C3UVB0
G	395	HIS	-	EXPRESSION TAG	UNP C3UVB0
G	396	HIS	-	EXPRESSION TAG	UNP C3UVB0
G	397	HIS	-	EXPRESSION TAG	UNP C3UVB0

- Molecule 2 is a protein called Octapeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	Y	8	Total	C	N	O	0	0	0
			72	44	20	8			

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		
4	E	1	Total	Cl	0	0
			1	1		
4	B	1	Total	Cl	0	0
			1	1		
4	A	1	Total	Cl	0	0
			1	1		
4	F	1	Total	Cl	0	0
			1	1		

- Molecule 5 is water.

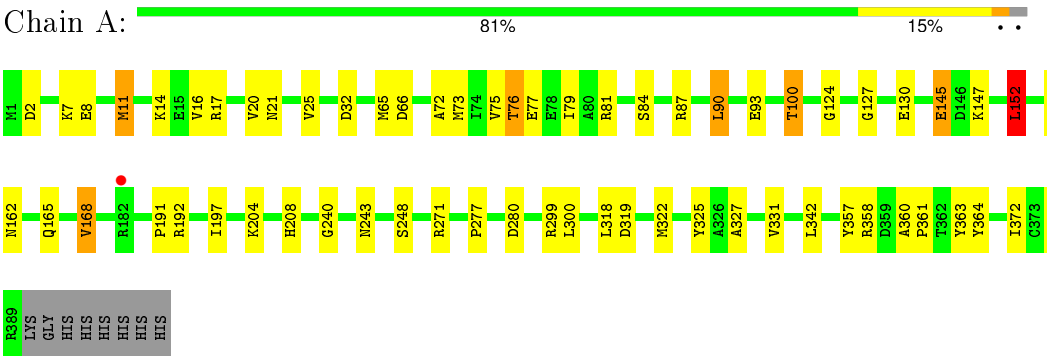
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	175	Total O 175 175	0	0
5	B	179	Total O 179 179	0	0
5	D	84	Total O 84 84	0	0
5	E	78	Total O 78 78	0	0
5	F	143	Total O 143 143	0	0
5	G	115	Total O 115 115	0	0
5	Y	3	Total O 3 3	0	0

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.

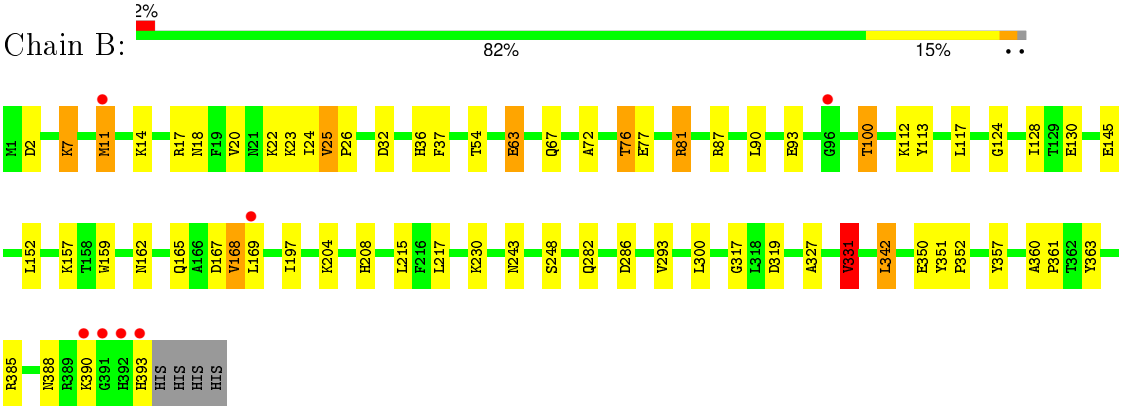
- Molecule 1: Glutaryl-CoA dehydrogenase

Chain A:



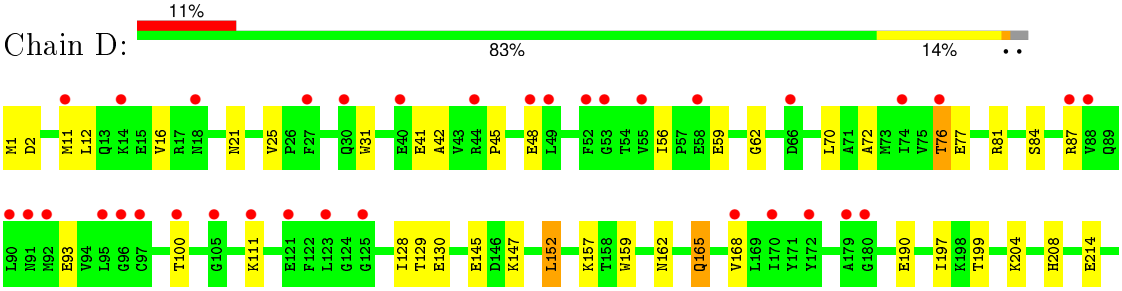
- Molecule 1: Glutaryl-CoA dehydrogenase

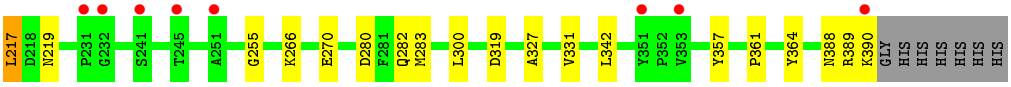
Chain B:



- Molecule 1: Glutaryl-CoA dehydrogenase

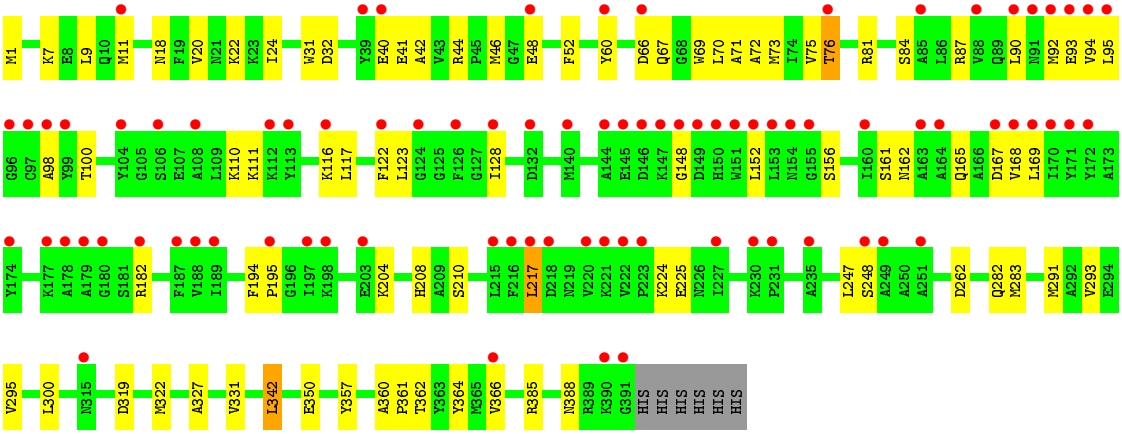
Chain D:





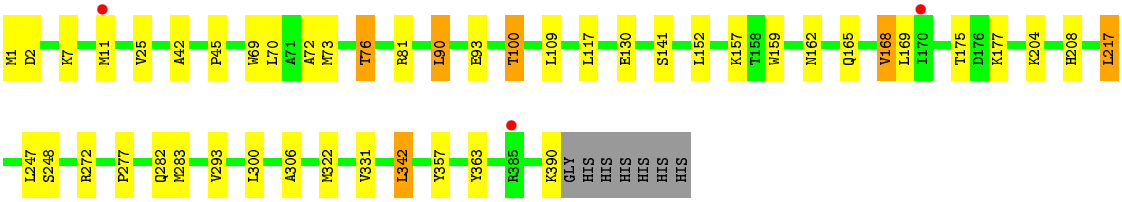
• Molecule 1: Glutaryl-CoA dehydrogenase

Chain E:



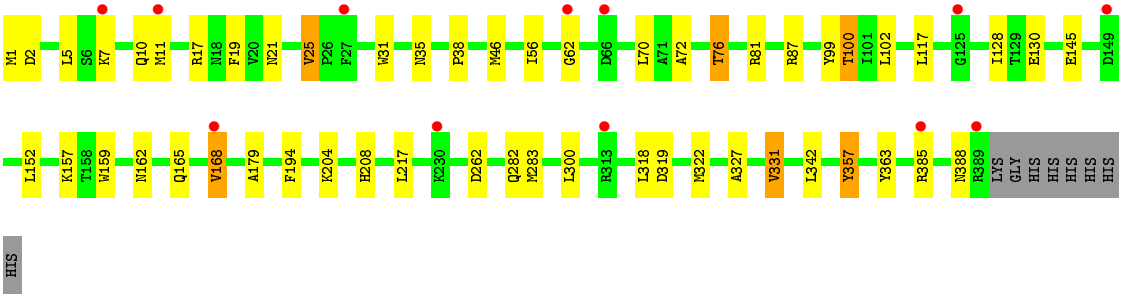
• Molecule 1: Glutaryl-CoA dehydrogenase

Chain F:



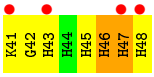
• Molecule 1: Glutaryl-CoA dehydrogenase

Chain G:



• Molecule 2: Octapeptide

Chain Y:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	152.40Å 250.60Å 62.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 29.87 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-2.10) 99.7 (29.87-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.74 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.6.0046	Depositor
R, R_{free}	0.181 , 0.225 0.217 , 0.246	Depositor DCC
R_{free} test set	7079 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	27.6	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 140757 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19170	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.59% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.94	1/3050 (0.0%)	0.88	8/4117 (0.2%)
1	B	0.90	2/3086 (0.1%)	0.83	4/4163 (0.1%)
1	D	0.68	0/3062	0.71	0/4131
1	E	0.68	0/3057	0.73	2/4124 (0.0%)
1	F	0.83	0/3062	0.79	2/4131 (0.0%)
1	G	0.77	1/3033 (0.0%)	0.77	1/4094 (0.0%)
2	Y	0.77	0/76	0.94	0/98
All	All	0.81	4/18426 (0.0%)	0.79	17/24858 (0.1%)

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
2	Y	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	357	TYR	CD1-CE1	7.49	1.50	1.39
1	A	357	TYR	CD1-CE1	6.58	1.49	1.39
1	B	331	VAL	CB-CG1	-5.24	1.41	1.52
1	G	357	TYR	CD1-CE1	5.04	1.47	1.39

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	192	ARG	NE-CZ-NH1	8.41	124.51	120.30
1	A	358	ARG	NE-CZ-NH1	6.84	123.72	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	342	LEU	CA-CB-CG	6.48	130.21	115.30
1	E	217	LEU	CA-CB-CG	6.07	129.25	115.30
1	A	192	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	A	152	LEU	CA-CB-CG	5.74	128.50	115.30
1	A	358	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	A	375	MET	CG-SD-CE	-5.71	91.06	100.20
1	A	73	MET	CG-SD-CE	5.71	109.33	100.20
1	B	81	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	271	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	G	217	LEU	CA-CB-CG	5.61	128.21	115.30
1	B	215	LEU	CA-CB-CG	5.34	127.57	115.30
1	B	342	LEU	CA-CB-CG	5.33	127.56	115.30
1	B	286	ASP	CB-CG-OD1	5.33	123.09	118.30
1	F	342	LEU	CA-CB-CG	5.30	127.50	115.30
1	F	217	LEU	CA-CB-CG	5.20	127.26	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	Y	46	HIS	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	2992	0	2945	45	0
1	B	3026	0	2984	47	0
1	D	3004	0	2967	37	0
1	E	2999	0	2965	52	0
1	F	3001	0	2968	33	1
1	G	2975	0	2937	40	0
2	Y	72	0	55	8	1
3	A	53	0	31	4	0
3	B	53	0	31	4	0
3	D	53	0	31	5	0
3	E	53	0	31	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	53	0	31	5	0
3	G	53	0	31	4	0
4	A	1	0	0	0	0
4	B	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
5	A	175	0	0	6	0
5	B	179	0	0	6	0
5	D	84	0	0	1	0
5	E	78	0	0	2	0
5	F	143	0	0	4	1
5	G	115	0	0	2	1
5	Y	3	0	0	0	0
All	All	19170	0	18007	245	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (245) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:72:ALA:O	1:G:76:THR:HG22	1.65	0.95
1:F:331:VAL:HG21	1:F:363:TYR:HB2	1.59	0.84
5:B:7089:HOH:O	2:Y:47:HIS:HB3	1.77	0.84
1:E:72:ALA:O	1:E:76:THR:HG22	1.78	0.83
1:B:36:HIS:HD2	2:Y:48:HIS:HA	1.43	0.83
2:Y:46:HIS:HB2	2:Y:48:HIS:HD2	1.44	0.83
2:Y:42:GLY:C	2:Y:43:HIS:CA	2.48	0.81
1:B:77:GLU:OE1	5:B:7219:HOH:O	1.98	0.81
1:D:72:ALA:O	1:D:76:THR:HG22	1.79	0.81
1:D:70:LEU:HD21	1:G:1:MET:HG2	1.63	0.80
1:B:76:THR:HG22	1:B:90:LEU:HD23	1.61	0.80
1:B:11:MET:HE2	1:B:14:LYS:HD2	1.63	0.80
1:F:100:THR:HG21	5:F:7538:HOH:O	1.80	0.79
1:G:327:ALA:O	1:G:331:VAL:HG12	1.84	0.78
2:Y:46:HIS:HB2	2:Y:48:HIS:CD2	2.18	0.77
1:G:72:ALA:O	1:G:76:THR:CG2	2.33	0.77
1:E:72:ALA:O	1:E:76:THR:CG2	2.35	0.75
1:B:327:ALA:O	1:B:331:VAL:HG13	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:ALA:O	1:A:331:VAL:HG13	1.87	0.73
1:A:77:GLU:OE1	5:A:7266:HOH:O	2.09	0.70
1:D:81[B]:ARG:O	1:D:81[B]:ARG:HG2	1.93	0.68
3:E:400:FAD:H2'	3:E:400:FAD:H9	1.76	0.67
3:F:400:FAD:H2'	3:F:400:FAD:H9	1.76	0.67
3:D:400:FAD:C9	3:D:400:FAD:H2'	2.25	0.67
3:F:400:FAD:H2'	3:F:400:FAD:C9	2.24	0.67
1:A:81:ARG:HD2	5:A:7957:HOH:O	1.93	0.67
1:G:17:ARG:HH12	1:G:81:ARG:HH21	1.40	0.67
3:G:400:FAD:H2'	3:G:400:FAD:C9	2.24	0.66
3:E:400:FAD:C9	3:E:400:FAD:H2'	2.25	0.66
1:A:76:THR:HG22	1:A:90:LEU:HD23	1.77	0.66
1:A:322:MET:CE	1:B:293:VAL:HA	2.24	0.66
1:G:17:ARG:HH12	1:G:81:ARG:NH2	1.95	0.64
1:F:272:ARG:NH1	1:F:277:PRO:HD3	2.13	0.64
1:F:72:ALA:O	1:F:76:THR:HG22	1.97	0.64
1:E:283:MET:H	1:G:282:GLN:HE21	1.46	0.64
1:E:282:GLN:HE21	1:G:283:MET:H	1.46	0.64
1:A:331:VAL:HG21	1:A:363:TYR:HB2	1.80	0.64
1:D:282:GLN:HE21	1:F:283:MET:H	1.45	0.64
1:E:162:ASN:HA	1:E:165:GLN:HE21	1.62	0.63
1:G:5:LEU:O	1:G:10:GLN:NE2	2.31	0.63
1:B:204:LYS:O	1:B:208:HIS:HE1	1.80	0.63
1:F:81:ARG:HD2	5:F:7589:HOH:O	1.98	0.63
3:G:400:FAD:H2'	3:G:400:FAD:H9	1.80	0.63
1:D:283:MET:H	1:F:282:GLN:HE21	1.47	0.62
1:E:81:ARG:HD2	5:E:7641:HOH:O	1.99	0.62
1:E:331:VAL:HG23	1:E:360:ALA:HB1	1.80	0.62
1:E:327:ALA:O	1:E:331:VAL:HG13	2.00	0.61
1:B:36:HIS:CD2	2:Y:48:HIS:HA	2.32	0.61
1:E:20:VAL:HG22	1:E:24:ILE:HD12	1.83	0.61
1:E:293:VAL:HA	1:F:322:MET:HE3	1.83	0.61
1:E:18:ASN:HD21	1:E:22:LYS:NZ	2.00	0.60
3:B:400:FAD:H2'	3:B:400:FAD:C9	2.31	0.60
1:G:204:LYS:O	1:G:208:HIS:HE1	1.84	0.59
1:G:35:ASN:HD22	1:G:208:HIS:HB3	1.66	0.59
1:D:21:ASN:ND2	1:D:81[B]:ARG:HH22	2.00	0.59
1:G:35:ASN:ND2	1:G:208:HIS:HB3	2.17	0.59
1:D:130:GLU:HG2	1:D:157:LYS:HD3	1.85	0.59
1:A:159:TRP:O	3:A:400:FAD:C4X	2.50	0.59
1:G:21:ASN:HA	1:G:25:VAL:HG13	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:162:ASN:HA	1:G:165:GLN:HE21	1.68	0.58
1:F:100:THR:HG22	5:F:7633:HOH:O	2.02	0.58
1:E:293:VAL:HA	1:F:322:MET:CE	2.33	0.58
1:E:1:MET:HG2	1:F:70:LEU:HD21	1.85	0.58
1:A:21:ASN:HA	1:A:25:VAL:HG13	1.86	0.58
1:E:282:GLN:HB2	1:G:282:GLN:HB2	1.86	0.57
1:D:152:LEU:HD21	1:D:219:ASN:HA	1.86	0.57
1:A:17:ARG:HH12	1:A:81:ARG:NH2	2.02	0.57
1:F:72:ALA:O	1:F:76:THR:CG2	2.52	0.57
1:D:1:MET:HG2	1:G:70:LEU:HD21	1.85	0.57
1:E:117:LEU:HD21	1:E:168:VAL:CG1	2.34	0.57
1:D:199:THR:HA	1:D:214:GLU:O	2.05	0.56
1:G:81:ARG:NH1	1:G:262:ASP:OD2	2.38	0.56
1:A:322:MET:HE2	1:B:293:VAL:HG22	1.87	0.56
1:B:319:ASP:H	1:B:388:ASN:HD21	1.54	0.56
1:B:72:ALA:O	1:B:76:THR:CG2	2.53	0.56
1:D:12:LEU:O	1:D:16:VAL:HG23	2.06	0.56
1:A:319:ASP:H	1:A:388:ASN:HD21	1.53	0.56
1:E:44:ARG:NH1	1:E:48:GLU:HG3	2.21	0.56
1:F:357:TYR:CE2	1:G:357:TYR:CE2	2.94	0.56
1:D:319:ASP:H	1:D:388:ASN:HD21	1.53	0.56
1:A:100:THR:HG21	5:A:7065:HOH:O	2.05	0.56
1:E:42:ALA:O	1:E:46:MET:HG3	2.05	0.56
1:D:31:TRP:CZ2	1:D:41:GLU:HG3	2.41	0.55
3:E:400:FAD:H2A	1:F:282:GLN:HE22	1.72	0.55
1:A:72:ALA:O	1:A:76:THR:CG2	2.55	0.55
1:D:147:LYS:HE3	1:D:152:LEU:HD12	1.89	0.55
1:B:124:GLY:HA2	1:B:168:VAL:O	2.06	0.55
1:E:319:ASP:H	1:E:388:ASN:HD21	1.55	0.54
1:B:130:GLU:HG2	1:B:157:LYS:HD3	1.90	0.54
1:A:145[B]:GLU:OE2	1:A:147:LYS:NZ	2.27	0.54
1:A:240:GLY:HA3	5:A:7283:HOH:O	2.07	0.54
1:D:84:SER:O	1:D:87:ARG:HG3	2.07	0.54
1:E:81:ARG:NH1	1:E:262:ASP:OD2	2.41	0.54
1:A:318:LEU:H	1:A:388:ASN:ND2	2.06	0.54
1:G:130:GLU:HG2	1:G:157:LYS:HD3	1.90	0.54
1:D:327:ALA:O	1:D:331:VAL:HG13	2.07	0.53
1:G:17:ARG:NH1	1:G:81:ARG:NH2	2.57	0.53
1:A:72:ALA:O	1:A:76:THR:HG22	2.09	0.53
1:B:72:ALA:O	1:B:76:THR:HG22	2.08	0.53
3:A:400:FAD:C9	3:A:400:FAD:H2'	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:84:SER:O	1:E:87:ARG:HG3	2.09	0.52
1:A:16:VAL:O	1:A:20:VAL:HG23	2.10	0.52
1:E:87:ARG:HD2	1:E:87:ARG:C	2.30	0.52
1:G:318:LEU:O	1:G:322:MET:HG3	2.10	0.52
1:B:162:ASN:HA	1:B:165:GLN:HE21	1.75	0.52
1:B:100:THR:HG21	5:B:7078:HOH:O	2.09	0.52
1:A:100:THR:HG22	5:A:7075:HOH:O	2.09	0.51
1:E:70:LEU:HD21	1:F:1:MET:HG2	1.91	0.51
3:D:400:FAD:H9	3:D:400:FAD:H2'	1.92	0.51
1:D:282:GLN:HB2	1:F:282:GLN:HB2	1.93	0.51
1:B:76:THR:CG2	1:B:90:LEU:HD23	2.37	0.51
1:A:277:PRO:HD2	1:A:280:ASP:OD2	2.11	0.51
1:G:100:THR:HG21	5:G:7411:HOH:O	2.10	0.50
1:F:162:ASN:HA	1:F:165:GLN:HE21	1.76	0.50
3:A:400:FAD:H2A	1:B:282:GLN:HE22	1.76	0.50
1:D:56:ILE:HB	1:D:62:GLY:HA3	1.94	0.50
1:E:116:LYS:HD2	1:E:122:PHE:CZ	2.47	0.50
1:G:117:LEU:HD21	1:G:168:VAL:HG13	1.92	0.50
1:D:162:ASN:HA	1:D:165:GLN:HE21	1.75	0.50
1:B:167:ASP:OD2	2:Y:45:HIS:HE1	1.95	0.50
1:E:283:MET:H	1:G:282:GLN:NE2	2.09	0.50
1:D:21:ASN:HD21	1:D:81[B]:ARG:HH22	1.60	0.49
1:F:73:MET:HG3	1:F:306:ALA:HB2	1.94	0.49
1:B:243:ASN:HD21	1:B:317:GLY:HA2	1.77	0.49
1:B:20:VAL:HG22	1:B:24:ILE:HD12	1.93	0.49
1:D:282:GLN:NE2	1:F:283:MET:H	2.10	0.49
1:A:243:ASN:HB3	5:A:7130:HOH:O	2.13	0.49
1:G:87:ARG:HD2	1:G:87:ARG:C	2.33	0.49
1:B:385:ARG:HH11	1:B:385:ARG:HG3	1.78	0.49
1:E:60:TYR:CZ	1:E:110:LYS:HD2	2.48	0.49
1:E:204:LYS:O	1:E:208:HIS:HE1	1.96	0.48
1:B:112:LYS:HE2	1:B:113:TYR:OH	2.13	0.48
1:G:331:VAL:HG11	1:G:363:TYR:CB	2.44	0.48
1:E:116:LYS:HB2	1:E:122:PHE:CD2	2.49	0.48
1:E:32:ASP:OD1	1:E:208:HIS:HD2	1.97	0.48
1:G:56:ILE:HB	1:G:62:GLY:HA3	1.96	0.48
1:E:94:VAL:HA	1:E:98:ALA:HB3	1.94	0.48
1:F:272:ARG:HH12	1:F:277:PRO:HD3	1.79	0.48
1:B:331:VAL:HG21	1:B:363:TYR:HB2	1.95	0.48
1:A:372:ILE:HA	1:A:375:MET:HE3	1.95	0.48
1:E:71:ALA:O	1:E:75:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:73:MET:SD	1:E:247:LEU:HG	2.53	0.48
1:A:32:ASP:OD1	1:A:208:HIS:HD2	1.98	0.47
1:A:322:MET:HE3	1:B:293:VAL:HA	1.94	0.47
1:E:92:MET:SD	1:E:161:SER:HB2	2.55	0.47
1:D:389:ARG:O	1:D:390:LYS:C	2.51	0.47
1:E:282:GLN:HE22	3:F:400:FAD:H2A	1.79	0.47
1:D:357:TYR:CE2	1:E:357:TYR:CE2	3.03	0.47
1:E:282:GLN:NE2	1:G:283:MET:H	2.13	0.47
1:A:127:GLY:O	1:A:157:LYS:HE3	2.15	0.47
1:E:128:ILE:HB	3:E:400:FAD:O2	2.16	0.46
1:D:152:LEU:CD2	1:D:219:ASN:HA	2.46	0.46
1:B:100:THR:HG22	5:B:7158:HOH:O	2.15	0.46
1:D:283:MET:H	1:F:282:GLN:NE2	2.12	0.46
1:B:243:ASN:ND2	1:B:317:GLY:HA2	2.30	0.46
1:A:11:MET:HE2	1:A:14:LYS:HD2	1.96	0.46
3:B:400:FAD:H2'	3:B:400:FAD:H9	1.97	0.46
1:E:282:GLN:HB3	1:G:283:MET:HG3	1.98	0.46
1:A:204:LYS:O	1:A:208:HIS:HE1	1.98	0.46
1:D:204:LYS:O	1:D:208:HIS:HE1	1.98	0.46
1:A:130:GLU:HG2	1:A:157:LYS:HD3	1.98	0.46
1:E:18:ASN:HD21	1:E:22:LYS:HZ3	1.62	0.46
1:D:190:GLU:HB3	5:D:7587:HOH:O	2.15	0.46
1:D:197:ILE:HG12	1:D:217:LEU:HD22	1.97	0.46
3:F:400:FAD:C2'	3:F:400:FAD:H9	2.44	0.46
1:D:159:TRP:O	3:D:400:FAD:C4X	2.64	0.46
1:E:81:ARG:NH2	5:E:7557:HOH:O	2.46	0.46
1:D:77:GLU:HG2	1:D:255:GLY:HA2	1.97	0.46
1:B:17:ARG:HH12	1:B:81:ARG:NH2	2.14	0.46
1:F:76:THR:HG21	1:F:248:SER:OG	2.16	0.45
1:A:8:GLU:HG2	1:A:65:MET:CE	2.46	0.45
1:F:109:LEU:HD12	5:F:7583:HOH:O	2.17	0.45
1:B:360:ALA:N	1:B:361:PRO:CD	2.80	0.45
1:G:194:PHE:N	1:G:194:PHE:CD1	2.83	0.45
1:B:159:TRP:O	3:B:400:FAD:C4X	2.64	0.45
1:D:361:PRO:HA	1:D:364:TYR:CZ	2.52	0.45
1:F:130:GLU:HG2	1:F:157:LYS:HD3	1.98	0.45
1:D:266:LYS:HE2	1:D:270:GLU:OE1	2.16	0.45
1:B:18:ASN:HD21	1:B:22:LYS:NZ	2.14	0.45
1:F:76:THR:HG22	1:F:90:LEU:HD23	1.99	0.45
1:F:73:MET:SD	1:F:247:LEU:HG	2.56	0.45
1:E:52:PHE:O	1:E:94:VAL:HG21	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:ILE:HB	3:D:400:FAD:O2	2.17	0.44
1:B:197:ILE:HG12	1:B:217:LEU:HD22	2.00	0.44
1:A:360:ALA:N	1:A:361:PRO:CD	2.80	0.44
1:A:322:MET:HE2	1:B:293:VAL:HA	1.98	0.44
1:D:129:THR:OG1	3:D:400:FAD:H1'1	2.17	0.44
1:A:159:TRP:O	3:A:400:FAD:C10	2.66	0.44
1:A:17:ARG:HH12	1:A:81:ARG:CZ	2.30	0.44
1:E:69:TRP:O	1:E:73:MET:HG2	2.17	0.44
1:F:204:LYS:O	1:F:208:HIS:HE1	2.01	0.44
1:B:76:THR:HG21	1:B:248:SER:OG	2.18	0.43
1:E:291:MET:O	1:E:295:VAL:HG23	2.18	0.43
1:B:11:MET:HE2	1:B:14:LYS:CD	2.43	0.43
1:B:351:TYR:HB3	1:B:352:PRO:HD2	2.01	0.43
1:F:141:SER:O	1:F:177:LYS:NZ	2.40	0.43
1:E:123:LEU:HD13	1:E:165:GLN:HB3	2.00	0.43
1:F:42:ALA:C	1:F:45:PRO:HD2	2.39	0.43
1:A:145[A]:GLU:HG2	1:A:152:LEU:O	2.18	0.43
1:B:7:LYS:HD2	1:B:7:LYS:HA	1.74	0.43
1:E:194:PHE:HA	1:E:195:PRO:HD3	1.88	0.43
1:G:159:TRP:O	3:G:400:FAD:C4X	2.67	0.43
1:E:95:LEU:HD12	1:E:248:SER:HB2	2.00	0.43
1:E:31:TRP:CZ2	1:E:41:GLU:HG3	2.53	0.43
1:B:72:ALA:O	1:B:76:THR:HG23	2.17	0.43
1:A:76:THR:HG21	1:A:248:SER:OG	2.19	0.43
1:F:117:LEU:HD21	1:F:168:VAL:HG13	2.00	0.43
1:E:361:PRO:HA	1:E:364:TYR:CZ	2.53	0.43
1:G:204:LYS:O	1:G:208:HIS:CE1	2.70	0.42
1:A:84:SER:O	1:A:87:ARG:HG3	2.19	0.42
1:A:72:ALA:O	1:A:76:THR:HG23	2.19	0.42
1:G:99:TYR:O	1:G:102:LEU:HB3	2.19	0.42
1:B:54:THR:HA	1:B:63:GLU:HB2	2.01	0.42
1:G:81:ARG:HD2	5:G:7596:HOH:O	2.18	0.42
1:B:67:GLN:NE2	5:B:7247:HOH:O	2.20	0.42
1:E:9:LEU:HD11	1:E:67:GLN:HE21	1.85	0.42
1:E:116:LYS:HB2	1:E:122:PHE:CE2	2.55	0.42
1:A:75:VAL:O	1:A:79:ILE:HG13	2.20	0.42
1:G:331:VAL:HG11	1:G:363:TYR:HB2	2.02	0.42
1:A:325:TYR:CE1	1:A:374:LYS:HE3	2.55	0.42
1:E:122:PHE:HA	1:E:167:ASP:OD2	2.20	0.42
1:A:191:PRO:HA	1:A:197:ILE:HD13	2.02	0.42
1:B:32:ASP:OD1	1:B:208:HIS:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:ILE:HB	3:B:400:FAD:O2	2.21	0.41
1:G:319:ASP:H	1:G:388:ASN:HD21	1.67	0.41
1:D:31:TRP:HZ2	1:D:41:GLU:HG3	1.82	0.41
1:B:25:VAL:N	1:B:26:PRO:CD	2.83	0.41
1:E:322:MET:HE2	1:F:293:VAL:HA	2.03	0.41
1:A:124:GLY:HA2	1:A:168:VAL:O	2.21	0.41
1:G:128:ILE:HB	3:G:400:FAD:O2	2.20	0.41
1:E:362:THR:O	1:E:366:VAL:HG22	2.21	0.41
1:F:69:TRP:O	1:F:73:MET:HG2	2.20	0.41
1:A:7:LYS:HD2	1:A:7:LYS:HA	1.57	0.41
1:G:19:PHE:CE2	1:G:46:MET:CG	3.03	0.41
1:G:31:TRP:CE3	1:G:38:PRO:HG3	2.56	0.41
1:F:159:TRP:O	3:F:400:FAD:C4X	2.69	0.41
1:A:299:ARG:HH11	1:A:299:ARG:HD2	1.70	0.41
1:D:42:ALA:C	1:D:45:PRO:HD2	2.41	0.41
1:B:117:LEU:HD21	1:B:168:VAL:HG13	2.03	0.40
1:B:37:PHE:HB3	2:Y:47:HIS:H	1.87	0.40
1:B:23:LYS:HE2	1:B:23:LYS:HB3	1.95	0.40
1:D:70:LEU:CD2	1:G:1:MET:HG2	2.43	0.40
1:B:81:ARG:NH2	5:B:8022:HOH:O	2.30	0.40
1:A:162:ASN:HA	1:A:165:GLN:HE21	1.87	0.40
1:A:361:PRO:HA	1:A:364:TYR:CZ	2.57	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:390:LYS:O	2:Y:41:LYS:CG[4_455]	1.78	0.42
5:F:7936:HOH:O	5:G:8014:HOH:O[1_556]	2.19	0.01

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	389/397 (98%)	376 (97%)	13 (3%)	0	100 100
1	B	393/397 (99%)	380 (97%)	13 (3%)	0	100 100
1	D	390/397 (98%)	379 (97%)	11 (3%)	0	100 100
1	E	390/397 (98%)	368 (94%)	21 (5%)	1 (0%)	46 45
1	F	390/397 (98%)	378 (97%)	12 (3%)	0	100 100
1	G	387/397 (98%)	375 (97%)	11 (3%)	1 (0%)	46 45
2	Y	4/8 (50%)	2 (50%)	2 (50%)	0	100 100
All	All	2343/2390 (98%)	2258 (96%)	83 (4%)	2 (0%)	56 58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	179	ALA
1	E	148	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	304/309 (98%)	290 (95%)	14 (5%)	33 31
1	B	307/309 (99%)	286 (93%)	21 (7%)	20 16
1	D	305/309 (99%)	287 (94%)	18 (6%)	24 20
1	E	304/309 (98%)	282 (93%)	22 (7%)	18 14
1	F	305/309 (99%)	290 (95%)	15 (5%)	31 28
1	G	302/309 (98%)	289 (96%)	13 (4%)	35 34
2	Y	6/7 (86%)	5 (83%)	1 (17%)	3 1
All	All	1833/1861 (98%)	1729 (94%)	104 (6%)	27 22

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	11	MET
1	A	66[A]	ASP
1	A	66[B]	ASP
1	A	76	THR
1	A	90	LEU
1	A	93	GLU
1	A	100	THR
1	A	145[A]	GLU
1	A	145[B]	GLU
1	A	152	LEU
1	A	168	VAL
1	A	300	LEU
1	A	342	LEU
1	B	2	ASP
1	B	7	LYS
1	B	11	MET
1	B	25	VAL
1	B	63	GLU
1	B	76	THR
1	B	87	ARG
1	B	93	GLU
1	B	100	THR
1	B	145[A]	GLU
1	B	145[B]	GLU
1	B	152	LEU
1	B	168	VAL
1	B	169	LEU
1	B	230	LYS
1	B	300	LEU
1	B	331	VAL
1	B	342	LEU
1	B	350	GLU
1	B	390	LYS
1	B	393	HIS
1	D	2	ASP
1	D	11	MET
1	D	25	VAL
1	D	48	GLU
1	D	59	GLU
1	D	76	THR
1	D	93	GLU
1	D	100	THR

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Mol	Chain	Res	Type
1	D	111	LYS
1	D	145[A]	GLU
1	D	145[B]	GLU
1	D	152	LEU
1	D	165	GLN
1	D	168	VAL
1	D	217	LEU
1	D	280	ASP
1	D	300	LEU
1	D	342	LEU
1	E	7	LYS
1	E	11	MET
1	E	40	GLU
1	E	66	ASP
1	E	76	THR
1	E	90	LEU
1	E	93	GLU
1	E	100	THR
1	E	111	LYS
1	E	152	LEU
1	E	156	SER
1	E	169	LEU
1	E	182	ARG
1	E	210	SER
1	E	217	LEU
1	E	224	LYS
1	E	225	GLU
1	E	300	LEU
1	E	342	LEU
1	E	350	GLU
1	E	385[A]	ARG
1	E	385[B]	ARG
1	F	2	ASP
1	F	7	LYS
1	F	11	MET
1	F	25	VAL
1	F	76	THR
1	F	90	LEU
1	F	93	GLU
1	F	100	THR
1	F	152	LEU
1	F	168	VAL

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Mol	Chain	Res	Type
1	F	169	LEU
1	F	175	THR
1	F	217	LEU
1	F	300	LEU
1	F	342	LEU
1	G	2	ASP
1	G	7	LYS
1	G	11	MET
1	G	25	VAL
1	G	76	THR
1	G	100	THR
1	G	145	GLU
1	G	152	LEU
1	G	168	VAL
1	G	300	LEU
1	G	331	VAL
1	G	342	LEU
1	G	385	ARG
2	Y	47	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	21	ASN
1	A	33	ASN
1	A	165	GLN
1	A	208	HIS
1	A	243	ASN
1	A	269	ASN
1	A	282	GLN
1	A	388	ASN
1	B	18	ASN
1	B	21	ASN
1	B	33	ASN
1	B	36	HIS
1	B	165	GLN
1	B	208	HIS
1	B	269	ASN
1	B	282	GLN
1	B	388	ASN
1	D	21	ASN

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Mol	Chain	Res	Type
1	D	165	GLN
1	D	208	HIS
1	D	243	ASN
1	D	269	ASN
1	D	282	GLN
1	D	388	ASN
1	E	18	ASN
1	E	21	ASN
1	E	33	ASN
1	E	67	GLN
1	E	165	GLN
1	E	208	HIS
1	E	243	ASN
1	E	269	ASN
1	E	282	GLN
1	E	388	ASN
1	F	21	ASN
1	F	33	ASN
1	F	165	GLN
1	F	208	HIS
1	F	269	ASN
1	F	282	GLN
1	F	388	ASN
1	G	21	ASN
1	G	33	ASN
1	G	35	ASN
1	G	36	HIS
1	G	89	GLN
1	G	162	ASN
1	G	165	GLN
1	G	208	HIS
1	G	243	ASN
1	G	269	ASN
1	G	282	GLN
1	G	388	ASN
2	Y	45	HIS
2	Y	48	HIS

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 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
3	FAD	A	400	-	48,58,58	1.51	7 (14%)	54,89,89	2.97	18 (33%)
3	FAD	B	400	-	48,58,58	1.55	9 (18%)	54,89,89	2.51	14 (25%)
3	FAD	D	400	-	48,58,58	1.70	11 (22%)	54,89,89	2.19	9 (16%)
3	FAD	E	400	-	48,58,58	1.37	6 (12%)	54,89,89	2.21	12 (22%)
3	FAD	F	400	-	48,58,58	1.47	9 (18%)	54,89,89	2.55	16 (29%)
3	FAD	G	400	-	48,58,58	1.58	5 (10%)	54,89,89	2.60	12 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	A	400	-	-	0/30/50/50	0/6/6/6
3	FAD	B	400	-	-	0/30/50/50	0/6/6/6
3	FAD	D	400	-	-	0/30/50/50	0/6/6/6
3	FAD	E	400	-	-	0/30/50/50	0/6/6/6
3	FAD	F	400	-	-	0/30/50/50	0/6/6/6
3	FAD	G	400	-	-	0/30/50/50	0/6/6/6

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	400	FAD	PA-O2A	-2.61	1.43	1.54
3	A	400	FAD	P-O2P	-2.57	1.44	1.54
3	F	400	FAD	C6-C5X	-2.44	1.38	1.41
3	B	400	FAD	C9A-C5X	-2.12	1.38	1.42
3	B	400	FAD	O4B-C4B	-2.11	1.40	1.45
3	A	400	FAD	C9-C9A	-2.02	1.36	1.40
3	D	400	FAD	C6-C5X	-2.00	1.38	1.41
3	D	400	FAD	C5X-N5	2.00	1.38	1.35
3	F	400	FAD	C5'-C4'	2.01	1.54	1.51
3	F	400	FAD	C9A-N10	2.02	1.41	1.38
3	E	400	FAD	C9A-N10	2.02	1.41	1.38
3	E	400	FAD	C4-N3	2.03	1.36	1.33
3	D	400	FAD	C2A-N3A	2.10	1.35	1.32
3	A	400	FAD	C5'-C4'	2.11	1.54	1.51
3	B	400	FAD	C4X-N5	2.18	1.36	1.33
3	D	400	FAD	C1'-N10	2.18	1.50	1.48
3	B	400	FAD	C10-N1	2.26	1.39	1.35
3	E	400	FAD	C2A-N1A	2.34	1.38	1.33
3	A	400	FAD	C4X-N5	2.40	1.37	1.33
3	D	400	FAD	C10-N10	2.52	1.42	1.39
3	B	400	FAD	C5X-N5	2.52	1.39	1.35
3	B	400	FAD	C2A-N1A	2.60	1.38	1.33
3	D	400	FAD	C2A-N1A	2.66	1.38	1.33
3	D	400	FAD	C10-N1	2.73	1.40	1.35
3	G	400	FAD	C2A-N1A	2.79	1.39	1.33
3	F	400	FAD	C1'-N10	2.96	1.51	1.48
3	F	400	FAD	C5X-N5	3.02	1.40	1.35
3	A	400	FAD	C5X-N5	3.02	1.40	1.35
3	F	400	FAD	C2A-N1A	3.19	1.40	1.33
3	G	400	FAD	C2A-N3A	3.20	1.37	1.32
3	E	400	FAD	C2A-N3A	3.28	1.38	1.32
3	A	400	FAD	C2A-N1A	3.36	1.40	1.33
3	F	400	FAD	C4-N3	3.47	1.39	1.33
3	F	400	FAD	C4X-N5	3.47	1.38	1.33
3	F	400	FAD	C2A-N3A	3.52	1.38	1.32
3	G	400	FAD	C4-N3	3.57	1.39	1.33
3	B	400	FAD	C2A-N3A	3.59	1.38	1.32
3	B	400	FAD	C4-N3	3.99	1.40	1.33
3	E	400	FAD	C4X-N5	4.19	1.39	1.33
3	G	400	FAD	C1'-N10	4.29	1.52	1.48
3	D	400	FAD	O4B-C1B	4.47	1.46	1.41
3	D	400	FAD	C4X-N5	4.57	1.40	1.33
3	E	400	FAD	C1'-N10	4.64	1.53	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	400	FAD	C1'-N10	4.86	1.53	1.48
3	D	400	FAD	C4-N3	5.08	1.42	1.33
3	A	400	FAD	C2A-N3A	5.51	1.41	1.32
3	G	400	FAD	C4X-N5	6.31	1.43	1.33

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	400	FAD	N3A-C2A-N1A	-14.87	117.51	128.89
3	G	400	FAD	N3A-C2A-N1A	-12.94	118.99	128.89
3	F	400	FAD	N3A-C2A-N1A	-11.93	119.76	128.89
3	B	400	FAD	N3A-C2A-N1A	-11.62	120.00	128.89
3	D	400	FAD	N3A-C2A-N1A	-11.57	120.03	128.89
3	E	400	FAD	N3A-C2A-N1A	-10.47	120.88	128.89
3	B	400	FAD	C4X-C4-N3	-4.84	116.97	123.59
3	A	400	FAD	C4X-C4-N3	-4.34	117.66	123.59
3	F	400	FAD	C4X-C4-N3	-4.30	117.70	123.59
3	B	400	FAD	C1B-N9A-C4A	-4.18	120.63	126.94
3	A	400	FAD	C1B-N9A-C4A	-4.12	120.72	126.94
3	F	400	FAD	P-O3P-PA	-3.74	122.22	132.73
3	F	400	FAD	O4'-C4'-C3'	-3.36	100.56	109.02
3	E	400	FAD	P-O3P-PA	-3.31	123.42	132.73
3	G	400	FAD	C9A-C5X-N5	-3.02	117.89	122.36
3	G	400	FAD	C4X-C4-N3	-2.97	119.52	123.59
3	G	400	FAD	C4-C4X-C10	-2.85	118.12	119.94
3	F	400	FAD	O3'-C3'-C4'	-2.79	101.72	108.75
3	B	400	FAD	O4'-C4'-C3'	-2.78	102.02	109.02
3	A	400	FAD	O4'-C4'-C3'	-2.65	102.35	109.02
3	A	400	FAD	C7-C6-C5X	-2.63	116.63	120.92
3	F	400	FAD	C1B-N9A-C4A	-2.62	122.99	126.94
3	A	400	FAD	P-O3P-PA	-2.56	125.53	132.73
3	E	400	FAD	C4X-C4-N3	-2.53	120.13	123.59
3	A	400	FAD	O3B-C3B-C4B	-2.46	103.66	111.05
3	D	400	FAD	P-O3P-PA	-2.42	125.94	132.73
3	B	400	FAD	C9A-C5X-N5	-2.30	118.95	122.36
3	B	400	FAD	O3P-PA-O5B	-2.22	97.05	102.94
3	G	400	FAD	C4X-C10-N10	-2.20	119.22	120.52
3	B	400	FAD	C4A-C5A-N7A	-2.19	107.47	109.48
3	G	400	FAD	C1B-N9A-C4A	-2.12	123.74	126.94
3	D	400	FAD	C5B-C4B-C3B	-2.12	106.81	115.21
3	A	400	FAD	C9A-C5X-N5	-2.09	119.27	122.36
3	F	400	FAD	O3B-C3B-C4B	-2.06	104.87	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	400	FAD	C1'-N10-C9A	2.03	121.14	118.86
3	A	400	FAD	O2'-C2'-C3'	2.05	114.17	109.02
3	G	400	FAD	C2A-N1A-C6A	2.05	122.43	118.77
3	D	400	FAD	C6-C5X-C9A	2.06	121.69	118.98
3	B	400	FAD	C5X-C9A-N10	2.10	119.22	117.62
3	F	400	FAD	O2A-PA-O3P	2.13	114.78	105.09
3	B	400	FAD	C2A-N1A-C6A	2.14	122.59	118.77
3	A	400	FAD	C5X-C9A-N10	2.14	119.25	117.62
3	G	400	FAD	C6-C5X-C9A	2.20	121.88	118.98
3	B	400	FAD	C4B-O4B-C1B	2.22	112.15	109.72
3	F	400	FAD	C4-C4X-N5	2.34	121.56	118.72
3	E	400	FAD	C6-C5X-C9A	2.41	122.16	118.98
3	A	400	FAD	C2A-N1A-C6A	2.44	123.13	118.77
3	A	400	FAD	C1'-N10-C9A	2.45	121.61	118.86
3	A	400	FAD	N6A-C6A-N1A	2.46	124.48	119.20
3	D	400	FAD	C4-N3-C2	2.53	117.43	115.25
3	E	400	FAD	C4B-O4B-C1B	2.61	112.58	109.72
3	E	400	FAD	O2A-PA-O3P	2.63	117.01	105.09
3	B	400	FAD	C4-C4X-C10	2.69	121.66	119.94
3	F	400	FAD	C5X-C9A-N10	2.70	119.67	117.62
3	A	400	FAD	C6-C5X-C9A	2.76	122.61	118.98
3	F	400	FAD	O3'-C3'-C2'	2.78	115.75	108.75
3	E	400	FAD	C1'-C2'-C3'	2.80	117.84	109.82
3	F	400	FAD	O2'-C2'-C3'	2.87	116.22	109.02
3	G	400	FAD	C4X-N5-C5X	2.90	120.10	116.76
3	E	400	FAD	C4X-N5-C5X	2.98	120.19	116.76
3	D	400	FAD	O3'-C3'-C2'	2.99	116.28	108.75
3	D	400	FAD	C5X-C9A-N10	3.03	119.92	117.62
3	E	400	FAD	O2'-C2'-C1'	3.19	117.79	109.94
3	A	400	FAD	O3'-C3'-C2'	3.33	117.14	108.75
3	F	400	FAD	O3P-P-O5'	3.57	112.40	102.94
3	F	400	FAD	C4X-N5-C5X	3.66	120.97	116.76
3	D	400	FAD	C4X-N5-C5X	3.69	121.01	116.76
3	G	400	FAD	O2'-C2'-C1'	3.81	119.31	109.94
3	F	400	FAD	C1'-N10-C9A	4.12	123.48	118.86
3	A	400	FAD	C4X-N5-C5X	4.42	121.85	116.76
3	B	400	FAD	C4X-N5-C5X	4.75	122.23	116.76
3	E	400	FAD	C4-N3-C2	4.77	119.37	115.25
3	E	400	FAD	C5X-C9A-N10	4.78	121.25	117.62
3	A	400	FAD	O2'-C2'-C1'	5.08	122.42	109.94
3	B	400	FAD	O2'-C2'-C1'	5.11	122.51	109.94
3	D	400	FAD	O2'-C2'-C1'	5.15	122.61	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	400	FAD	C5X-C9A-N10	5.57	121.85	117.62
3	B	400	FAD	C4-N3-C2	6.15	120.56	115.25
3	F	400	FAD	C4-N3-C2	6.42	120.80	115.25
3	G	400	FAD	C4-N3-C2	7.02	121.32	115.25
3	A	400	FAD	C4-N3-C2	8.87	122.91	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	400	FAD	4	0
3	B	400	FAD	4	0
3	D	400	FAD	5	0
3	E	400	FAD	4	0
3	F	400	FAD	5	0
3	G	400	FAD	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	389/397 (97%)	-0.28	1 (0%) 94 95	13, 25, 43, 57	0
1	B	393/397 (98%)	-0.10	7 (1%) 71 76	13, 27, 48, 92	0
1	D	390/397 (98%)	0.83	43 (11%) 7 10	23, 47, 75, 88	0
1	E	391/397 (98%)	0.96	84 (21%) 1 1	18, 51, 99, 141	0
1	F	390/397 (98%)	-0.10	3 (0%) 87 90	16, 31, 50, 64	0
1	G	389/397 (97%)	0.30	12 (3%) 52 61	22, 39, 61, 77	0
2	Y	8/8 (100%)	1.99	4 (50%) 0 0	29, 48, 58, 76	0
All	All	2350/2390 (98%)	0.27	154 (6%) 22 29	13, 35, 73, 141	0

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	393	HIS	5.5
1	E	108	ALA	5.4
1	E	155	GLY	5.1
1	E	169	LEU	5.1
1	E	144	ALA	4.8
2	Y	41	LYS	4.8
1	D	11	MET	4.7
1	E	90	LEU	4.6
1	E	122	PHE	4.5
1	E	170	ILE	4.5
1	D	40	GLU	4.3
1	E	189	ILE	4.3
1	E	227	ILE	4.2
1	E	96	GLY	4.2
1	D	390	LYS	4.1
1	D	95	LEU	4.0
1	E	168	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	E	150	HIS	3.9
1	E	88	VAL	3.8
1	E	148	GLY	3.6
1	E	217	LEU	3.6
1	D	245	THR	3.5
1	E	187	PHE	3.5
1	D	90	LEU	3.4
1	E	153	LEU	3.4
1	E	222	VAL	3.4
1	E	391	GLY	3.4
1	E	92	MET	3.4
1	E	151	TRP	3.4
1	D	76	THR	3.3
1	E	40	GLU	3.3
1	D	92	MET	3.3
1	B	391	GLY	3.3
1	E	180	GLY	3.2
1	E	95	LEU	3.2
1	G	66	ASP	3.2
1	E	97	CYS	3.2
1	E	188	VAL	3.2
1	D	66	ASP	3.1
1	D	58	GLU	3.1
1	E	116	LYS	3.1
1	D	91	ASN	3.1
1	E	218	ASP	3.1
1	E	126	PHE	3.1
1	E	152	LEU	3.0
1	E	178	ALA	3.0
1	D	52	PHE	3.0
1	E	249	ALA	3.0
1	E	104	TYR	2.9
1	D	27	PHE	2.9
1	G	389	ARG	2.9
1	E	98	ALA	2.9
1	D	97	CYS	2.9
1	E	220	VAL	2.9
1	E	174	TYR	2.9
1	E	221	LYS	2.9
1	D	30	GLN	2.9
1	G	313	ARG	2.9
1	B	11	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	146	ASP	2.9
1	E	171	TYR	2.9
1	E	94	VAL	2.9
2	Y	48	HIS	2.8
1	E	215	LEU	2.8
1	B	392	HIS	2.8
1	D	123	LEU	2.8
1	E	106	SER	2.8
1	E	124	GLY	2.8
1	G	230	LYS	2.8
1	D	44	ARG	2.8
1	G	385	ARG	2.8
1	D	351	TYR	2.7
1	G	27	PHE	2.7
1	D	121	GLU	2.7
1	E	198	LYS	2.7
1	E	164	ALA	2.7
1	E	113	TYR	2.7
2	Y	43	HIS	2.7
1	E	128	ILE	2.6
2	Y	47	HIS	2.6
1	D	100	THR	2.6
1	E	177	LYS	2.6
1	G	11	MET	2.6
1	E	132	ASP	2.6
1	E	163	ALA	2.6
1	E	366	VAL	2.6
1	D	105	GLY	2.6
1	E	66	ASP	2.6
1	D	88	VAL	2.6
1	E	145	GLU	2.6
1	E	223	PRO	2.5
1	E	197	ILE	2.5
1	E	91	ASN	2.5
1	E	154	ASN	2.5
1	E	182	ARG	2.5
1	E	39	TYR	2.5
1	E	149	ASP	2.5
1	D	168	VAL	2.5
1	E	112	LYS	2.4
1	G	168	VAL	2.4
1	E	390	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	87	ARG	2.4
1	F	385[A]	ARG	2.4
1	E	99	TYR	2.4
1	E	147	LYS	2.4
1	E	203	GLU	2.4
1	E	248	SER	2.4
1	D	48	GLU	2.4
1	E	216	PHE	2.4
1	D	18	ASN	2.4
1	D	125	GLY	2.4
1	D	353	VAL	2.3
1	E	76	THR	2.3
1	D	49	LEU	2.3
1	D	231	PRO	2.3
1	D	14	LYS	2.3
1	G	7	LYS	2.3
1	D	251	ALA	2.3
1	D	53	GLY	2.3
1	E	230	LYS	2.3
1	G	62	GLY	2.3
1	A	182	ARG	2.3
1	E	251	ALA	2.3
1	D	241	SER	2.2
1	E	172	TYR	2.2
1	D	74	ILE	2.2
1	D	96	GLY	2.2
1	E	60	TYR	2.2
1	E	140	MET	2.2
1	D	111	LYS	2.2
1	D	172	TYR	2.2
1	D	55	VAL	2.2
1	D	170	ILE	2.2
1	E	235	ALA	2.2
1	E	167	ASP	2.2
1	F	11	MET	2.1
1	B	169	LEU	2.1
1	F	170	ILE	2.1
1	E	48	GLU	2.1
1	E	85	ALA	2.1
1	E	231	PRO	2.1
1	E	93	GLU	2.1
1	E	160	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	232	GLY	2.1
1	E	315	ASN	2.1
1	D	179	ALA	2.1
1	E	179	ALA	2.0
1	E	11	MET	2.0
1	B	390	LYS	2.0
1	G	125	GLY	2.0
1	E	195	PRO	2.0
1	B	96	GLY	2.0
1	D	180	GLY	2.0
1	G	149	ASP	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^{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
3	FAD	D	400	53/53	0.95	0.13	0.10	21,27,37,39	0
3	FAD	G	400	53/53	0.94	0.11	0.04	24,29,35,36	0
3	FAD	B	400	53/53	0.96	0.10	0.02	15,20,25,26	0
3	FAD	A	400	53/53	0.96	0.09	-0.11	16,20,24,27	0
3	FAD	F	400	53/53	0.97	0.09	-0.34	19,23,28,32	0
3	FAD	E	400	53/53	0.89	0.14	-0.40	32,43,55,62	0
4	CL	E	401	1/1	0.89	0.16	-0.73	54,54,54,54	0
4	CL	F	401	1/1	0.98	0.05	-1.44	36,36,36,36	0
4	CL	G	401	1/1	0.98	0.05	-1.69	38,38,38,38	0
4	CL	B	401	1/1	0.98	0.07	-1.69	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	CL	D	401	1/1	0.89	0.06	-2.11	45,45,45,45	0
4	CL	A	401	1/1	0.98	0.04	-2.56	32,32,32,32	0

6.5 Other polymers (i)

There are no such residues in this entry.