



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:38 AM GMT

PDB ID : 3BG6
Title : Pyranose 2-oxidase from Trametes multicolor, E542K mutant
Authors : Tan, T.C.; Divne, C.
Deposited on : 2007-11-26
Resolution : 1.70 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 ⓘ symbol.

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

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

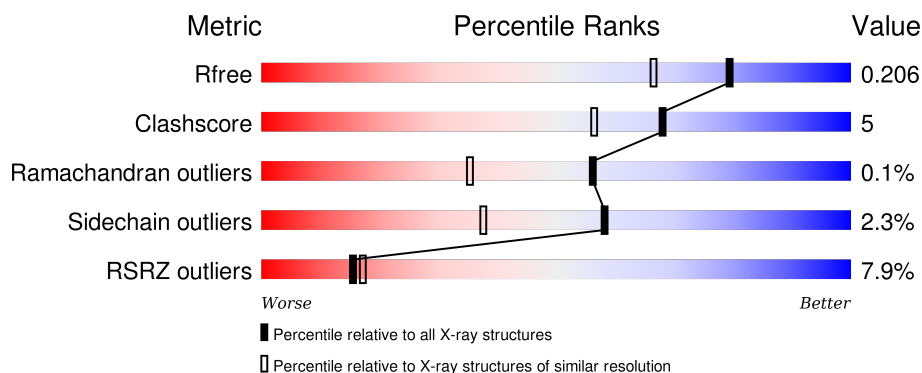
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	623	
1	B	623	
1	C	623	
1	D	623	
1	E	623	

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Mol	Chain	Length	Quality of chain
1	F	623	<div><div></div><div>9%</div><div>83%</div><div>8% • 7%</div></div>
1	G	623	<div><div></div><div>8%</div><div>83%</div><div>9% • 7%</div></div>
1	H	623	<div><div></div><div>6%</div><div>83%</div><div>9% • 7%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 39362 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 Pyranose oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	577	Total	C	N	O	S	0	0	0
			4549	2873	779	872	25			
1	B	577	Total	C	N	O	S	0	0	0
			4549	2873	779	872	25			
1	C	577	Total	C	N	O	S	0	0	0
			4549	2873	779	872	25			
1	D	577	Total	C	N	O	S	0	0	0
			4549	2873	779	872	25			
1	E	577	Total	C	N	O	S	0	0	0
			4549	2873	779	872	25			
1	F	577	Total	C	N	O	S	0	0	0
			4549	2873	779	872	25			
1	G	577	Total	C	N	O	S	0	0	0
			4549	2873	779	872	25			
1	H	577	Total	C	N	O	S	0	0	0
			4549	2873	779	872	25			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	542	LYS	GLU	ENGINEERED	UNP Q7ZA32
B	542	LYS	GLU	ENGINEERED	UNP Q7ZA32
C	542	LYS	GLU	ENGINEERED	UNP Q7ZA32
D	542	LYS	GLU	ENGINEERED	UNP Q7ZA32
E	542	LYS	GLU	ENGINEERED	UNP Q7ZA32
F	542	LYS	GLU	ENGINEERED	UNP Q7ZA32
G	542	LYS	GLU	ENGINEERED	UNP Q7ZA32
H	542	LYS	GLU	ENGINEERED	UNP Q7ZA32

- 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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	359	Total	O	0	0
			359	359		
3	B	373	Total	O	0	0
			373	373		
3	C	267	Total	O	0	0
			267	267		
3	D	314	Total	O	0	0
			314	314		

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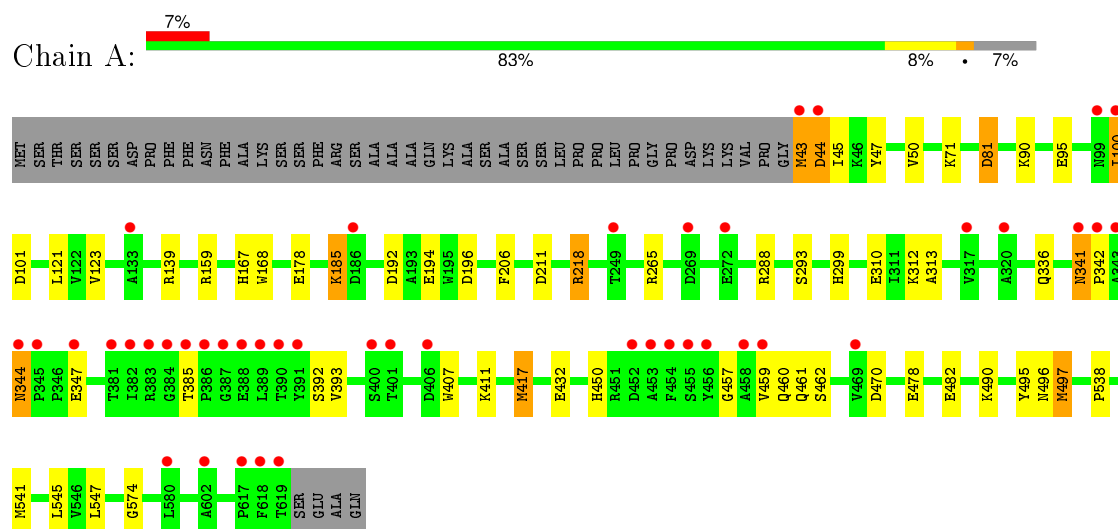
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	301	Total 301	O 301	0	0
3	F	262	Total 262	O 262	0	0
3	G	315	Total 315	O 315	0	0
3	H	355	Total 355	O 355	0	0

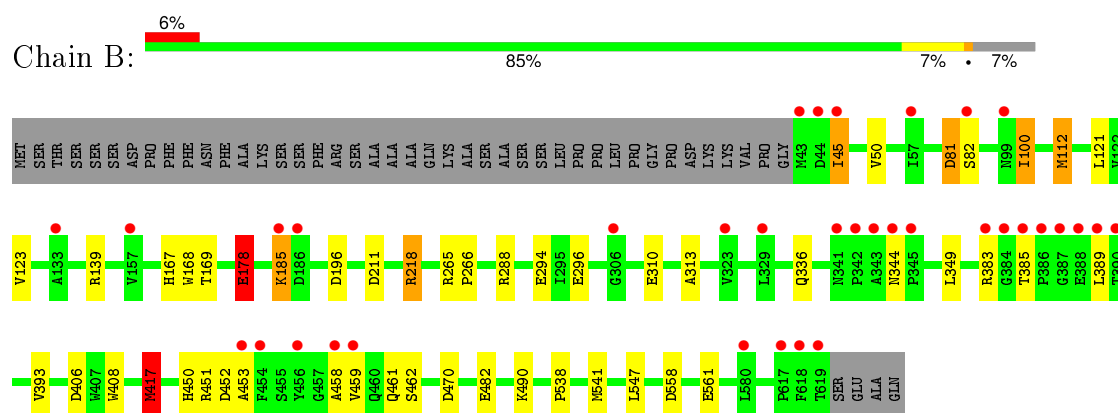
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

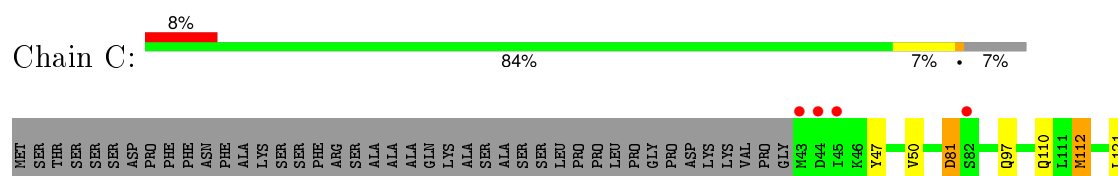
• Molecule 1: Pyranose oxidase

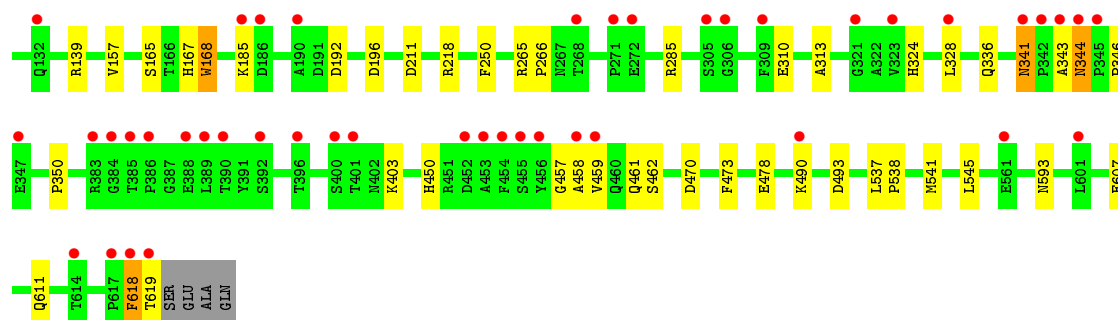


• Molecule 1: Pyranose oxidase

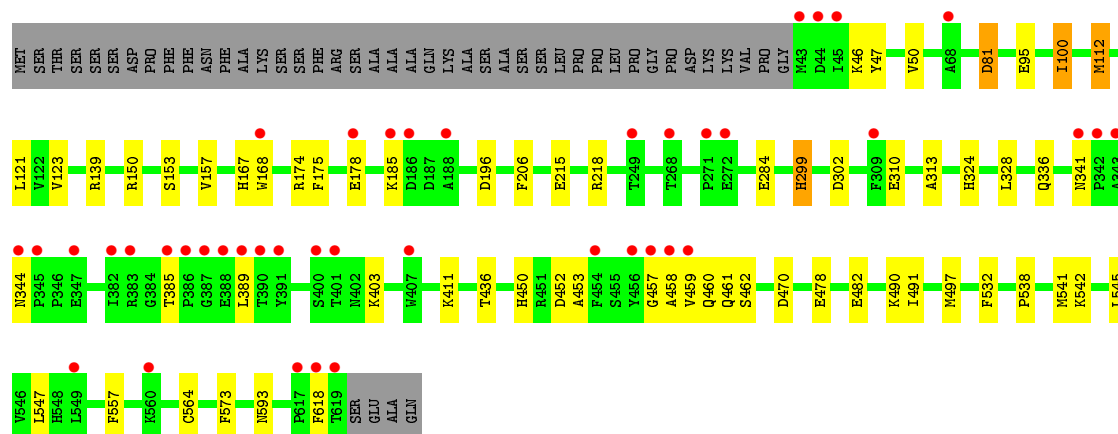
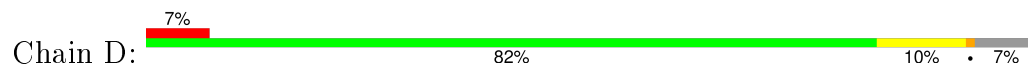


• Molecule 1: Pyranose oxidase

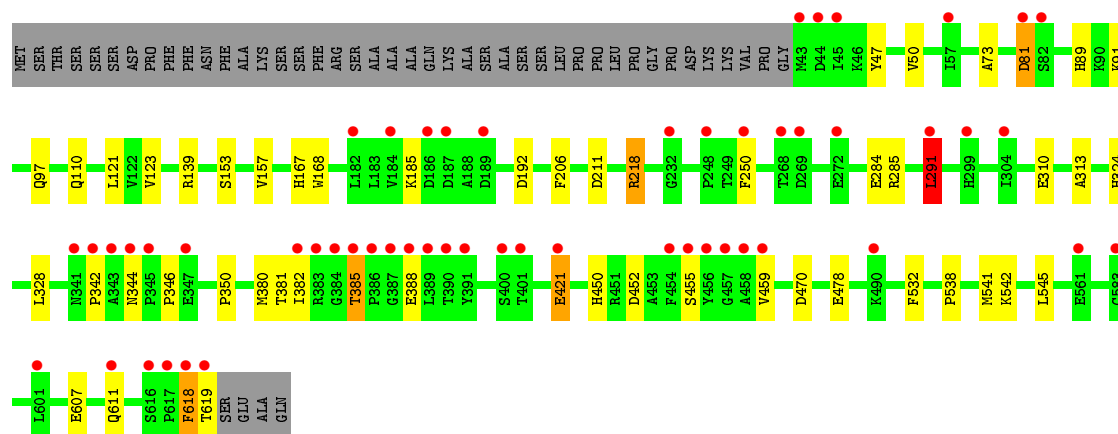
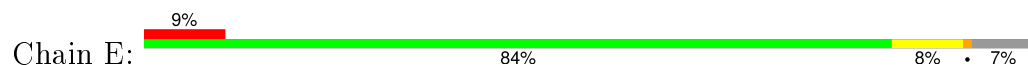




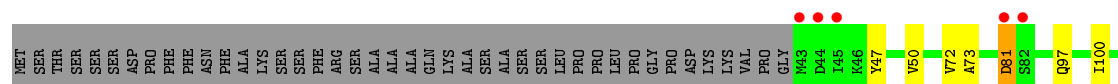
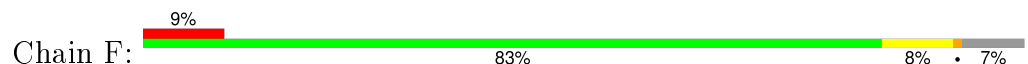
- Molecule 1: Pyranose oxidase

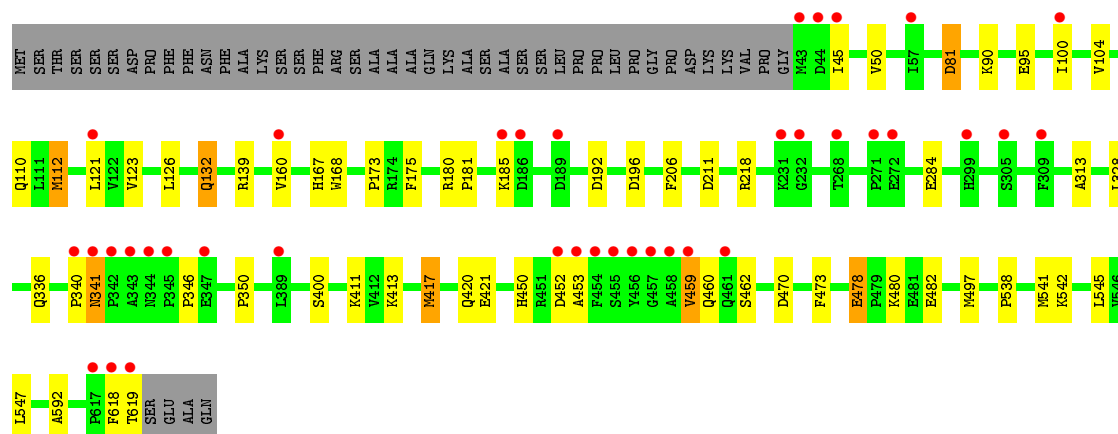


- Molecule 1: Pyranose oxidase



- Molecule 1: Pyranose oxidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	168.86Å 103.75Å 169.33Å 90.00° 106.31° 90.00°	Depositor
Resolution (Å)	40.00 – 1.70 39.18 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.3 (40.00-1.70) 98.3 (39.18-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.166 , 0.198 0.177 , 0.206	Depositor DCC
R_{free} test set	6061 reflections (1.01%)	DCC
Wilson B-factor (Å ²)	17.8	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 50.3	EDS
Estimated twinning fraction	0.014 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 603616 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	39362	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.09	11/4665 (0.2%)	1.03	18/6342 (0.3%)
1	B	1.11	7/4665 (0.2%)	1.05	17/6342 (0.3%)
1	C	0.91	2/4665 (0.0%)	0.94	13/6342 (0.2%)
1	D	0.97	6/4665 (0.1%)	0.96	13/6342 (0.2%)
1	E	0.98	5/4665 (0.1%)	0.96	10/6342 (0.2%)
1	F	0.96	5/4665 (0.1%)	0.99	10/6342 (0.2%)
1	G	1.01	6/4665 (0.1%)	0.96	11/6342 (0.2%)
1	H	1.07	11/4665 (0.2%)	1.03	18/6342 (0.3%)
All	All	1.01	53/37320 (0.1%)	0.99	110/50736 (0.2%)

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	A	0	1
1	D	0	1
All	All	0	2

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	291	LEU	CG-CD1	12.75	1.99	1.51
1	A	194	GLU	CG-CD	-8.00	1.40	1.51
1	H	478	GLU	CD-OE1	7.85	1.34	1.25
1	B	482	GLU	CD-OE1	7.83	1.34	1.25
1	E	478	GLU	CD-OE1	7.68	1.34	1.25
1	A	478	GLU	CD-OE1	7.51	1.33	1.25
1	H	81	ASP	CB-CG	-7.37	1.36	1.51
1	F	371	GLU	CG-CD	7.14	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	310	GLU	CB-CG	-7.14	1.38	1.52
1	B	482	GLU	CG-CD	7.08	1.62	1.51
1	D	112	MET	CB-CG	6.89	1.73	1.51
1	D	482	GLU	CG-CD	6.77	1.62	1.51
1	C	478	GLU	CD-OE1	6.74	1.33	1.25
1	B	310	GLU	CB-CG	-6.72	1.39	1.52
1	B	112	MET	CB-CG	6.66	1.72	1.51
1	A	482	GLU	CD-OE1	6.54	1.32	1.25
1	H	421	GLU	CB-CG	6.51	1.64	1.52
1	C	310	GLU	CG-CD	6.45	1.61	1.51
1	H	421	GLU	CD-OE1	-6.43	1.18	1.25
1	A	482	GLU	CG-CD	6.38	1.61	1.51
1	H	95	GLU	CB-CG	-6.27	1.40	1.52
1	H	160	VAL	CB-CG1	6.24	1.66	1.52
1	F	112	MET	CB-CG	6.23	1.71	1.51
1	A	81	ASP	CB-CG	-6.20	1.38	1.51
1	E	310	GLU	CG-CD	6.11	1.61	1.51
1	B	139	ARG	CD-NE	-6.05	1.36	1.46
1	F	478	GLU	CD-OE1	6.03	1.32	1.25
1	D	478	GLU	CD-OE1	6.00	1.32	1.25
1	G	91	LYS	CE-NZ	5.98	1.64	1.49
1	B	178	GLU	CB-CG	-5.97	1.40	1.52
1	H	478	GLU	CG-CD	5.86	1.60	1.51
1	D	139	ARG	CD-NE	-5.83	1.36	1.46
1	F	72	VAL	CB-CG2	5.76	1.65	1.52
1	D	482	GLU	CD-OE1	5.73	1.31	1.25
1	G	478	GLU	CD-OE2	5.69	1.31	1.25
1	H	482	GLU	CG-CD	5.63	1.60	1.51
1	A	196	ASP	CB-CG	5.62	1.63	1.51
1	A	139	ARG	CD-NE	-5.61	1.36	1.46
1	F	139	ARG	CD-NE	-5.50	1.37	1.46
1	A	178	GLU	CG-CD	5.46	1.60	1.51
1	D	482	GLU	CD-OE2	5.46	1.31	1.25
1	H	139	ARG	CD-NE	-5.43	1.37	1.46
1	A	95	GLU	CB-CG	-5.41	1.41	1.52
1	H	482	GLU	CD-OE1	5.29	1.31	1.25
1	A	478	GLU	CG-CD	5.28	1.59	1.51
1	E	478	GLU	CG-CD	5.25	1.59	1.51
1	G	122	VAL	CB-CG2	5.18	1.63	1.52
1	H	104	VAL	CB-CG2	-5.14	1.42	1.52
1	G	139	ARG	CD-NE	-5.12	1.37	1.46
1	B	82	SER	N-CA	5.11	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	81	ASP	CB-CG	-5.07	1.41	1.51
1	G	482	GLU	CG-CD	5.05	1.59	1.51
1	A	432	GLU	CD-OE2	5.03	1.31	1.25

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	139	ARG	NE-CZ-NH2	-23.75	108.43	120.30
1	B	139	ARG	NE-CZ-NH2	-19.64	110.48	120.30
1	E	139	ARG	NE-CZ-NH1	18.29	129.44	120.30
1	F	139	ARG	NE-CZ-NH1	18.25	129.43	120.30
1	D	139	ARG	NE-CZ-NH2	-18.23	111.18	120.30
1	H	139	ARG	NE-CZ-NH2	-17.91	111.34	120.30
1	A	139	ARG	NE-CZ-NH2	-17.80	111.40	120.30
1	E	139	ARG	NE-CZ-NH2	-17.80	111.40	120.30
1	C	139	ARG	NE-CZ-NH2	-17.64	111.48	120.30
1	G	139	ARG	NE-CZ-NH1	17.16	128.88	120.30
1	B	139	ARG	NE-CZ-NH1	16.29	128.45	120.30
1	C	139	ARG	NE-CZ-NH1	16.28	128.44	120.30
1	G	139	ARG	NE-CZ-NH2	-15.21	112.69	120.30
1	H	139	ARG	NE-CZ-NH1	14.75	127.67	120.30
1	A	139	ARG	NE-CZ-NH1	14.18	127.39	120.30
1	D	139	ARG	NE-CZ-NH1	13.37	126.99	120.30
1	F	218	ARG	NE-CZ-NH1	12.72	126.66	120.30
1	H	81	ASP	CB-CG-OD1	-11.80	107.68	118.30
1	H	211	ASP	CB-CG-OD1	11.18	128.36	118.30
1	E	81	ASP	CB-CG-OD1	-10.82	108.56	118.30
1	A	81	ASP	CB-CG-OD1	-10.68	108.69	118.30
1	B	218	ARG	NE-CZ-NH1	10.30	125.45	120.30
1	B	81	ASP	CB-CG-OD1	-10.10	109.22	118.30
1	C	81	ASP	CB-CG-OD1	-9.84	109.45	118.30
1	A	211	ASP	CB-CG-OD1	9.62	126.96	118.30
1	E	218	ARG	NE-CZ-NH1	9.33	124.97	120.30
1	F	81	ASP	CB-CG-OD1	-9.25	109.98	118.30
1	C	81	ASP	CB-CG-OD2	9.01	126.41	118.30
1	B	417	MET	CG-SD-CE	-8.69	86.30	100.20
1	A	218	ARG	NE-CZ-NH1	8.41	124.51	120.30
1	G	196	ASP	CB-CG-OD1	7.97	125.47	118.30
1	B	211	ASP	CB-CG-OD1	7.93	125.44	118.30
1	C	211	ASP	CB-CG-OD1	7.92	125.42	118.30
1	A	196	ASP	CB-CG-OD1	7.34	124.91	118.30
1	B	451	ARG	NE-CZ-NH1	7.30	123.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	470	ASP	CB-CG-OD1	7.25	124.83	118.30
1	G	211	ASP	CB-CG-OD1	7.17	124.75	118.30
1	A	159	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	B	470	ASP	CB-CG-OD2	-6.96	112.03	118.30
1	E	211	ASP	CB-CG-OD1	6.89	124.50	118.30
1	A	417	MET	CG-SD-CE	-6.86	89.22	100.20
1	D	81	ASP	CB-CG-OD1	-6.85	112.13	118.30
1	H	112	MET	CG-SD-CE	6.76	111.01	100.20
1	H	211	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	G	218	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	D	470	ASP	CB-CG-OD1	6.51	124.16	118.30
1	H	218	ARG	NE-CZ-NH1	6.51	123.55	120.30
1	F	314	ASP	CB-CG-OD1	6.45	124.11	118.30
1	B	81	ASP	CB-CG-OD2	6.43	124.09	118.30
1	H	473	PHE	CB-CG-CD2	-6.43	116.30	120.80
1	B	196	ASP	CB-CG-OD1	6.42	124.08	118.30
1	D	196	ASP	CB-CG-OD1	6.37	124.03	118.30
1	C	470	ASP	CB-CG-OD2	-6.37	112.57	118.30
1	C	192	ASP	CB-CG-OD1	6.26	123.94	118.30
1	A	288	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	E	81	ASP	CB-CG-OD2	6.22	123.90	118.30
1	H	192	ASP	CB-CG-OD1	6.21	123.89	118.30
1	B	218	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	H	139	ARG	CA-CB-CG	6.07	126.75	113.40
1	A	497	MET	CG-SD-CE	6.06	109.89	100.20
1	H	192	ASP	CB-CG-OD2	-6.06	112.85	118.30
1	H	470	ASP	CB-CG-OD1	6.05	123.75	118.30
1	F	139	ARG	CD-NE-CZ	6.04	132.06	123.60
1	B	470	ASP	CB-CG-OD1	6.02	123.72	118.30
1	D	218	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	G	288	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	C	139	ARG	CD-NE-CZ	5.82	131.75	123.60
1	B	349	LEU	CB-CG-CD2	5.80	120.85	111.00
1	B	406	ASP	CB-CG-OD1	5.77	123.49	118.30
1	B	139	ARG	CD-NE-CZ	5.75	131.65	123.60
1	B	288	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	D	139	ARG	CD-NE-CZ	5.68	131.55	123.60
1	A	265	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	H	175	PHE	CB-CG-CD1	5.60	124.72	120.80
1	F	261	ASP	CB-CG-OD1	5.57	123.31	118.30
1	H	196	ASP	CB-CG-OD1	5.56	123.30	118.30
1	E	192	ASP	CB-CG-OD1	5.54	123.28	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	470	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	495	TYR	CD1-CE1-CZ	-5.50	114.85	119.80
1	G	470	ASP	CB-CG-OD2	-5.45	113.40	118.30
1	F	470	ASP	CB-CG-OD1	5.44	123.20	118.30
1	E	291	LEU	CB-CG-CD1	5.41	120.20	111.00
1	A	81	ASP	CB-CG-OD2	5.37	123.14	118.30
1	E	470	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	A	470	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	H	411	LYS	CD-CE-NZ	-5.29	99.53	111.70
1	G	265	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	F	81	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	211	ASP	CB-CG-OD2	-5.25	113.57	118.30
1	B	383	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	G	150	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	C	473	PHE	CB-CG-CD2	-5.23	117.14	120.80
1	D	81	ASP	CB-CG-OD2	5.22	123.00	118.30
1	F	472	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	G	234	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	H	175	PHE	CB-CG-CD2	-5.19	117.17	120.80
1	H	473	PHE	CB-CG-CD1	5.18	124.43	120.80
1	D	389	LEU	CA-CB-CG	5.17	127.19	115.30
1	G	473	PHE	CB-CG-CD2	-5.15	117.20	120.80
1	A	139	ARG	CD-NE-CZ	5.10	130.74	123.60
1	D	175	PHE	CB-CG-CD2	-5.10	117.23	120.80
1	D	302	ASP	CB-CG-OD1	5.09	122.89	118.30
1	C	211	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	D	174	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	D	150	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	H	497	MET	CG-SD-CE	5.02	108.24	100.20
1	C	493	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	A	192	ASP	CB-CG-OD1	5.02	122.82	118.30
1	E	291	LEU	CB-CG-CD2	-5.01	102.49	111.00
1	C	196	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	43	MET	Peptide
1	D	436	THR	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4549	0	4402	46	0
1	B	4549	0	4402	43	0
1	C	4549	0	4402	42	0
1	D	4549	0	4402	46	0
1	E	4549	0	4402	49	0
1	F	4549	0	4402	42	0
1	G	4549	0	4402	46	0
1	H	4549	0	4402	43	0
2	A	53	0	30	11	0
2	B	53	0	31	12	0
2	C	53	0	29	4	0
2	D	53	0	31	10	0
2	E	53	0	30	5	0
2	F	53	0	29	8	0
2	G	53	0	31	13	0
2	H	53	0	30	5	0
3	A	359	0	0	5	0
3	B	373	0	0	6	0
3	C	267	0	0	3	0
3	D	314	0	0	2	0
3	E	301	0	0	2	0
3	F	262	0	0	5	0
3	G	315	0	0	6	0
3	H	355	0	0	4	0
All	All	39362	0	35457	330	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 5.

All (330) 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:D:167:HIS:HE2	2:D:801:FAD:C8M	0.96	1.56
1:B:167:HIS:HE2	2:B:801:FAD:C8M	0.92	1.55
1:G:167:HIS:HE2	2:G:801:FAD:C8M	0.90	1.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:HIS:HE2	2:A:801:FAD:C8M	0.89	1.51
1:F:167:HIS:HE2	2:F:801:FAD:C8M	0.88	1.51
1:E:291:LEU:CG	1:E:291:LEU:CD1	1.99	1.40
1:B:167:HIS:NE2	2:B:801:FAD:HM82	1.05	1.36
1:G:167:HIS:NE2	2:G:801:FAD:HM82	0.96	1.28
1:D:167:HIS:NE2	2:D:801:FAD:HM82	0.94	1.27
1:A:167:HIS:NE2	2:A:801:FAD:HM82	0.92	1.25
1:F:167:HIS:NE2	2:F:801:FAD:HM82	0.89	1.20
1:F:132:GLN:HG2	3:F:922:HOH:O	1.50	1.09
1:F:167:HIS:CD2	2:F:801:FAD:HM82	1.90	1.06
1:G:167:HIS:CE1	2:G:801:FAD:HM82	1.93	1.03
1:D:167:HIS:CD2	2:D:801:FAD:HM82	1.97	0.99
1:A:167:HIS:CD2	2:A:801:FAD:HM82	1.98	0.98
1:B:167:HIS:HE2	2:B:801:FAD:HM81	1.26	0.98
1:A:167:HIS:CE1	2:A:801:FAD:HM82	1.99	0.96
1:G:167:HIS:HE2	2:G:801:FAD:C8	1.79	0.96
1:D:167:HIS:CE1	2:D:801:FAD:HM82	2.01	0.95
1:F:167:HIS:HE2	2:F:801:FAD:HM81	1.31	0.95
1:D:100:ILE:HD13	1:D:100:ILE:O	1.67	0.94
1:B:167:HIS:HE2	2:B:801:FAD:C8	1.84	0.91
1:F:167:HIS:CE1	2:F:801:FAD:HM82	2.04	0.91
1:B:167:HIS:CD2	2:B:801:FAD:HM82	2.05	0.91
1:B:45:ILE:H	1:B:45:ILE:HD12	1.35	0.89
1:D:167:HIS:HE2	2:D:801:FAD:HM81	1.36	0.89
1:G:481:GLU:HG2	3:G:970:HOH:O	1.73	0.89
1:E:167:HIS:NE2	2:E:801:FAD:HM81	1.86	0.88
1:G:167:HIS:CD2	2:G:801:FAD:HM82	2.08	0.87
1:B:167:HIS:CE1	2:B:801:FAD:HM82	2.08	0.87
1:H:110:GLN:HE21	1:H:167:HIS:HD1	1.24	0.86
1:A:167:HIS:HE2	2:A:801:FAD:HM81	1.34	0.84
1:G:490:LYS:HD3	1:G:491:ILE:HD13	1.61	0.82
1:A:167:HIS:HE2	2:A:801:FAD:C8	1.88	0.82
1:E:110:GLN:HE21	1:E:167:HIS:HD1	1.27	0.81
1:B:178:GLU:HG3	3:B:1035:HOH:O	1.80	0.81
1:E:97:GLN:HG3	1:E:250:PHE:CE2	2.16	0.80
1:C:110:GLN:HE21	1:C:167:HIS:HD1	1.27	0.80
1:C:285:ARG:HA	1:C:328:LEU:HD11	1.63	0.79
1:F:97:GLN:HG3	1:F:250:PHE:CE2	2.17	0.79
1:G:167:HIS:HE2	2:G:801:FAD:HM81	1.37	0.79
1:C:97:GLN:HG3	1:C:250:PHE:CD2	2.18	0.79
1:E:459:VAL:HG22	1:F:121:LEU:HD13	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:VAL:HG22	1:B:121:LEU:HD13	1.66	0.77
1:E:541:MET:CE	1:E:545:LEU:HD23	2.16	0.76
1:F:132:GLN:CG	3:F:922:HOH:O	2.18	0.75
1:A:81:ASP:OD1	1:A:81:ASP:C	2.22	0.74
1:B:393:VAL:HB	1:B:417:MET:HG2	1.69	0.74
1:B:81:ASP:C	1:B:81:ASP:OD1	2.21	0.74
1:D:167:HIS:HE2	2:D:801:FAD:C8	1.94	0.74
1:C:167:HIS:CD2	2:C:801:FAD:C8M	2.69	0.73
1:E:97:GLN:HG3	1:E:250:PHE:CD2	2.23	0.73
1:C:167:HIS:CE1	2:C:801:FAD:C8M	2.70	0.72
1:E:167:HIS:CE1	2:E:801:FAD:C8M	2.69	0.72
1:E:167:HIS:CD2	2:E:801:FAD:C8M	2.69	0.71
1:H:167:HIS:CD2	2:H:801:FAD:C8M	2.71	0.71
1:A:167:HIS:CE1	2:A:801:FAD:C8M	2.69	0.71
1:C:97:GLN:HG3	1:C:250:PHE:CE2	2.26	0.71
1:F:538:PRO:HG2	1:H:538:PRO:HG2	1.73	0.70
1:C:541:MET:HE3	3:C:929:HOH:O	1.91	0.70
1:H:167:HIS:CE1	2:H:801:FAD:C8M	2.69	0.69
1:C:541:MET:CE	3:C:929:HOH:O	2.40	0.69
1:H:619:THR:HG23	1:H:619:THR:O	1.93	0.69
1:F:541:MET:HE3	3:F:925:HOH:O	1.91	0.69
1:B:541:MET:CE	3:B:964:HOH:O	2.40	0.68
1:H:167:HIS:NE2	2:H:801:FAD:HM81	1.99	0.67
1:E:541:MET:HE2	1:E:545:LEU:HD23	1.76	0.67
1:A:336:GLN:NE2	1:A:344:ASN:O	2.27	0.67
1:C:285:ARG:HA	1:C:328:LEU:CD1	2.24	0.67
1:G:167:HIS:CE1	2:G:801:FAD:C8M	2.65	0.66
1:B:541:MET:HE3	3:B:964:HOH:O	1.95	0.66
1:H:417:MET:HA	1:H:417:MET:HE3	1.78	0.66
1:B:167:HIS:NE2	2:B:801:FAD:C8	2.52	0.66
1:C:459:VAL:HG12	1:D:123:VAL:HG22	1.77	0.66
1:G:132:GLN:HG2	3:G:891:HOH:O	1.96	0.66
1:E:291:LEU:CD1	1:E:291:LEU:HG	2.19	0.66
1:B:167:HIS:CE1	2:B:801:FAD:C8M	2.73	0.65
1:D:458:ALA:HA	1:D:461:GLN:HE21	1.61	0.65
1:H:417:MET:CE	1:H:420:GLN:NE2	2.60	0.64
1:C:341:ASN:HD21	1:C:343:ALA:HB3	1.62	0.64
1:C:607:GLU:O	1:C:611:GLN:NE2	2.31	0.64
1:H:417:MET:CE	1:H:417:MET:HA	2.27	0.64
1:G:97:GLN:HG3	1:G:250:PHE:CE2	2.32	0.63
1:A:541:MET:CE	1:A:545:LEU:HD23	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:167:HIS:NE2	2:G:801:FAD:C8	2.49	0.63
1:E:291:LEU:H	1:E:291:LEU:HD12	1.63	0.63
1:D:497:MET:HE1	3:D:1202:HOH:O	1.99	0.62
1:E:167:HIS:NE2	2:E:801:FAD:C8	2.57	0.62
1:D:541:MET:HE2	1:D:545:LEU:HD23	1.83	0.61
1:C:541:MET:HE2	1:C:545:LEU:HD23	1.81	0.61
1:F:541:MET:CE	3:F:925:HOH:O	2.47	0.61
1:E:421:GLU:H	1:E:421:GLU:CD	2.04	0.61
1:F:459:VAL:O	1:F:462:SER:HB3	2.00	0.61
1:C:81:ASP:OD1	1:C:81:ASP:C	2.37	0.61
1:C:50:VAL:HG13	1:C:313:ALA:HB2	1.81	0.61
1:E:291:LEU:H	1:E:291:LEU:CD1	2.14	0.60
1:A:167:HIS:NE2	2:A:801:FAD:HM81	2.02	0.60
1:D:497:MET:CE	3:D:1202:HOH:O	2.48	0.60
1:F:417:MET:O	1:F:417:MET:HE3	2.01	0.60
1:G:100:ILE:C	1:G:100:ILE:HD13	2.22	0.60
1:G:459:VAL:HG22	1:H:121:LEU:HD13	1.82	0.60
1:C:167:HIS:NE2	2:C:801:FAD:HM81	2.02	0.60
1:E:291:LEU:HD13	3:E:1365:HOH:O	2.01	0.60
1:E:81:ASP:OD1	1:E:81:ASP:C	2.37	0.60
1:B:417:MET:HE3	1:B:417:MET:HA	1.82	0.60
1:A:299:HIS:CD2	1:A:310:GLU:HG2	2.37	0.60
1:E:381:THR:C	1:E:382:ILE:HD12	2.23	0.59
1:H:132:GLN:HG2	3:H:1000:HOH:O	2.02	0.59
1:A:167:HIS:NE2	2:A:801:FAD:C8	2.57	0.59
1:A:393:VAL:H	1:A:417:MET:HE2	1.66	0.59
1:A:299:HIS:NE2	1:A:310:GLU:HG2	2.17	0.59
1:G:167:HIS:NE2	2:G:801:FAD:HM81	2.04	0.59
1:D:100:ILE:HD13	1:D:100:ILE:C	2.23	0.59
1:C:541:MET:CE	1:C:545:LEU:HD23	2.33	0.58
1:C:619:THR:HG23	1:C:619:THR:O	2.03	0.58
1:E:541:MET:HE3	1:E:545:LEU:HD23	1.85	0.58
1:B:538:PRO:HG2	1:D:538:PRO:HG2	1.85	0.58
1:G:132:GLN:CG	3:G:891:HOH:O	2.50	0.58
1:H:167:HIS:NE2	2:H:801:FAD:C8	2.61	0.57
1:C:457:GLY:O	1:C:461:GLN:HG3	2.03	0.57
1:C:121:LEU:HD13	1:D:459:VAL:CG2	2.33	0.57
1:F:81:ASP:C	1:F:81:ASP:OD1	2.41	0.57
1:G:459:VAL:HG12	1:H:123:VAL:HG22	1.87	0.57
1:A:459:VAL:HG12	1:B:123:VAL:HG22	1.86	0.57
1:H:417:MET:CE	1:H:420:GLN:HE21	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:VAL:HG13	1:A:313:ALA:HB2	1.86	0.57
1:F:167:HIS:CE1	2:F:801:FAD:C8M	2.75	0.56
1:E:382:ILE:N	1:E:382:ILE:HD12	2.20	0.56
1:D:167:HIS:CE1	2:D:801:FAD:C8M	2.76	0.56
1:D:541:MET:CE	1:D:545:LEU:HD23	2.35	0.56
1:C:285:ARG:CA	1:C:328:LEU:HD11	2.34	0.56
1:F:167:HIS:NE2	2:F:801:FAD:HM81	2.02	0.56
1:A:392:SER:HA	1:A:417:MET:HE1	1.88	0.56
1:C:121:LEU:HD13	1:D:459:VAL:HG22	1.87	0.55
1:A:541:MET:HE3	1:A:545:LEU:HD23	1.89	0.55
1:F:541:MET:HE3	1:F:545:LEU:HD23	1.89	0.55
1:D:50:VAL:HG13	1:D:313:ALA:HB2	1.88	0.55
1:F:459:VAL:O	1:F:462:SER:CB	2.55	0.54
1:C:121:LEU:HD12	1:D:458:ALA:O	2.06	0.54
1:F:541:MET:CE	1:F:545:LEU:HD23	2.36	0.54
1:C:167:HIS:NE2	2:C:801:FAD:C8	2.64	0.54
1:A:185:LYS:HG2	3:A:1080:HOH:O	2.08	0.53
1:A:45:ILE:C	1:A:45:ILE:HD12	2.28	0.53
1:G:459:VAL:O	1:G:462:SER:HB2	2.08	0.53
1:D:46:LYS:HE3	1:D:47:TYR:O	2.09	0.53
1:C:157:VAL:HG21	1:C:324:HIS:HE1	1.74	0.53
1:F:167:HIS:NE2	2:F:801:FAD:C8	2.66	0.53
1:E:123:VAL:HG22	1:F:459:VAL:HG12	1.91	0.53
1:D:457:GLY:O	1:D:461:GLN:HG3	2.09	0.52
1:E:47:TYR:O	1:E:313:ALA:HA	2.09	0.52
1:D:157:VAL:HG21	1:D:324:HIS:HE1	1.74	0.52
1:B:50:VAL:HG13	1:B:313:ALA:HB2	1.92	0.52
1:B:167:HIS:NE2	2:B:801:FAD:HM81	1.97	0.52
1:E:89:HIS:CE1	1:E:91:LYS:HG2	2.44	0.52
1:G:82:SER:O	1:H:81:ASP:HA	2.10	0.52
1:G:459:VAL:O	1:G:462:SER:CB	2.57	0.52
1:A:459:VAL:O	1:A:462:SER:CB	2.58	0.52
1:C:459:VAL:O	1:C:462:SER:CB	2.59	0.51
1:G:50:VAL:HG13	1:G:313:ALA:HB2	1.93	0.51
1:B:547:LEU:HD12	2:B:801:FAD:HM83	1.92	0.51
1:E:157:VAL:HG21	1:E:324:HIS:HE1	1.75	0.51
1:E:607:GLU:O	1:E:611:GLN:HG3	2.11	0.51
1:E:618:PHE:HD1	1:E:619:THR:N	2.10	0.50
1:H:417:MET:CE	1:H:417:MET:CA	2.89	0.50
1:E:346:PRO:HG2	1:E:350:PRO:HA	1.94	0.50
1:B:336:GLN:NE2	1:B:344:ASN:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:MET:HE3	3:A:1067:HOH:O	2.12	0.49
1:A:121:LEU:HD12	1:B:458:ALA:O	2.12	0.49
1:A:538:PRO:HG2	1:C:538:PRO:HG2	1.94	0.49
1:C:346:PRO:HG2	1:C:350:PRO:HA	1.93	0.49
1:G:336:GLN:NE2	1:G:344:ASN:O	2.45	0.49
1:F:478:GLU:CD	1:F:480:LYS:HE2	2.32	0.49
1:E:618:PHE:C	1:E:618:PHE:HD1	2.15	0.49
1:E:452:ASP:OD1	1:E:452:ASP:N	2.46	0.49
1:H:619:THR:CG2	1:H:619:THR:O	2.61	0.49
1:A:541:MET:HE2	1:A:545:LEU:HD23	1.92	0.49
1:H:284:GLU:C	1:H:328:LEU:CD1	2.81	0.49
1:C:218:ARG:HD2	3:C:911:HOH:O	2.11	0.49
1:H:452:ASP:O	1:H:453:ALA:C	2.51	0.49
1:H:50:VAL:HG13	1:H:313:ALA:HB2	1.95	0.49
1:F:47:TYR:O	1:F:313:ALA:HA	2.13	0.49
1:D:167:HIS:NE2	2:D:801:FAD:C8	2.65	0.49
1:B:100:ILE:HD13	1:B:100:ILE:C	2.33	0.49
1:B:459:VAL:O	1:B:462:SER:CB	2.60	0.49
1:B:547:LEU:CD1	2:B:801:FAD:HM83	2.43	0.49
1:C:459:VAL:CG1	1:D:123:VAL:HG22	2.43	0.49
1:H:459:VAL:O	1:H:462:SER:CB	2.61	0.48
1:D:490:LYS:HD3	1:D:491:ILE:HD13	1.95	0.48
1:G:541:MET:HE2	1:G:545:LEU:HD23	1.95	0.48
1:A:457:GLY:H	1:A:460:GLN:HE21	1.60	0.48
1:G:457:GLY:O	1:G:461:GLN:HG3	2.13	0.48
1:D:167:HIS:NE2	2:D:801:FAD:HM81	2.10	0.48
1:B:417:MET:HB3	1:B:417:MET:HE2	1.68	0.48
1:E:618:PHE:CD1	1:E:618:PHE:C	2.87	0.47
1:E:50:VAL:HG13	1:E:313:ALA:HB2	1.96	0.47
1:F:417:MET:HE3	1:F:417:MET:CA	2.44	0.47
1:G:547:LEU:CD1	2:G:801:FAD:HM83	2.44	0.47
1:H:81:ASP:O	1:H:90:LYS:HE2	2.14	0.47
1:E:385:THR:O	1:E:388:GLU:HB3	2.15	0.47
1:A:547:LEU:HD12	2:A:801:FAD:HM83	1.97	0.47
1:F:121:LEU:CD2	1:G:121:LEU:CD2	2.93	0.47
1:E:385:THR:O	1:E:388:GLU:CB	2.63	0.47
1:H:341:ASN:HD22	1:H:341:ASN:C	2.18	0.47
1:B:452:ASP:O	1:B:453:ALA:C	2.54	0.47
1:H:542:LYS:CE	3:H:1138:HOH:O	2.62	0.47
3:G:1107:HOH:O	1:H:112:MET:HB3	2.16	0.46
1:D:81:ASP:C	1:D:81:ASP:OD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:618:PHE:C	1:C:618:PHE:HD1	2.18	0.46
1:C:112:MET:HE3	1:D:95:GLU:HG3	1.96	0.46
1:D:547:LEU:HD12	2:D:801:FAD:HM83	1.98	0.46
1:D:153:SER:OG	1:D:542:LYS:CG	2.64	0.46
1:F:218:ARG:HG3	1:F:430:ASP:OD2	2.16	0.46
1:F:50:VAL:HG12	1:F:73:ALA:HB3	1.98	0.46
1:A:123:VAL:HG22	1:B:459:VAL:HG12	1.98	0.46
1:C:47:TYR:O	1:C:313:ALA:HA	2.15	0.45
1:A:497:MET:CE	3:A:1109:HOH:O	2.65	0.45
1:F:324:HIS:HD2	1:F:327:GLN:OE1	1.99	0.45
1:G:341:ASN:HD21	1:G:343:ALA:HB3	1.80	0.45
1:E:218:ARG:HD2	3:E:1194:HOH:O	2.16	0.45
1:E:541:MET:HE3	1:E:545:LEU:CD2	2.45	0.45
1:H:346:PRO:HG2	1:H:350:PRO:HA	1.98	0.45
1:B:81:ASP:O	1:B:81:ASP:OD1	2.33	0.45
1:C:336:GLN:NE2	1:C:344:ASN:O	2.49	0.45
1:B:169:THR:O	1:B:169:THR:HG22	2.17	0.45
1:C:618:PHE:C	1:C:618:PHE:CD1	2.89	0.45
1:A:497:MET:HE2	3:A:1109:HOH:O	2.17	0.45
1:G:547:LEU:HD12	2:G:801:FAD:HM83	1.99	0.45
1:A:459:VAL:O	1:A:462:SER:HB3	2.16	0.45
1:H:417:MET:HE1	1:H:420:GLN:NE2	2.30	0.45
1:E:47:TYR:CD2	1:E:73:ALA:HB2	2.52	0.45
1:F:121:LEU:HD21	1:G:121:LEU:CD2	2.47	0.45
1:C:343:ALA:C	1:C:344:ASN:HD22	2.20	0.45
1:A:393:VAL:H	1:A:417:MET:CE	2.29	0.45
1:H:459:VAL:O	1:H:462:SER:HB3	2.17	0.45
1:B:294:GLU:OE1	1:B:296:GLU:OE2	2.35	0.45
1:B:167:HIS:CD2	2:B:801:FAD:C8	3.00	0.45
1:A:100:ILE:HG23	1:A:101:ASP:N	2.32	0.45
1:C:537:LEU:HB3	1:C:538:PRO:HD2	1.98	0.45
1:G:363:PHE:HA	1:G:471:TRP:O	2.17	0.45
1:E:342:PRO:C	1:E:344:ASN:H	2.20	0.45
1:D:100:ILE:CD1	1:D:453:ALA:HA	2.47	0.44
1:G:541:MET:CE	1:G:545:LEU:HD23	2.48	0.44
1:H:542:LYS:HE2	3:H:1138:HOH:O	2.17	0.44
1:B:265:ARG:HA	1:B:266:PRO:C	2.38	0.44
1:G:312:LYS:HE3	3:G:941:HOH:O	2.17	0.44
1:F:610:LYS:NZ	3:F:976:HOH:O	2.48	0.44
1:H:126:LEU:HD12	1:H:132:GLN:HG3	1.99	0.44
1:G:47:TYR:O	1:G:313:ALA:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:541:MET:HE3	3:H:962:HOH:O	2.18	0.44
1:A:541:MET:HE3	1:A:545:LEU:CD2	2.47	0.44
1:F:97:GLN:HG3	1:F:250:PHE:CD2	2.53	0.44
1:C:458:ALA:O	1:D:121:LEU:HD12	2.17	0.44
1:F:121:LEU:CD2	1:G:121:LEU:HD21	2.48	0.44
1:E:291:LEU:HD12	1:E:291:LEU:N	2.29	0.43
1:H:81:ASP:C	1:H:81:ASP:OD1	2.51	0.43
1:B:185:LYS:NZ	1:B:185:LYS:CB	2.81	0.43
1:D:47:TYR:O	1:D:313:ALA:HA	2.18	0.43
1:B:100:ILE:HD13	1:B:100:ILE:O	2.18	0.43
1:G:104:VAL:HG22	1:G:453:ALA:HB1	2.00	0.43
1:B:218:ARG:HD2	3:B:838:HOH:O	2.18	0.43
1:F:564:CYS:HG	1:F:573:PHE:HE2	1.66	0.43
1:E:167:HIS:CD2	2:E:801:FAD:C8	3.01	0.43
1:B:45:ILE:H	1:B:45:ILE:CD1	2.07	0.43
1:F:336:GLN:HB2	1:F:346:PRO:HG3	2.00	0.43
1:G:167:HIS:CD2	2:G:801:FAD:C8	3.02	0.43
1:A:47:TYR:O	1:A:313:ALA:HA	2.19	0.43
1:A:44:ASP:OD2	1:A:71:LYS:NZ	2.41	0.43
1:E:284:GLU:C	1:E:328:LEU:CD1	2.87	0.43
1:A:293:SER:HA	1:A:574:GLY:O	2.19	0.43
1:H:173:PRO:HG2	1:H:592:ALA:HB1	2.00	0.43
1:E:153:SER:OG	1:E:542:LYS:HG2	2.19	0.42
1:H:45:ILE:C	1:H:45:ILE:HD12	2.39	0.42
1:G:167:HIS:CD2	1:G:167:HIS:C	2.93	0.42
1:D:541:MET:CE	1:D:545:LEU:CD2	2.97	0.42
1:E:380:MET:CB	1:E:382:ILE:HD11	2.49	0.42
1:H:541:MET:CE	1:H:545:LEU:HD23	2.49	0.42
1:A:341:ASN:HA	1:A:342:PRO:HD2	1.89	0.42
1:G:537:LEU:HB3	1:G:538:PRO:HD2	2.00	0.42
1:B:541:MET:HE1	3:B:964:HOH:O	2.11	0.42
1:G:459:VAL:CG1	1:H:123:VAL:HG22	2.48	0.42
1:G:201:LYS:HE2	1:G:205:TYR:OH	2.20	0.42
1:D:284:GLU:C	1:D:328:LEU:CD1	2.87	0.42
1:A:218:ARG:HD2	3:A:906:HOH:O	2.19	0.42
1:D:336:GLN:NE2	1:D:344:ASN:O	2.53	0.42
1:F:417:MET:C	1:F:417:MET:HE3	2.39	0.42
1:B:121:LEU:CD2	1:C:121:LEU:CD2	2.98	0.42
1:C:459:VAL:O	1:C:462:SER:HB3	2.20	0.42
1:D:185:LYS:HE3	1:D:557:PHE:CD2	2.55	0.42
1:H:478:GLU:CD	1:H:480:LYS:HE2	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:299:HIS:CE1	1:D:310:GLU:HG3	2.54	0.42
1:F:293:SER:HA	1:F:574:GLY:O	2.20	0.42
1:A:81:ASP:O	1:A:90:LYS:HE2	2.20	0.41
1:D:284:GLU:O	1:D:328:LEU:CD1	2.68	0.41
1:D:564:CYS:HG	1:D:573:PHE:HE2	1.68	0.41
1:A:547:LEU:CD1	2:A:801:FAD:HM83	2.51	0.41
1:G:393:VAL:O	1:G:413:LYS:HE2	2.20	0.41
1:D:215:GLU:O	1:D:411:LYS:NZ	2.53	0.41
1:G:97:GLN:HG3	1:G:250:PHE:CD2	2.56	0.41
1:F:383:ARG:O	1:F:391:TYR:HA	2.20	0.41
1:E:121:LEU:HD12	1:F:458:ALA:O	2.21	0.41
1:A:341:ASN:C	1:A:341:ASN:HD22	2.24	0.41
1:H:459:VAL:CG1	1:H:460:GLN:N	2.83	0.41
1:E:285:ARG:HA	1:E:328:LEU:CD1	2.51	0.41
1:H:336:GLN:OE1	1:H:340:PRO:HA	2.21	0.41
1:E:291:LEU:CD1	1:E:291:LEU:N	2.83	0.41
1:G:481:GLU:CG	3:G:970:HOH:O	2.48	0.41
1:H:417:MET:HE2	1:H:417:MET:O	2.21	0.41
1:E:121:LEU:CD2	1:H:121:LEU:HD21	2.51	0.41
1:F:157:VAL:HG21	1:F:324:HIS:HE1	1.85	0.41
1:F:181:PRO:HG3	1:F:587:PRO:HD2	2.03	0.41
1:H:547:LEU:HD12	2:H:801:FAD:HM83	2.02	0.41
1:G:104:VAL:HG21	1:G:454:PHE:C	2.41	0.41
1:C:265:ARG:HA	1:C:266:PRO:C	2.41	0.41
1:G:478:GLU:CD	1:G:480:LYS:HE2	2.40	0.41
1:B:558:ASP:OD2	1:B:561:GLU:HG3	2.21	0.41
1:C:165:SER:HA	1:C:168:TRP:CD1	2.56	0.41
1:A:167:HIS:C	1:A:167:HIS:CD2	2.95	0.40
1:D:284:GLU:O	1:D:328:LEU:HD12	2.22	0.40
1:H:180:ARG:HA	1:H:181:PRO:HD3	1.84	0.40
1:E:532:PHE:CZ	1:E:538:PRO:HG3	2.57	0.40
1:E:167:HIS:CD2	1:E:167:HIS:C	2.95	0.40
1:E:459:VAL:HG12	1:F:123:VAL:HG22	2.02	0.40
1:B:459:VAL:O	1:B:462:SER:HB2	2.20	0.40
1:A:407:TRP:O	1:A:411:LYS:HG3	2.20	0.40
1:D:452:ASP:OD1	1:D:452:ASP:N	2.54	0.40
1:D:460:GLN:C	1:D:462:SER:H	2.22	0.40
1:G:159:ARG:HA	2:G:801:FAD:O2B	2.22	0.40
1:B:121:LEU:HD23	3:B:1050:HOH:O	2.20	0.40
1:D:532:PHE:CZ	1:D:538:PRO:HG3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	575/623 (92%)	557 (97%)	17 (3%)	1 (0%)	52	32
1	B	575/623 (92%)	555 (96%)	18 (3%)	2 (0%)	46	26
1	C	575/623 (92%)	561 (98%)	14 (2%)	0	100	100
1	D	575/623 (92%)	560 (97%)	15 (3%)	0	100	100
1	E	575/623 (92%)	558 (97%)	17 (3%)	0	100	100
1	F	575/623 (92%)	562 (98%)	13 (2%)	0	100	100
1	G	575/623 (92%)	558 (97%)	15 (3%)	2 (0%)	46	26
1	H	575/623 (92%)	557 (97%)	18 (3%)	0	100	100
All	All	4600/4984 (92%)	4468 (97%)	127 (3%)	5 (0%)	56	35

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	389	LEU
1	G	453	ALA
1	A	44	ASP
1	B	461	GLN
1	G	45	ILE

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	505/542 (93%)	491 (97%)	14 (3%)	51	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	505/542 (93%)	494 (98%)	11 (2%)	60	39
1	C	505/542 (93%)	495 (98%)	10 (2%)	63	44
1	D	505/542 (93%)	493 (98%)	12 (2%)	57	36
1	E	505/542 (93%)	496 (98%)	9 (2%)	66	49
1	F	505/542 (93%)	489 (97%)	16 (3%)	46	24
1	G	505/542 (93%)	495 (98%)	10 (2%)	63	44
1	H	505/542 (93%)	493 (98%)	12 (2%)	57	36
All	All	4040/4336 (93%)	3946 (98%)	94 (2%)	58	37

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	MET
1	A	100	ILE
1	A	168	TRP
1	A	185	LYS
1	A	206	PHE
1	A	312	LYS
1	A	341	ASN
1	A	344	ASN
1	A	347	GLU
1	A	385	THR
1	A	450	HIS
1	A	461	GLN
1	A	490	LYS
1	A	496	ASN
1	B	45	ILE
1	B	100	ILE
1	B	112	MET
1	B	168	TRP
1	B	178	GLU
1	B	185	LYS
1	B	385	THR
1	B	408	TRP
1	B	417	MET
1	B	450	HIS
1	B	490	LYS
1	C	112	MET
1	C	168	TRP
1	C	185	LYS

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Mol	Chain	Res	Type
1	C	341	ASN
1	C	344	ASN
1	C	403	LYS
1	C	450	HIS
1	C	490	LYS
1	C	593	ASN
1	C	618	PHE
1	D	100	ILE
1	D	112	MET
1	D	168	TRP
1	D	178	GLU
1	D	206	PHE
1	D	299	HIS
1	D	341	ASN
1	D	385	THR
1	D	403	LYS
1	D	450	HIS
1	D	593	ASN
1	D	618	PHE
1	E	168	TRP
1	E	185	LYS
1	E	206	PHE
1	E	291	LEU
1	E	385	THR
1	E	421	GLU
1	E	450	HIS
1	E	455	SER
1	E	618	PHE
1	F	100	ILE
1	F	112	MET
1	F	132	GLN
1	F	168	TRP
1	F	206	PHE
1	F	272	GLU
1	F	328	LEU
1	F	341	ASN
1	F	385	THR
1	F	408	TRP
1	F	417	MET
1	F	450	HIS
1	F	461	GLN
1	F	576	LYS

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Mol	Chain	Res	Type
1	F	593	ASN
1	F	618	PHE
1	G	45	ILE
1	G	100	ILE
1	G	168	TRP
1	G	385	THR
1	G	408	TRP
1	G	450	HIS
1	G	496	ASN
1	G	593	ASN
1	G	618	PHE
1	G	619	THR
1	H	100	ILE
1	H	132	GLN
1	H	168	TRP
1	H	185	LYS
1	H	206	PHE
1	H	341	ASN
1	H	400	SER
1	H	413	LYS
1	H	417	MET
1	H	450	HIS
1	H	459	VAL
1	H	618	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	341	ASN
1	A	344	ASN
1	A	460	GLN
1	A	461	GLN
1	B	341	ASN
1	B	460	GLN
1	C	341	ASN
1	C	344	ASN
1	C	611	GLN
1	D	299	HIS
1	D	324	HIS
1	D	341	ASN
1	D	460	GLN
1	D	461	GLN

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Mol	Chain	Res	Type
1	E	341	ASN
1	E	460	GLN
1	E	461	GLN
1	E	611	GLN
1	F	324	HIS
1	F	341	ASN
1	F	460	GLN
1	F	461	GLN
1	G	263	GLN
1	G	324	HIS
1	G	341	ASN
1	G	460	GLN
1	H	263	GLN
1	H	341	ASN
1	H	460	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	A	801	1	48,58,58	1.47	9 (18%)	54,89,89	3.69	14 (25%)
2	FAD	B	801	1	48,58,58	1.54	9 (18%)	54,89,89	3.37	16 (29%)
2	FAD	C	801	1	48,58,58	1.60	9 (18%)	54,89,89	2.75	15 (27%)
2	FAD	D	801	1	48,58,58	1.24	5 (10%)	54,89,89	2.72	17 (31%)
2	FAD	E	801	1	48,58,58	1.43	9 (18%)	54,89,89	2.63	15 (27%)
2	FAD	F	801	1	48,58,58	1.44	8 (16%)	54,89,89	2.77	17 (31%)
2	FAD	G	801	1	48,58,58	1.54	9 (18%)	54,89,89	2.86	16 (29%)
2	FAD	H	801	1	48,58,58	1.47	9 (18%)	54,89,89	2.65	16 (29%)

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	801	1	-	0/30/50/50	0/6/6/6
2	FAD	B	801	1	-	0/30/50/50	0/6/6/6
2	FAD	C	801	1	-	0/30/50/50	0/6/6/6
2	FAD	D	801	1	-	0/30/50/50	0/6/6/6
2	FAD	E	801	1	-	0/30/50/50	0/6/6/6
2	FAD	F	801	1	-	0/30/50/50	0/6/6/6
2	FAD	G	801	1	-	0/30/50/50	0/6/6/6
2	FAD	H	801	1	-	0/30/50/50	0/6/6/6

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	FAD	C10-N10	-4.29	1.34	1.39
2	B	801	FAD	C8A-N7A	-3.75	1.27	1.34
2	B	801	FAD	O4B-C4B	-3.63	1.36	1.45
2	F	801	FAD	C10-N10	-3.49	1.35	1.39
2	E	801	FAD	O4B-C4B	-3.40	1.37	1.45
2	H	801	FAD	C1'-N10	-3.23	1.45	1.48
2	A	801	FAD	C2B-C3B	-3.22	1.44	1.53
2	G	801	FAD	C2B-C3B	-3.17	1.44	1.53
2	F	801	FAD	O3B-C3B	-3.10	1.35	1.43
2	E	801	FAD	C2B-C3B	-3.02	1.45	1.53
2	D	801	FAD	C2B-C3B	-3.00	1.45	1.53
2	A	801	FAD	O3B-C3B	-2.81	1.36	1.43
2	A	801	FAD	O4B-C4B	-2.68	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	801	FAD	C2B-C3B	-2.67	1.46	1.53
2	D	801	FAD	O4B-C4B	-2.66	1.38	1.45
2	C	801	FAD	C10-N10	-2.64	1.36	1.39
2	C	801	FAD	O2B-C2B	-2.58	1.36	1.43
2	A	801	FAD	O2B-C2B	-2.54	1.36	1.43
2	E	801	FAD	O2B-C2B	-2.51	1.37	1.43
2	C	801	FAD	C2B-C3B	-2.50	1.46	1.53
2	B	801	FAD	C2B-C3B	-2.49	1.46	1.53
2	H	801	FAD	C10-N10	-2.40	1.36	1.39
2	G	801	FAD	O4B-C4B	-2.28	1.39	1.45
2	E	801	FAD	O3B-C3B	-2.07	1.38	1.43
2	F	801	FAD	C9A-C5X	-2.06	1.38	1.42
2	G	801	FAD	PA-O1A	-2.06	1.43	1.51
2	H	801	FAD	C2B-C3B	-2.03	1.47	1.53
2	G	801	FAD	O2B-C2B	-2.01	1.38	1.43
2	H	801	FAD	C9A-C5X	-2.00	1.38	1.42
2	H	801	FAD	C4-C4X	2.01	1.45	1.41
2	D	801	FAD	C5X-N5	2.04	1.38	1.35
2	C	801	FAD	C9A-N10	2.06	1.41	1.38
2	B	801	FAD	C4-N3	2.11	1.37	1.33
2	E	801	FAD	C4X-N5	2.11	1.36	1.33
2	F	801	FAD	C5'-C4'	2.15	1.54	1.51
2	A	801	FAD	C4-C4X	2.17	1.45	1.41
2	G	801	FAD	C6-C7	2.19	1.43	1.37
2	B	801	FAD	C6-C5X	2.26	1.45	1.41
2	E	801	FAD	C2A-N1A	2.28	1.38	1.33
2	C	801	FAD	O4B-C1B	2.32	1.44	1.41
2	C	801	FAD	C5'-C4'	2.34	1.55	1.51
2	G	801	FAD	C2A-N3A	2.35	1.36	1.32
2	F	801	FAD	C6-C5X	2.40	1.45	1.41
2	H	801	FAD	C5X-N5	2.42	1.39	1.35
2	H	801	FAD	C2A-N1A	2.42	1.38	1.33
2	C	801	FAD	C2A-N1A	2.44	1.38	1.33
2	D	801	FAD	C2A-N3A	2.44	1.36	1.32
2	A	801	FAD	O4B-C1B	2.45	1.44	1.41
2	B	801	FAD	C2A-N1A	2.57	1.38	1.33
2	A	801	FAD	C5'-C4'	2.59	1.55	1.51
2	B	801	FAD	C10-N1	2.64	1.40	1.35
2	H	801	FAD	C10-N1	2.73	1.40	1.35
2	F	801	FAD	C5X-N5	2.79	1.39	1.35
2	C	801	FAD	C4X-N5	2.80	1.37	1.33
2	E	801	FAD	C9A-N10	2.85	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	FAD	O4B-C1B	2.86	1.44	1.41
2	E	801	FAD	C4-C4X	2.88	1.47	1.41
2	F	801	FAD	C9A-N10	3.00	1.42	1.38
2	A	801	FAD	C4X-N5	3.01	1.38	1.33
2	E	801	FAD	C4-N3	3.15	1.38	1.33
2	G	801	FAD	C9A-N10	3.22	1.43	1.38
2	G	801	FAD	C4-N3	3.54	1.39	1.33
2	D	801	FAD	C4-N3	3.56	1.39	1.33
2	G	801	FAD	O4B-C1B	3.99	1.46	1.41
2	H	801	FAD	C4-N3	4.26	1.41	1.33
2	B	801	FAD	C4X-N5	4.36	1.40	1.33
2	C	801	FAD	C4-N3	5.21	1.42	1.33

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	FAD	N3A-C2A-N1A	-13.70	118.41	128.89
2	A	801	FAD	N3A-C2A-N1A	-11.81	119.85	128.89
2	C	801	FAD	N3A-C2A-N1A	-10.90	120.55	128.89
2	D	801	FAD	N3A-C2A-N1A	-9.93	121.29	128.89
2	G	801	FAD	N3A-C2A-N1A	-9.77	121.41	128.89
2	A	801	FAD	C4X-C4-N3	-8.48	111.99	123.59
2	G	801	FAD	C4-C4X-C10	-8.12	114.74	119.94
2	H	801	FAD	N3A-C2A-N1A	-7.84	122.89	128.89
2	F	801	FAD	N3A-C2A-N1A	-7.82	122.91	128.89
2	F	801	FAD	C4-C4X-C10	-6.72	115.64	119.94
2	E	801	FAD	N3A-C2A-N1A	-6.70	123.76	128.89
2	C	801	FAD	C4X-C4-N3	-6.70	114.42	123.59
2	D	801	FAD	C4-C4X-C10	-6.32	115.90	119.94
2	H	801	FAD	C4X-C4-N3	-5.74	115.74	123.59
2	E	801	FAD	C4-C4X-C10	-5.66	116.32	119.94
2	B	801	FAD	C4-C4X-C10	-5.03	116.72	119.94
2	E	801	FAD	C4X-C4-N3	-4.77	117.07	123.59
2	B	801	FAD	C4X-C4-N3	-4.62	117.27	123.59
2	A	801	FAD	C4-C4X-C10	-4.58	117.01	119.94
2	G	801	FAD	C4X-C4-N3	-4.53	117.40	123.59
2	H	801	FAD	C4-C4X-C10	-4.22	117.24	119.94
2	F	801	FAD	C4X-C4-N3	-3.93	118.22	123.59
2	A	801	FAD	C4X-C10-N10	-3.83	118.26	120.52
2	F	801	FAD	C4X-C10-N10	-3.51	118.45	120.52
2	G	801	FAD	C4X-C10-N10	-3.38	118.53	120.52
2	D	801	FAD	C4X-C4-N3	-3.37	118.98	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	FAD	C4A-C5A-N7A	-3.06	106.66	109.48
2	C	801	FAD	C4X-C10-N10	-3.01	118.75	120.52
2	E	801	FAD	C4X-C10-N10	-2.87	118.83	120.52
2	D	801	FAD	C8M-C8-C9	-2.78	112.71	120.28
2	E	801	FAD	C4B-O4B-C1B	-2.68	106.77	109.72
2	F	801	FAD	C9A-C5X-N5	-2.54	118.60	122.36
2	H	801	FAD	C4X-C10-N10	-2.48	119.06	120.52
2	C	801	FAD	C4A-C5A-N7A	-2.36	107.31	109.48
2	D	801	FAD	C6-C5X-N5	-2.25	116.06	118.96
2	B	801	FAD	C7M-C7-C6	-2.14	114.47	120.28
2	G	801	FAD	C4A-C5A-N7A	-2.13	107.52	109.48
2	H	801	FAD	C6-C5X-N5	-2.11	116.25	118.96
2	H	801	FAD	C4A-C5A-N7A	-2.05	107.59	109.48
2	C	801	FAD	N6A-C6A-N1A	-2.05	114.81	119.20
2	E	801	FAD	C7M-C7-C6	-2.04	114.74	120.28
2	G	801	FAD	C7-C6-C5X	-2.02	117.62	120.92
2	B	801	FAD	O2A-PA-O1A	2.04	123.58	112.53
2	F	801	FAD	O2A-PA-O1A	2.06	123.71	112.53
2	B	801	FAD	C1'-N10-C9A	2.11	121.23	118.86
2	C	801	FAD	O2B-C2B-C3B	2.12	118.72	111.83
2	H	801	FAD	C6-C5X-C9A	2.13	121.79	118.98
2	A	801	FAD	C2B-C3B-C4B	2.14	107.02	102.61
2	H	801	FAD	O4B-C4B-C5B	2.15	117.00	109.32
2	A	801	FAD	C1'-N10-C9A	2.16	121.28	118.86
2	B	801	FAD	C7M-C7-C8	2.17	125.50	120.73
2	E	801	FAD	O2A-PA-O1A	2.23	124.62	112.53
2	D	801	FAD	O4B-C1B-N9A	2.23	112.78	108.10
2	H	801	FAD	C1'-N10-C9A	2.25	121.39	118.86
2	B	801	FAD	O4B-C4B-C3B	2.29	109.76	105.15
2	F	801	FAD	O4B-C1B-N9A	2.32	112.95	108.10
2	H	801	FAD	O2'-C2'-C3'	2.36	114.94	109.02
2	C	801	FAD	O2A-PA-O1A	2.36	125.34	112.53
2	E	801	FAD	O4'-C4'-C5'	2.39	115.41	110.19
2	D	801	FAD	C2A-N1A-C6A	2.42	123.09	118.77
2	A	801	FAD	O4'-C4'-C3'	2.43	115.12	109.02
2	H	801	FAD	C2B-C3B-C4B	2.44	107.62	102.61
2	A	801	FAD	O2'-C2'-C3'	2.45	115.17	109.02
2	G	801	FAD	C6-C5X-C9A	2.45	122.21	118.98
2	C	801	FAD	C1'-N10-C9A	2.47	121.63	118.86
2	G	801	FAD	C4X-N5-C5X	2.48	119.62	116.76
2	C	801	FAD	C6-C5X-C9A	2.51	122.28	118.98
2	H	801	FAD	O4'-C4'-C3'	2.52	115.35	109.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	FAD	O3B-C3B-C4B	2.52	118.62	111.05
2	A	801	FAD	C2A-N1A-C6A	2.57	123.36	118.77
2	E	801	FAD	O4B-C1B-N9A	2.62	113.57	108.10
2	D	801	FAD	O4B-C4B-C5B	2.64	118.76	109.32
2	F	801	FAD	O4B-C4B-C5B	2.64	118.76	109.32
2	E	801	FAD	O2B-C2B-C3B	2.65	120.44	111.83
2	F	801	FAD	C2A-N1A-C6A	2.66	123.53	118.77
2	D	801	FAD	O4'-C4'-C3'	2.67	115.74	109.02
2	D	801	FAD	C4-C4X-N5	2.76	122.06	118.72
2	F	801	FAD	C4X-N5-C5X	2.81	120.00	116.76
2	G	801	FAD	C2A-N1A-C6A	2.82	123.80	118.77
2	C	801	FAD	C4B-O4B-C1B	2.83	112.83	109.72
2	D	801	FAD	O2B-C2B-C3B	2.96	121.45	111.83
2	D	801	FAD	O4B-C4B-C3B	2.97	111.13	105.15
2	G	801	FAD	O4'-C4'-C3'	3.02	116.61	109.02
2	A	801	FAD	O2B-C2B-C3B	3.05	121.76	111.83
2	C	801	FAD	O4'-C4'-C3'	3.07	116.74	109.02
2	F	801	FAD	C2B-C3B-C4B	3.13	109.05	102.61
2	G	801	FAD	C2B-C3B-C4B	3.13	109.05	102.61
2	G	801	FAD	O3B-C3B-C4B	3.21	120.67	111.05
2	E	801	FAD	C1'-N10-C9A	3.28	122.54	118.86
2	G	801	FAD	O2B-C2B-C3B	3.30	122.56	111.83
2	A	801	FAD	C5X-C9A-N10	3.33	120.15	117.62
2	H	801	FAD	O3B-C3B-C4B	3.34	121.07	111.05
2	B	801	FAD	C2A-N1A-C6A	3.43	124.89	118.77
2	B	801	FAD	O2B-C2B-C3B	3.48	123.14	111.83
2	F	801	FAD	C5X-C9A-N10	3.53	120.30	117.62
2	F	801	FAD	O2B-C2B-C3B	3.63	123.63	111.83
2	F	801	FAD	O3B-C3B-C4B	3.63	121.94	111.05
2	H	801	FAD	O2B-C2B-C3B	3.64	123.68	111.83
2	E	801	FAD	O3B-C3B-C4B	3.70	122.16	111.05
2	A	801	FAD	C2B-C1B-N9A	3.78	120.07	114.29
2	B	801	FAD	O4B-C1B-N9A	3.80	116.05	108.10
2	B	801	FAD	C4X-N5-C5X	3.82	121.16	116.76
2	G	801	FAD	C2B-C1B-N9A	3.86	120.18	114.29
2	E	801	FAD	O4B-C4B-C3B	3.87	112.94	105.15
2	F	801	FAD	C4-C4X-N5	3.98	123.55	118.72
2	B	801	FAD	O3B-C3B-C4B	3.98	123.00	111.05
2	G	801	FAD	C4-C4X-N5	4.20	123.82	118.72
2	C	801	FAD	O3B-C3B-C4B	4.24	123.77	111.05
2	D	801	FAD	O3B-C3B-C4B	4.68	125.08	111.05
2	D	801	FAD	C1'-N10-C9A	4.88	124.33	118.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	FAD	C2B-C1B-N9A	5.12	122.11	114.29
2	B	801	FAD	C2B-C1B-N9A	5.30	122.39	114.29
2	E	801	FAD	C2B-C1B-N9A	5.51	122.72	114.29
2	C	801	FAD	O4B-C1B-N9A	5.54	119.70	108.10
2	F	801	FAD	C2B-C1B-N9A	5.64	122.91	114.29
2	B	801	FAD	C4-C4X-N5	5.79	125.75	118.72
2	D	801	FAD	C2B-C1B-N9A	5.89	123.28	114.29
2	D	801	FAD	C4-N3-C2	7.04	121.33	115.25
2	H	801	FAD	C2B-C1B-N9A	7.55	125.83	114.29
2	C	801	FAD	C4-N3-C2	8.14	122.29	115.25
2	H	801	FAD	C4-N3-C2	10.00	123.89	115.25
2	G	801	FAD	C4-N3-C2	10.09	123.97	115.25
2	F	801	FAD	C4-N3-C2	10.39	124.23	115.25
2	E	801	FAD	C4-N3-C2	10.68	124.48	115.25
2	B	801	FAD	C4-N3-C2	13.22	126.67	115.25
2	A	801	FAD	C4-N3-C2	19.36	131.98	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 68 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	FAD	11	0
2	B	801	FAD	12	0
2	C	801	FAD	4	0
2	D	801	FAD	10	0
2	E	801	FAD	5	0
2	F	801	FAD	8	0
2	G	801	FAD	13	0
2	H	801	FAD	5	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, 95th 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	577/623 (92%)	0.68	44 (7%) 17 19	15, 21, 40, 56	0
1	B	577/623 (92%)	0.63	35 (6%) 25 26	17, 22, 39, 65	0
1	C	577/623 (92%)	0.78	48 (8%) 14 16	20, 27, 45, 65	0
1	D	577/623 (92%)	0.66	42 (7%) 18 20	19, 25, 41, 62	0
1	E	577/623 (92%)	0.74	54 (9%) 11 12	18, 26, 42, 63	0
1	F	577/623 (92%)	0.81	57 (9%) 9 10	19, 27, 42, 64	0
1	G	577/623 (92%)	0.66	47 (8%) 15 16	18, 24, 42, 59	0
1	H	577/623 (92%)	0.63	38 (6%) 22 23	18, 23, 38, 61	0
All	All	4616/4984 (92%)	0.70	365 (7%) 15 17	15, 25, 42, 65	0

All (365) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	389	LEU	15.4
1	H	619	THR	15.2
1	C	619	THR	14.3
1	A	459	VAL	14.1
1	B	619	THR	12.9
1	D	619	THR	12.7
1	A	619	THR	12.5
1	F	619	THR	11.9
1	A	343	ALA	11.8
1	F	343	ALA	11.2
1	G	619	THR	11.0
1	E	459	VAL	11.0
1	B	45	ILE	10.7
1	C	389	LEU	10.6
1	G	389	LEU	10.5
1	E	619	THR	10.3

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Mol	Chain	Res	Type	RSRZ
1	H	43	MET	9.3
1	C	618	PHE	9.2
1	D	459	VAL	9.2
1	G	343	ALA	9.2
1	B	43	MET	9.1
1	A	389	LEU	8.8
1	F	43	MET	8.8
1	G	43	MET	8.8
1	F	459	VAL	8.7
1	B	343	ALA	8.7
1	B	44	ASP	8.7
1	A	43	MET	8.6
1	F	389	LEU	8.6
1	H	45	ILE	8.5
1	C	345	PRO	8.1
1	F	344	ASN	8.0
1	F	342	PRO	8.0
1	C	456	TYR	7.8
1	G	459	VAL	7.8
1	H	343	ALA	7.7
1	G	458	ALA	7.7
1	B	459	VAL	7.7
1	B	345	PRO	7.7
1	G	345	PRO	7.5
1	A	458	ALA	7.5
1	C	385	THR	7.5
1	D	345	PRO	7.5
1	B	456	TYR	7.4
1	D	343	ALA	7.3
1	G	44	ASP	7.2
1	E	44	ASP	7.1
1	C	459	VAL	7.1
1	E	43	MET	7.1
1	D	618	PHE	7.1
1	D	454	PHE	7.0
1	E	618	PHE	7.0
1	H	459	VAL	6.9
1	D	458	ALA	6.9
1	C	44	ASP	6.9
1	F	345	PRO	6.8
1	E	385	THR	6.7
1	D	45	ILE	6.7

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Mol	Chain	Res	Type	RSRZ
1	F	44	ASP	6.7
1	E	45	ILE	6.6
1	C	343	ALA	6.6
1	E	343	ALA	6.6
1	H	344	ASN	6.5
1	C	390	THR	6.5
1	D	344	ASN	6.4
1	B	389	LEU	6.3
1	A	345	PRO	6.3
1	D	43	MET	6.3
1	D	389	LEU	6.2
1	F	618	PHE	6.2
1	D	388	GLU	6.1
1	E	458	ALA	6.1
1	G	385	THR	6.0
1	H	342	PRO	6.0
1	E	384	GLY	6.0
1	F	385	THR	6.0
1	A	388	GLU	5.9
1	A	344	ASN	5.9
1	E	390	THR	5.9
1	C	45	ILE	5.9
1	H	453	ALA	5.9
1	B	344	ASN	5.8
1	E	388	GLU	5.8
1	G	186	ASP	5.8
1	F	458	ALA	5.8
1	C	43	MET	5.7
1	E	342	PRO	5.6
1	A	401	THR	5.5
1	H	345	PRO	5.5
1	C	344	ASN	5.5
1	E	387	GLY	5.5
1	A	385	THR	5.4
1	B	618	PHE	5.4
1	H	456	TYR	5.3
1	C	383	ARG	5.3
1	C	342	PRO	5.3
1	C	388	GLU	5.3
1	G	618	PHE	5.2
1	G	344	ASN	5.2
1	B	454	PHE	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	385	THR	5.1
1	B	458	ALA	5.0
1	F	384	GLY	4.9
1	H	617	PRO	4.9
1	D	385	THR	4.9
1	H	44	ASP	4.9
1	C	400	SER	4.9
1	B	341	ASN	4.9
1	E	344	ASN	4.9
1	C	458	ALA	4.8
1	G	45	ILE	4.8
1	H	458	ALA	4.7
1	C	384	GLY	4.7
1	F	45	ILE	4.7
1	G	401	THR	4.7
1	F	341	ASN	4.7
1	G	400	SER	4.7
1	G	455	SER	4.6
1	F	232	GLY	4.6
1	F	454	PHE	4.6
1	C	617	PRO	4.5
1	C	401	THR	4.5
1	F	387	GLY	4.5
1	G	100	ILE	4.4
1	C	396	THR	4.3
1	H	389	LEU	4.3
1	B	342	PRO	4.3
1	D	617	PRO	4.3
1	H	618	PHE	4.3
1	A	390	THR	4.3
1	D	44	ASP	4.3
1	D	341	ASN	4.3
1	A	456	TYR	4.2
1	A	384	GLY	4.2
1	D	342	PRO	4.2
1	C	309	PHE	4.1
1	F	390	THR	4.1
1	A	341	ASN	4.1
1	E	383	ARG	4.0
1	E	345	PRO	4.0
1	D	456	TYR	4.0
1	G	617	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	341	ASN	3.9
1	B	388	GLU	3.9
1	E	341	ASN	3.9
1	B	453	ALA	3.9
1	H	454	PHE	3.9
1	F	456	TYR	3.9
1	G	342	PRO	3.8
1	B	387	GLY	3.8
1	A	342	PRO	3.8
1	H	185	LYS	3.8
1	D	186	ASP	3.8
1	F	388	GLU	3.8
1	E	617	PRO	3.8
1	A	618	PHE	3.7
1	G	341	ASN	3.7
1	B	390	THR	3.7
1	D	390	THR	3.7
1	F	347	GLU	3.7
1	D	309	PHE	3.6
1	A	383	ARG	3.6
1	C	268	THR	3.6
1	A	44	ASP	3.6
1	G	382	ILE	3.6
1	H	100	ILE	3.6
1	G	390	THR	3.5
1	E	457	GLY	3.5
1	H	341	ASN	3.5
1	G	384	GLY	3.5
1	F	382	ILE	3.5
1	F	383	ARG	3.5
1	F	186	ASP	3.5
1	C	455	SER	3.5
1	E	400	SER	3.5
1	H	340	PRO	3.5
1	D	457	GLY	3.4
1	E	347	GLU	3.4
1	G	388	GLU	3.4
1	F	452	ASP	3.4
1	F	272	GLU	3.4
1	H	347	GLU	3.3
1	H	452	ASP	3.3
1	A	454	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	454	PHE	3.3
1	F	455	SER	3.3
1	B	82	SER	3.3
1	E	382	ILE	3.3
1	E	186	ASP	3.2
1	A	391	TYR	3.2
1	A	406	ASP	3.2
1	A	386	PRO	3.2
1	E	454	PHE	3.1
1	F	386	PRO	3.1
1	E	269	ASP	3.1
1	F	561	GLU	3.1
1	H	231	LYS	3.1
1	D	400	SER	3.1
1	C	271	PRO	3.1
1	C	82	SER	3.1
1	A	186	ASP	3.1
1	E	250	PHE	3.1
1	F	401	THR	3.0
1	F	391	TYR	3.0
1	D	271	PRO	3.0
1	A	99	ASN	3.0
1	A	249	THR	3.0
1	C	186	ASP	3.0
1	A	400	SER	3.0
1	C	305	SER	3.0
1	A	381	THR	2.9
1	E	391	TYR	2.9
1	D	382	ILE	2.9
1	H	457	GLY	2.9
1	E	272	GLU	2.9
1	H	189	ASP	2.9
1	A	272	GLU	2.9
1	B	186	ASP	2.9
1	E	456	TYR	2.9
1	F	453	ALA	2.9
1	G	185	LYS	2.9
1	G	399	ALA	2.9
1	D	383	ARG	2.9
1	G	340	PRO	2.8
1	C	306	GLY	2.8
1	F	189	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	382	ILE	2.8
1	H	57	ILE	2.7
1	C	347	GLU	2.7
1	E	268	THR	2.7
1	C	272	GLU	2.7
1	F	346	PRO	2.7
1	C	392	SER	2.7
1	G	309	PHE	2.7
1	G	453	ALA	2.7
1	D	272	GLU	2.7
1	D	560	LYS	2.7
1	E	184	VAL	2.7
1	F	546	VAL	2.7
1	C	323	VAL	2.6
1	H	305	SER	2.6
1	G	456	TYR	2.6
1	E	182	LEU	2.6
1	E	187	ASP	2.6
1	E	616	SER	2.6
1	C	454	PHE	2.6
1	C	561	GLU	2.6
1	A	617	PRO	2.6
1	F	490	LYS	2.6
1	F	187	ASP	2.6
1	H	232	GLY	2.6
1	G	188	ALA	2.6
1	D	549	LEU	2.6
1	G	187	ASP	2.6
1	F	394	THR	2.5
1	E	421	GLU	2.5
1	E	601	LEU	2.5
1	H	271	PRO	2.5
1	F	309	PHE	2.5
1	D	386	PRO	2.5
1	H	455	SER	2.5
1	H	121	LEU	2.5
1	E	561	GLU	2.5
1	G	396	THR	2.5
1	C	386	PRO	2.5
1	E	248	PRO	2.5
1	E	57	ILE	2.5
1	E	304	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	407	TRP	2.5
1	F	188	ALA	2.5
1	F	617	PRO	2.4
1	A	100	ILE	2.4
1	B	57	ILE	2.4
1	F	308	ARG	2.4
1	F	185	LYS	2.4
1	E	386	PRO	2.4
1	D	391	TYR	2.4
1	B	617	PRO	2.4
1	D	68	ALA	2.4
1	B	329	LEU	2.4
1	C	614	THR	2.4
1	B	386	PRO	2.4
1	H	186	ASP	2.4
1	A	602	ALA	2.4
1	A	347	GLU	2.3
1	G	386	PRO	2.3
1	C	601	LEU	2.3
1	H	272	GLU	2.3
1	C	453	ALA	2.3
1	D	188	ALA	2.3
1	E	490	LYS	2.3
1	B	383	ARG	2.3
1	F	168	TRP	2.3
1	E	455	SER	2.3
1	B	580	LEU	2.3
1	G	347	GLU	2.3
1	F	249	THR	2.3
1	B	133	ALA	2.3
1	C	490	LYS	2.3
1	D	268	THR	2.3
1	H	299	HIS	2.3
1	A	317	VAL	2.3
1	E	189	ASP	2.3
1	F	81	ASP	2.3
1	A	133	ALA	2.2
1	F	299	HIS	2.2
1	E	401	THR	2.2
1	F	549	LEU	2.2
1	F	586	ILE	2.2
1	G	582	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	413	LYS	2.2
1	E	583	CYS	2.2
1	E	82	SER	2.2
1	H	461	GLN	2.2
1	F	133	ALA	2.2
1	G	387	GLY	2.2
1	A	580	LEU	2.2
1	E	611	GLN	2.2
1	D	387	GLY	2.2
1	F	580	LEU	2.2
1	H	268	THR	2.2
1	D	185	LYS	2.1
1	E	232	GLY	2.1
1	C	132	GLN	2.1
1	B	323	VAL	2.1
1	A	455	SER	2.1
1	E	81	ASP	2.1
1	A	387	GLY	2.1
1	B	306	GLY	2.1
1	H	309	PHE	2.1
1	A	453	ALA	2.1
1	G	583	CYS	2.1
1	A	452	ASP	2.1
1	G	57	ILE	2.1
1	F	82	SER	2.1
1	B	157	VAL	2.1
1	B	384	GLY	2.1
1	H	160	VAL	2.1
1	D	168	TRP	2.1
1	A	320	ALA	2.1
1	D	347	GLU	2.1
1	C	185	LYS	2.1
1	C	452	ASP	2.1
1	G	461	GLN	2.1
1	C	328	LEU	2.1
1	A	269	ASP	2.1
1	G	189	ASP	2.1
1	A	469	VAL	2.0
1	D	249	THR	2.0
1	F	268	THR	2.0
1	B	185	LYS	2.0
1	F	315	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	190	ALA	2.0
1	D	178	GLU	2.0
1	E	299	HIS	2.0
1	E	291	LEU	2.0
1	G	549	LEU	2.0
1	B	99	ASN	2.0
1	D	401	THR	2.0
1	F	285	ARG	2.0
1	C	321	GLY	2.0
1	G	232	GLY	2.0
1	G	133	ALA	2.0
1	G	383	ARG	2.0
1	G	182	LEU	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, 95th 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	D	801	53/53	0.94	0.16	1.51	14,17,20,20	0
2	FAD	B	801	53/53	0.94	0.17	1.44	10,15,17,21	0
2	FAD	A	801	53/53	0.95	0.15	0.79	12,17,21,23	0
2	FAD	C	801	53/53	0.94	0.14	0.40	7,16,21,24	0
2	FAD	H	801	53/53	0.95	0.14	0.20	11,15,18,19	0
2	FAD	F	801	53/53	0.94	0.12	-0.25	16,19,21,22	0
2	FAD	G	801	53/53	0.95	0.12	-0.31	14,18,20,21	0
2	FAD	E	801	53/53	0.93	0.12	-0.58	14,18,21,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.