Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:23 PM GMT

PDB ID	:	1FCD
Title	:	THE STRUCTURE OF FLAVOCYTOCHROME C SULFIDE DEHYDROGENASE FROM A PURPLE PHOTOTROPHIC BACTERIUM CHROMATIUM VINOSUM AT 2.5 ANGSTROMS RESOLUTION
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Deposited on	:	1994-08-18
Resolution	:	2.53 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 (i)) were used in the production of this report:

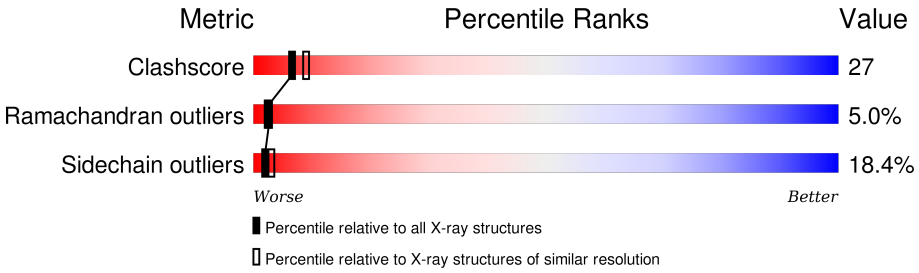
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.53 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))
Clashscore	102246	4968 (2.54-2.50)
Ramachandran outliers	100387	4873 (2.54-2.50)
Sidechain outliers	100360	4875 (2.54-2.50)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	401	46% 37% 13% •
1	B	401	42% 40% 14% •
2	C	174	56% 31% 13%
2	D	174	51% 35% 11% •

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FAD	A	699	X	-	-	-
3	FAD	B	699	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9002 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 FLAVOCYTOCHROME C SULFIDE DEHYDROGENASE (FLAVIN-BINDING SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	0	0
			3018	1918	505	584	11			
1	B	401	Total	C	N	O	S	0	0	0
			3018	1918	505	584	11			

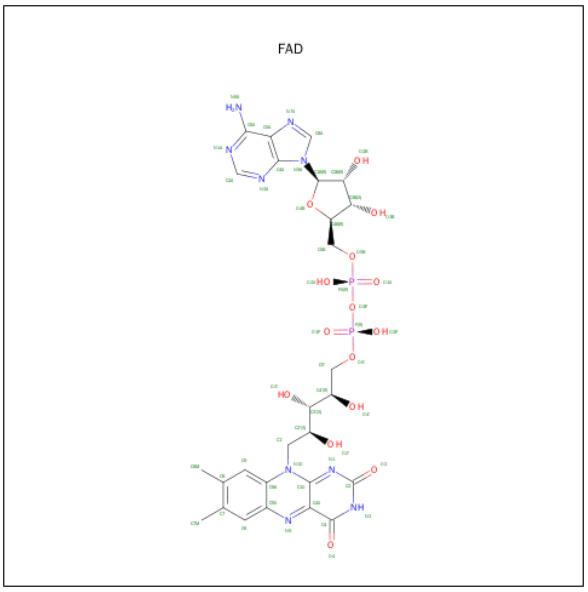
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	182	MET	LYS	CONFLICT	UNP Q06530
A	296	SER	CYS	CONFLICT	UNP Q06530
A	321	VAL	ALA	CONFLICT	UNP Q06530
B	182	MET	LYS	CONFLICT	UNP Q06530
B	296	SER	CYS	CONFLICT	UNP Q06530
B	321	VAL	ALA	CONFLICT	UNP Q06530

- Molecule 2 is a protein called FLAVOCYTOCHROME C SULFIDE DEHYDROGENASE (CYTOCHROME SUBUNIT).

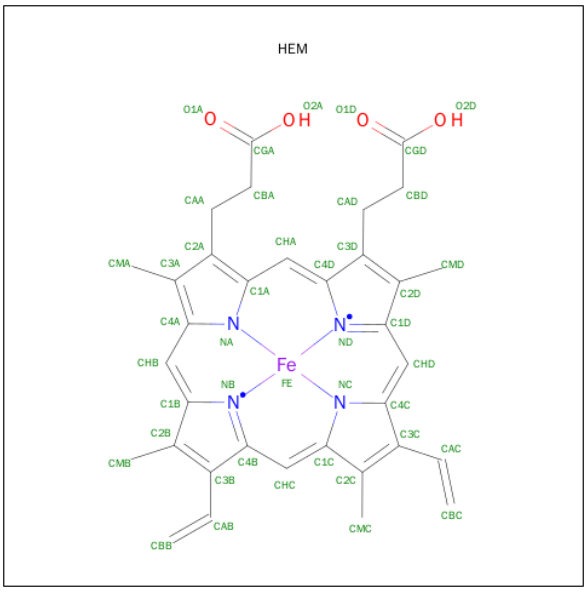
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	174	Total	C	N	O	S	0	0	0
			1344	842	225	264	13			
2	D	174	Total	C	N	O	S	0	0	0
			1344	842	225	264	13			

- 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		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

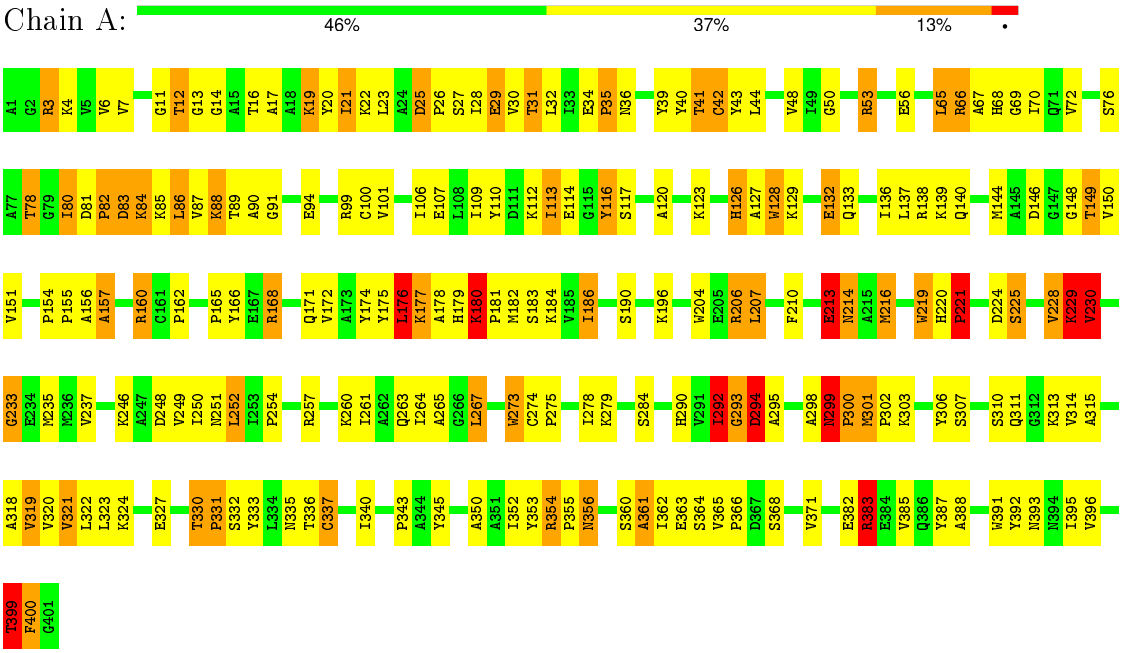
3 Residue-property plots (i)

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.

Note EDS was not executed.

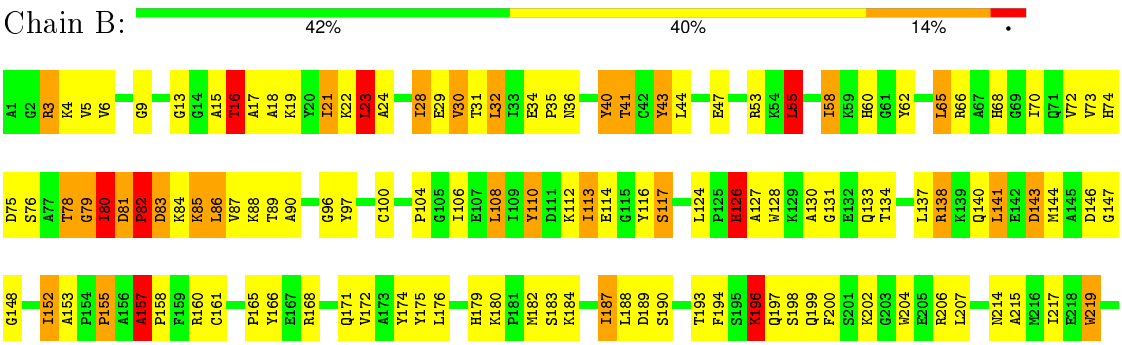
• Molecule 1: FLAVOCYTOCHROME C SULFIDE DEHYDROGENASE (FLAVIN-BINDING SUBUNIT)

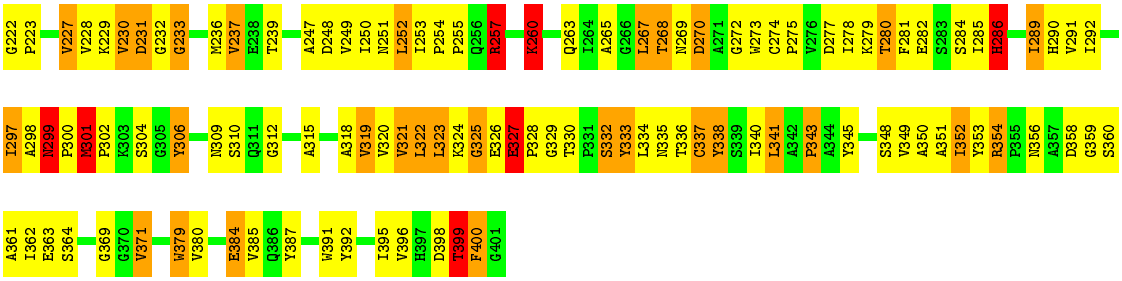
Chain A:



• Molecule 1: FLAVOCYTOCHROME C SULFIDE DEHYDROGENASE (FLAVIN-BINDING SUBUNIT)

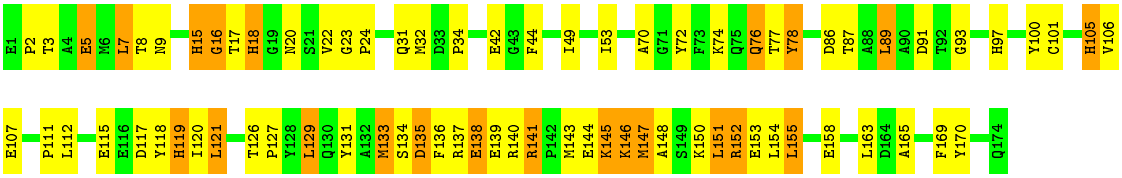
Chain B:





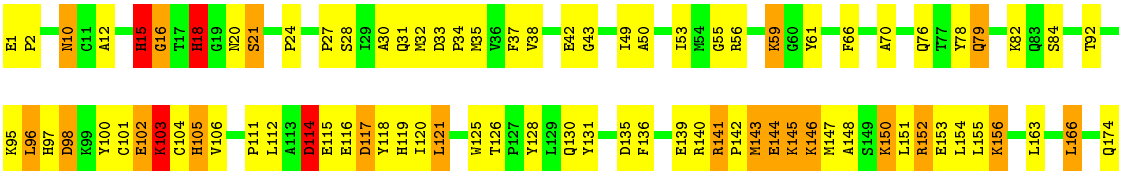
• Molecule 2: FLAVOCYTOCHROME C SULFIDE DEHYDROGENASE (CYTOCHROME SUBUNIT)

Chain C:



• Molecule 2: FLAVOCYTOCHROME C SULFIDE DEHYDROGENASE (CYTOCHROME SUBUNIT)

Chain D:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	168.60Å 84.60Å 106.40Å 90.00° 107.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.53	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.53)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.237 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9002	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.96	2/3093 (0.1%)	1.77	62/4209 (1.5%)
1	B	0.97	4/3093 (0.1%)	1.75	75/4209 (1.8%)
2	C	0.86	0/1374	1.46	13/1847 (0.7%)
2	D	0.87	1/1374 (0.1%)	1.54	22/1847 (1.2%)
All	All	0.94	7/8934 (0.1%)	1.68	172/12112 (1.4%)

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	4
1	B	0	2
2	C	0	1
All	All	0	7

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	399	THR	C-O	-9.50	1.05	1.23
2	D	30	ALA	C-O	-8.60	1.07	1.23
1	B	400	PHE	N-CA	7.31	1.60	1.46
1	A	399	THR	C-O	-7.15	1.09	1.23
1	B	233	GLY	CA-C	5.67	1.60	1.51
1	A	400	PHE	CA-C	5.54	1.67	1.52
1	B	230	VAL	CA-CB	5.36	1.66	1.54

All (172) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	400	PHE	CA-C-O	-20.26	77.56	120.10
1	A	400	PHE	CA-C-N	19.11	154.43	116.20
1	B	399	THR	O-C-N	-13.51	101.08	122.70
1	B	230	VAL	CG1-CB-CG2	-11.48	92.53	110.90
1	B	160	ARG	NE-CZ-NH2	-10.70	114.95	120.30
1	A	230	VAL	CA-C-N	-10.53	94.04	117.20
1	B	128	TRP	CD1-CG-CD2	10.30	114.54	106.30
1	A	399	THR	O-C-N	-10.11	106.52	122.70
1	A	230	VAL	CG1-CB-CG2	-9.90	95.06	110.90
1	A	225	SER	N-CA-CB	-9.81	95.78	110.50
1	B	43	TYR	CB-CG-CD2	-9.73	115.17	121.00
1	B	126	HIS	CA-CB-CG	9.41	129.60	113.60
1	A	219	TRP	CD1-CG-CD2	9.34	113.77	106.30
2	D	125	TRP	CD1-CG-CD2	9.09	113.58	106.30
1	A	180	LYS	O-C-N	-8.98	104.05	121.10
1	A	337	CYS	CA-CB-SG	8.92	130.06	114.00
1	B	379	TRP	CD1-CG-CD2	8.87	113.40	106.30
2	D	18	HIS	CA-CB-CG	8.69	128.38	113.60
1	B	128	TRP	CE2-CD2-CG	-8.68	100.35	107.30
1	A	128	TRP	CD1-CG-CD2	8.60	113.18	106.30
1	B	273	TRP	CG-CD2-CE3	8.53	141.57	133.90
1	B	273	TRP	CD1-CG-CD2	8.51	113.10	106.30
1	B	204	TRP	CD1-CG-CD2	8.49	113.10	106.30
1	B	273	TRP	CE2-CD2-CG	-8.44	100.55	107.30
1	B	126	HIS	CA-C-N	8.22	135.30	117.20
1	B	323	LEU	O-C-N	-8.21	109.56	122.70
1	B	379	TRP	CE2-CD2-CG	-8.21	100.73	107.30
1	A	219	TRP	CE2-CD2-CG	-8.04	100.87	107.30
1	B	399	THR	CA-C-N	7.98	134.75	117.20
1	A	273	TRP	CE2-CD2-CG	-7.95	100.94	107.30
1	A	32	LEU	CA-CB-CG	7.93	133.55	115.30
1	B	228	VAL	CA-C-N	-7.86	99.92	117.20
1	A	204	TRP	CD1-CG-CD2	7.85	112.58	106.30
1	A	214	ASN	N-CA-C	-7.83	89.87	111.00
1	B	379	TRP	CG-CD2-CE3	7.83	140.94	133.90
1	A	273	TRP	CD1-CG-CD2	7.68	112.45	106.30
1	B	338	TYR	CB-CG-CD1	-7.63	116.42	121.00
1	A	354	ARG	NE-CZ-NH2	7.61	124.11	120.30
1	B	354	ARG	NE-CZ-NH2	7.55	124.08	120.30
2	D	125	TRP	CE2-CD2-CG	-7.53	101.28	107.30
2	C	141	ARG	NE-CZ-NH2	7.48	124.04	120.30
1	A	273	TRP	CG-CD2-CE3	7.47	140.62	133.90
1	B	337	CYS	CA-CB-SG	7.43	127.37	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	257	ARG	NE-CZ-NH2	7.42	124.01	120.30
1	A	148	GLY	CA-C-N	7.42	133.52	117.20
1	A	204	TRP	CE2-CD2-CG	-7.37	101.40	107.30
1	A	128	TRP	CE2-CD2-CG	-7.36	101.41	107.30
2	C	140	ARG	NE-CZ-NH2	7.35	123.97	120.30
1	B	379	TRP	CB-CG-CD1	-7.34	117.45	127.00
1	B	204	TRP	CE2-CD2-CG	-7.31	101.45	107.30
2	D	114	ASP	N-CA-C	-7.27	91.38	111.00
1	B	273	TRP	CB-CG-CD1	-7.26	117.57	127.00
1	A	273	TRP	CB-CG-CD1	-7.18	117.66	127.00
1	A	213	GLU	CA-C-N	-7.17	101.42	117.20
1	A	66	ARG	NE-CZ-NH2	7.15	123.87	120.30
1	B	138	ARG	NE-CZ-NH2	7.13	123.86	120.30
1	B	384	GLU	CA-CB-CG	-7.13	97.72	113.40
1	A	230	VAL	O-C-N	7.12	134.10	122.70
2	D	140	ARG	NE-CZ-NH2	7.12	123.86	120.30
1	B	126	HIS	O-C-N	-7.12	111.31	122.70
2	C	137	ARG	NE-CZ-NH2	7.09	123.85	120.30
1	A	228	VAL	CA-C-N	-7.05	101.68	117.20
2	C	152	ARG	NE-CZ-NH2	7.03	123.81	120.30
2	D	144	GLU	CB-CA-C	6.86	124.11	110.40
1	A	168	ARG	NE-CZ-NH1	6.82	123.71	120.30
2	D	141	ARG	NE-CZ-NH2	6.81	123.70	120.30
2	D	15	HIS	CB-CG-ND1	-6.74	106.35	123.20
2	C	78	TYR	CB-CG-CD1	-6.65	117.01	121.00
1	A	39	TYR	CB-CG-CD1	-6.63	117.02	121.00
1	A	292	ILE	O-C-N	6.60	134.42	123.20
1	B	286	HIS	CA-CB-CG	6.58	124.79	113.60
2	D	103	LYS	N-CA-C	-6.54	93.35	111.00
1	B	66	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	B	166	TYR	CB-CG-CD2	-6.48	117.11	121.00
1	A	225	SER	CB-CA-C	6.38	122.22	110.10
1	B	301	MET	CG-SD-CE	6.31	110.29	100.20
1	A	166	TYR	CB-CG-CD2	-6.30	117.22	121.00
2	D	125	TRP	CG-CD1-NE1	-6.30	103.80	110.10
1	A	168	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	A	292	ILE	C-N-CA	6.29	135.51	122.30
1	B	126	HIS	N-CA-C	-6.26	94.08	111.00
2	D	15	HIS	CG-CD2-NE2	-6.23	97.36	109.20
1	B	219	TRP	CD1-CG-CD2	6.20	111.26	106.30
1	B	53	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	A	40	TYR	CB-CG-CD1	-6.19	117.28	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	204	TRP	CG-CD2-CE3	6.17	139.45	133.90
1	B	55	LEU	CA-CB-CG	6.15	129.45	115.30
1	B	16	THR	O-C-N	-6.14	112.87	122.70
2	C	143	MET	CG-SD-CE	6.14	110.02	100.20
1	B	228	VAL	CG1-CB-CG2	6.14	120.72	110.90
2	C	133	MET	CG-SD-CE	6.13	110.02	100.20
1	B	9	GLY	O-C-N	-6.12	112.79	123.20
1	B	379	TRP	CG-CD1-NE1	-6.12	103.98	110.10
1	B	144	MET	CG-SD-CE	6.08	109.93	100.20
1	A	182	MET	CG-SD-CE	6.03	109.85	100.20
1	A	186	ILE	CG1-CB-CG2	-6.03	98.13	111.40
1	A	160	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	B	128	TRP	CG-CD1-NE1	-6.01	104.09	110.10
1	B	110	TYR	CB-CG-CD1	-6.00	117.40	121.00
1	B	341	LEU	CA-CB-CG	6.00	129.10	115.30
1	A	301	MET	CG-SD-CE	5.98	109.77	100.20
1	B	41	THR	N-CA-CB	-5.97	98.95	110.30
1	B	143	ASP	CB-CA-C	-5.97	98.47	110.40
1	A	138	ARG	NE-CZ-NH1	5.93	123.27	120.30
2	D	35	MET	CG-SD-CE	5.93	109.69	100.20
1	A	128	TRP	CG-CD1-NE1	-5.89	104.20	110.10
2	D	105	HIS	CA-CB-CG	-5.87	103.62	113.60
2	C	121	LEU	CA-CB-CG	5.87	128.79	115.30
2	D	125	TRP	CG-CD2-CE3	5.81	139.13	133.90
1	B	73	VAL	N-CA-C	-5.81	95.32	111.00
1	B	82	PRO	O-C-N	5.78	131.95	122.70
1	B	236	MET	CG-SD-CE	-5.75	91.00	100.20
1	B	179	HIS	CA-CB-CG	5.75	123.37	113.60
1	B	40	TYR	CB-CG-CD2	-5.72	117.57	121.00
1	A	148	GLY	CA-C-O	-5.71	110.32	120.60
1	B	53	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	206	ARG	NE-CZ-NH1	5.68	123.14	120.30
2	D	147	MET	CG-SD-CE	5.66	109.26	100.20
1	A	180	LYS	CA-C-N	5.62	132.85	117.10
1	A	230	VAL	CA-C-O	5.60	131.85	120.10
1	B	157	ALA	CA-C-N	5.60	132.77	117.10
1	A	383	ARG	NE-CZ-NH2	5.59	123.09	120.30
1	A	219	TRP	CG-CD2-CE3	5.59	138.93	133.90
2	D	32	MET	CG-SD-CE	5.57	109.12	100.20
1	B	79	GLY	O-C-N	5.57	131.61	122.70
1	B	9	GLY	CA-C-N	5.57	127.33	116.20
1	B	219	TRP	CE2-CD2-CG	-5.54	102.86	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	216	MET	CA-CB-CG	5.54	122.72	113.30
1	A	31	THR	CA-CB-CG2	-5.54	104.65	112.40
1	B	237	VAL	CG1-CB-CG2	5.54	119.76	110.90
1	A	207	LEU	CA-CB-CG	5.52	128.00	115.30
1	A	229	LYS	N-CA-CB	-5.51	100.68	110.60
2	C	119	HIS	CA-C-N	-5.45	105.20	117.20
1	A	219	TRP	CB-CG-CD1	-5.45	119.92	127.00
1	A	219	TRP	CG-CD1-NE1	-5.45	104.65	110.10
1	B	280	THR	N-CA-C	-5.43	96.34	111.00
2	D	15	HIS	N-CA-C	-5.42	96.36	111.00
2	C	15	HIS	CG-CD2-NE2	-5.39	98.96	109.20
1	B	193	THR	N-CA-CB	-5.36	100.12	110.30
1	A	292	ILE	CA-C-N	-5.35	105.50	116.20
2	C	18	HIS	CG-CD2-NE2	-5.32	99.10	109.20
2	D	143	MET	CG-SD-CE	5.31	108.70	100.20
1	A	36	ASN	CA-C-N	-5.29	105.56	117.20
2	D	121	LEU	CA-CB-CG	5.29	127.46	115.30
1	A	299	ASN	CB-CA-C	5.28	120.96	110.40
1	A	399	THR	CA-C-N	5.28	128.81	117.20
1	A	41	THR	N-CA-C	5.26	125.19	111.00
2	C	147	MET	CG-SD-CE	5.25	108.60	100.20
1	B	80	ILE	N-CA-C	-5.24	96.85	111.00
1	B	160	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	196	LYS	CA-C-N	-5.16	105.84	117.20
1	B	58	ILE	N-CA-CB	-5.16	98.94	110.80
1	B	43	TYR	CA-CB-CG	5.15	123.19	113.40
1	A	144	MET	CG-SD-CE	-5.14	91.97	100.20
1	B	380	VAL	CG1-CB-CG2	-5.14	102.68	110.90
1	B	232	GLY	CA-C-N	5.13	126.47	116.20
2	D	166	LEU	CA-CB-CG	5.13	127.10	115.30
1	B	43	TYR	CB-CA-C	-5.11	100.17	110.40
1	A	400	PHE	N-CA-CB	-5.10	101.41	110.60
1	B	189	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	B	128	TRP	CG-CD2-CE3	5.09	138.48	133.90
1	B	237	VAL	N-CA-CB	-5.08	100.32	111.50
2	D	15	HIS	ND1-CG-CD2	5.07	115.90	108.80
1	A	216	MET	CG-SD-CE	-5.07	92.09	100.20
1	B	44	LEU	CA-CB-CG	5.06	126.93	115.30
1	B	175	TYR	CB-CG-CD2	-5.05	117.97	121.00
1	A	129	LYS	N-CA-C	-5.04	97.39	111.00
1	B	273	TRP	CG-CD1-NE1	-5.04	105.06	110.10
1	A	78	THR	N-CA-CB	-5.04	100.73	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	204	TRP	CG-CD1-NE1	-5.03	105.07	110.10
2	D	21	SER	CA-C-N	-5.01	106.19	117.20
2	C	5	GLU	CA-CB-CG	-5.00	102.39	113.40

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	HIS	Sidechain
1	A	220	HIS	Sidechain
1	A	400	PHE	Mainchain,Peptide
1	B	60	HIS	Sidechain
1	B	68	HIS	Sidechain
2	C	105	HIS	Sidechain

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	3018	0	2953	168	0
1	B	3018	0	2954	208	0
2	C	1344	0	1282	58	0
2	D	1344	0	1282	60	0
3	A	53	0	30	7	0
3	B	53	0	30	2	0
4	C	86	0	60	3	0
4	D	86	0	60	4	0
All	All	9002	0	8651	482	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 27.

All (482) 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:A:180:LYS:HA	1:A:180:LYS:NZ	1.25	1.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:GLY:HA3	1:A:311:GLN:HE22	1.09	1.15
1:B:300:PRO:O	1:B:301:MET:HB2	1.47	1.11
1:A:293:GLY:HA3	1:A:311:GLN:NE2	1.70	1.06
1:B:19:LYS:O	1:B:23:LEU:HB2	1.55	1.06
1:B:81:ASP:HB3	1:B:82:PRO:CD	1.86	1.05
1:A:180:LYS:NZ	1:A:180:LYS:CA	2.20	1.04
1:B:299:ASN:HB3	1:B:300:PRO:HD2	1.37	1.04
1:A:298:ALA:O	1:A:299:ASN:O	1.75	1.02
1:B:81:ASP:HB3	1:B:82:PRO:HD3	1.41	1.00
1:A:25:ASP:O	1:A:25:ASP:OD1	1.79	1.00
1:B:298:ALA:O	1:B:300:PRO:O	1.81	0.97
1:A:299:ASN:O	1:A:301:MET:N	1.99	0.96
1:B:17:ALA:O	1:B:21:ILE:HB	1.66	0.94
1:A:180:LYS:HZ2	1:A:180:LYS:CA	1.79	0.93
1:A:180:LYS:HA	1:A:180:LYS:HZ3	1.13	0.91
1:B:80:ILE:O	1:B:81:ASP:HB2	1.69	0.90
2:C:145:LYS:H	2:C:145:LYS:HD3	1.37	0.89
1:B:299:ASN:HB3	1:B:300:PRO:CD	2.02	0.89
1:A:88:LYS:HG3	1:A:94:GLU:HG2	1.54	0.89
1:B:22:LYS:HZ2	1:B:29:GLU:HA	1.36	0.88
1:B:82:PRO:C	1:B:84:LYS:H	1.75	0.88
1:B:15:ALA:HB3	1:B:399:THR:HG22	1.56	0.86
1:B:290:HIS:NE2	1:B:319:VAL:HG23	1.91	0.86
1:B:153:ALA:HB1	1:B:227:VAL:HG11	1.57	0.86
2:D:145:LYS:HD3	2:D:145:LYS:N	1.90	0.85
1:A:146:ASP:OD1	1:A:179:HIS:O	1.95	0.85
1:B:16:THR:HG22	1:B:17:ALA:N	1.91	0.83
1:A:53:ARG:HH11	1:A:53:ARG:HB2	1.44	0.83
1:A:293:GLY:CA	1:A:311:GLN:HE22	1.92	0.82
2:C:145:LYS:HD3	2:C:145:LYS:N	1.91	0.82
1:B:290:HIS:CD2	1:B:319:VAL:HG23	2.14	0.81
1:B:82:PRO:C	1:B:84:LYS:N	2.34	0.80
1:B:260:LYS:HD2	1:B:260:LYS:H	1.44	0.80
1:B:299:ASN:HD21	1:B:361:ALA:HA	1.46	0.80
1:A:22:LYS:HE2	1:A:69:GLY:HA3	1.63	0.79
1:B:299:ASN:CG	1:B:362:ILE:H	1.86	0.79
1:B:3:ARG:NH2	1:B:323:LEU:HB3	1.99	0.78
1:B:17:ALA:HB1	1:B:21:ILE:CD1	2.15	0.77
2:D:145:LYS:HD3	2:D:145:LYS:H	1.49	0.77
1:A:109:ILE:HD11	1:A:257:ARG:HD2	1.66	0.77
1:B:112:LYS:HG3	1:B:255:PRO:HG2	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:HIS:HE2	1:B:319:VAL:HG23	1.45	0.77
1:A:180:LYS:HA	1:A:180:LYS:HZ2	0.97	0.77
1:B:84:LYS:O	1:B:85:LYS:HB3	1.85	0.76
1:B:299:ASN:OD1	1:B:361:ALA:HB1	1.86	0.76
1:B:80:ILE:O	1:B:81:ASP:CB	2.32	0.76
1:A:213:GLU:HG2	1:B:223:PRO:HD3	1.67	0.76
1:B:19:LYS:O	1:B:23:LEU:CB	2.33	0.75
1:A:21:ILE:CG2	1:A:30:VAL:HG21	2.16	0.75
1:B:321:VAL:HG11	1:B:328:PRO:HA	1.69	0.75
2:C:18:HIS:HB3	2:C:76:GLN:HG2	1.69	0.74
1:A:19:LYS:O	1:A:23:LEU:HB2	1.87	0.73
1:B:100:CYS:HB3	1:B:289:ILE:HG23	1.69	0.73
2:D:146:LYS:HE3	2:D:146:LYS:H	1.54	0.73
1:B:81:ASP:O	1:B:83:ASP:N	2.22	0.72
2:C:145:LYS:H	2:C:145:LYS:CD	1.96	0.72
1:A:99:ARG:HH11	1:A:290:HIS:HE1	1.36	0.72
1:B:81:ASP:CB	1:B:82:PRO:CD	2.63	0.72
1:A:150:VAL:HG13	1:A:249:VAL:HB	1.72	0.72
1:A:315:ALA:O	1:A:319:VAL:HG13	1.90	0.71
1:B:148:GLY:O	1:B:183:SER:HB3	1.90	0.71
1:B:22:LYS:NZ	1:B:29:GLU:HA	2.04	0.71
2:D:31:GLN:HB2	2:D:76:GLN:O	1.91	0.70
1:B:83:ASP:N	1:B:83:ASP:OD1	2.23	0.70
1:A:331:PRO:HD2	1:A:355:PRO:HG3	1.72	0.70
1:A:382:GLU:O	1:A:385:VAL:HG12	1.91	0.69
1:B:292:ILE:HD11	1:B:315:ALA:CB	2.22	0.69
1:B:279:LYS:NZ	1:B:329:GLY:O	2.25	0.69
2:C:138:GLU:O	2:C:139:GLU:HB2	1.93	0.69
1:B:34:GLU:O	1:B:74:HIS:HA	1.92	0.69
1:B:392:TYR:O	1:B:396:VAL:HB	1.92	0.69
1:B:32:LEU:HD23	1:B:72:VAL:HG23	1.74	0.68
1:A:260:LYS:H	1:A:260:LYS:HD2	1.58	0.68
1:B:260:LYS:CD	1:B:260:LYS:H	2.07	0.68
1:B:141:LEU:HD21	1:B:172:VAL:HG13	1.76	0.67
1:B:334:LEU:HD12	1:B:352:ILE:HD13	1.77	0.67
1:A:313:LYS:HD3	2:C:9:ASN:HB3	1.75	0.67
1:B:81:ASP:CB	1:B:82:PRO:HD3	2.21	0.67
1:B:131:GLY:HA2	1:B:134:THR:OG1	1.95	0.67
1:B:110:TYR:HB3	1:B:117:SER:HA	1.77	0.67
1:A:299:ASN:HB2	1:A:362:ILE:HB	1.78	0.66
1:B:275:PRO:HG2	1:B:285:ILE:HD11	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ILE:HD12	1:A:252:LEU:HD23	1.77	0.66
1:A:265:ALA:HB3	1:A:267:LEU:HD22	1.76	0.66
1:A:160:ARG:HD3	3:A:699:FAD:H9	1.78	0.65
1:B:79:GLY:O	1:B:88:LYS:N	2.28	0.65
1:A:350:ALA:HB2	2:C:53:ILE:HD11	1.77	0.65
1:B:81:ASP:HB3	1:B:82:PRO:HD2	1.76	0.65
1:A:19:LYS:HG3	1:A:20:TYR:N	2.11	0.65
1:A:319:VAL:O	1:A:323:LEU:N	2.24	0.65
1:B:252:LEU:O	1:B:254:PRO:HD3	1.95	0.65
1:B:17:ALA:O	1:B:21:ILE:CB	2.44	0.65
1:B:297:ILE:HG22	1:B:297:ILE:O	1.96	0.64
2:C:97:HIS:HD1	2:C:101:CYS:HB2	1.61	0.64
1:A:298:ALA:C	1:A:299:ASN:O	2.35	0.64
1:A:146:ASP:CG	1:A:179:HIS:O	2.36	0.64
1:A:300:PRO:HD2	1:A:362:ILE:O	1.98	0.64
1:B:80:ILE:HG22	1:B:265:ALA:HB2	1.79	0.64
1:B:280:THR:HG22	1:B:318:ALA:HB1	1.80	0.64
2:D:136:PHE:CE1	2:D:141:ARG:HD3	2.32	0.64
2:C:24:PRO:O	2:C:127:PRO:HG2	1.98	0.64
1:B:15:ALA:O	1:B:16:THR:C	2.35	0.64
2:D:145:LYS:H	2:D:145:LYS:CD	2.11	0.64
1:A:65:LEU:O	1:A:68:HIS:HB3	1.97	0.64
1:B:108:LEU:HD13	1:B:126:HIS:NE2	2.14	0.63
1:A:221:PRO:O	1:A:225:SER:HB3	1.99	0.63
2:D:49:ILE:HG13	2:D:141:ARG:HG3	1.81	0.63
1:A:319:VAL:CG2	1:A:320:VAL:N	2.61	0.63
2:D:1:GLU:HG2	2:D:2:PRO:HD2	1.81	0.63
2:C:49:ILE:HG23	2:C:141:ARG:HG2	1.81	0.62
1:A:19:LYS:HA	1:A:70:ILE:HD11	1.80	0.62
2:D:153:GLU:HB3	2:D:154:LEU:HD12	1.81	0.62
1:B:153:ALA:CB	1:B:227:VAL:HG11	2.27	0.62
1:A:156:ALA:HB2	1:A:190:SER:HB2	1.82	0.62
1:A:99:ARG:HH11	1:A:290:HIS:CE1	2.17	0.62
1:A:180:LYS:HD2	1:A:180:LYS:N	2.15	0.61
1:A:365:VAL:HG13	1:A:368:SER:OG	2.00	0.61
1:A:66:ARG:C	1:A:68:HIS:H	2.03	0.61
1:A:84:LYS:O	1:A:86:LEU:HD23	1.99	0.61
1:B:112:LYS:CG	1:B:255:PRO:HG2	2.30	0.61
2:D:27:PRO:HG3	2:D:128:TYR:CD1	2.35	0.61
1:B:85:LYS:HG2	1:B:85:LYS:O	2.01	0.61
1:B:153:ALA:HB1	1:B:227:VAL:CG1	2.27	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:ASP:O	1:B:360:SER:N	2.33	0.61
2:D:126:THR:O	2:D:130:GLN:HG3	1.99	0.61
1:A:180:LYS:HZ3	1:A:180:LYS:CA	1.96	0.60
1:B:80:ILE:HG22	1:B:265:ALA:CB	2.30	0.60
2:D:20:ASN:HD21	2:D:78:TYR:HA	1.66	0.60
1:B:85:LYS:O	1:B:96:GLY:HA2	2.01	0.60
1:B:17:ALA:HB1	1:B:21:ILE:HG13	1.84	0.60
1:B:168:ARG:HH11	1:B:251:ASN:HD21	1.48	0.60
1:B:5:VAL:O	1:B:30:VAL:HA	2.01	0.60
2:D:55:GLY:O	2:D:59:LYS:HG3	2.02	0.60
1:A:319:VAL:O	1:A:323:LEU:HB2	2.02	0.60
1:B:130:ALA:O	1:B:134:THR:HG23	2.02	0.60
2:C:111:PRO:HB3	2:C:120:ILE:HD12	1.82	0.59
2:C:89:LEU:HD23	2:C:165:ALA:HA	1.84	0.59
1:A:11:GLY:O	1:A:13:GLY:N	2.35	0.59
1:A:114:GLU:N	1:A:229:LYS:HA	2.17	0.59
1:B:78:THR:OG1	1:B:90:ALA:HB2	2.02	0.59
1:B:6:VAL:HG11	1:B:87:VAL:HG21	1.85	0.59
1:B:28:ILE:HD12	1:B:323:LEU:HD21	1.85	0.59
1:B:351:ALA:O	1:B:352:ILE:O	2.21	0.59
1:B:65:LEU:O	1:B:70:ILE:HG12	2.03	0.59
1:B:304:SER:HA	3:B:699:FAD:H1'2	1.85	0.59
1:A:80:ILE:HG21	1:A:265:ALA:HB1	1.85	0.58
1:B:300:PRO:HD2	1:B:362:ILE:O	2.03	0.58
2:D:156:LYS:HZ2	2:D:163:LEU:HD21	1.68	0.58
1:B:40:TYR:HD2	1:B:58:ILE:HG22	1.69	0.58
1:B:356:ASN:CG	1:B:363:GLU:HB3	2.24	0.58
1:B:5:VAL:HG23	1:B:30:VAL:HB	1.85	0.58
1:A:387:TYR:HH	2:C:131:TYR:HD2	1.52	0.57
2:D:141:ARG:HG2	2:D:142:PRO:HD2	1.86	0.57
1:B:299:ASN:CB	1:B:362:ILE:HB	2.34	0.57
1:A:7:VAL:HG22	1:A:101:VAL:HB	1.87	0.57
1:A:53:ARG:HB2	1:A:53:ARG:NH1	2.17	0.57
1:A:179:HIS:O	1:A:180:LYS:HB2	2.05	0.57
1:B:302:PRO:HG2	1:B:335:ASN:OD1	2.03	0.57
1:A:356:ASN:HB2	1:A:363:GLU:HB2	1.87	0.56
1:A:302:PRO:HG2	1:A:335:ASN:ND2	2.20	0.56
1:A:183:SER:O	1:A:184:LYS:HG3	2.05	0.56
1:A:206:ARG:HD2	1:A:345:TYR:HE2	1.69	0.56
1:B:274:CYS:SG	1:B:291:VAL:HG11	2.46	0.56
1:B:17:ALA:HB1	1:B:21:ILE:CG1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:38:VAL:O	2:D:42:GLU:HB2	2.06	0.56
1:B:299:ASN:CB	1:B:300:PRO:CD	2.80	0.56
1:B:16:THR:HG22	1:B:17:ALA:H	1.70	0.56
1:A:87:VAL:O	1:A:94:GLU:HA	2.06	0.55
1:B:126:HIS:O	1:B:126:HIS:ND1	2.39	0.55
1:A:25:ASP:C	1:A:25:ASP:OD1	2.45	0.55
2:D:100:TYR:HE2	2:D:154:LEU:HB3	1.71	0.55
2:C:153:GLU:HB2	2:C:154:LEU:HD12	1.86	0.55
2:D:95:LYS:HG3	2:D:96:LEU:N	2.21	0.55
1:A:21:ILE:CG2	1:A:22:LYS:N	2.70	0.55
1:B:282:GLU:HG3	1:B:290:HIS:CE1	2.41	0.55
1:B:112:LYS:CB	1:B:255:PRO:HG2	2.37	0.55
1:B:114:GLU:H	1:B:229:LYS:HA	1.72	0.55
1:A:327:GLU:O	1:A:327:GLU:HG3	2.07	0.55
1:A:11:GLY:O	1:A:12:THR:C	2.45	0.55
2:C:5:GLU:HG3	2:C:72:TYR:CE2	2.41	0.55
1:B:157:ALA:HB1	1:B:158:PRO:HD3	1.89	0.55
1:B:227:VAL:HA	1:B:239:THR:HA	1.89	0.54
1:B:292:ILE:HD11	1:B:315:ALA:HB3	1.87	0.54
1:A:117:SER:H	1:A:120:ALA:HB3	1.72	0.54
2:D:33:ASP:OD2	2:D:117:ASP:HA	2.07	0.54
1:A:293:GLY:CA	1:A:311:GLN:NE2	2.58	0.54
2:D:114:ASP:O	2:D:116:GLU:HG2	2.07	0.54
1:A:228:VAL:O	1:A:230:VAL:N	2.40	0.54
2:C:31:GLN:HG3	2:C:76:GLN:O	2.07	0.54
1:B:114:GLU:O	1:B:230:VAL:HA	2.07	0.54
1:A:12:THR:HA	1:A:399:THR:HG21	1.89	0.53
1:A:383:ARG:HH11	1:A:383:ARG:CG	2.21	0.53
2:C:20:ASN:HD21	2:C:78:TYR:HA	1.73	0.53
1:B:4:LYS:HD3	1:B:29:GLU:HB3	1.89	0.53
1:B:279:LYS:NZ	1:B:279:LYS:HB3	2.24	0.53
1:B:85:LYS:CG	1:B:85:LYS:O	2.56	0.53
1:B:21:ILE:HD11	1:B:319:VAL:HG11	1.89	0.53
1:B:321:VAL:HG13	1:B:326:GLU:O	2.08	0.53
1:B:229:LYS:O	1:B:230:VAL:HG23	2.09	0.53
1:B:13:GLY:O	1:B:16:THR:HB	2.08	0.53
2:D:27:PRO:HG3	2:D:128:TYR:CE1	2.43	0.53
1:B:147:GLY:HA2	1:B:182:MET:O	2.08	0.53
1:B:326:GLU:O	1:B:327:GLU:O	2.27	0.52
1:B:333:TYR:HD1	1:B:353:TYR:HB2	1.74	0.52
1:B:257:ARG:HB2	1:B:272:GLY:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:GLN:O	1:A:174:TYR:HB3	2.08	0.52
1:A:229:LYS:O	1:A:230:VAL:HG23	2.09	0.52
2:D:97:HIS:NE2	2:D:102:GLU:HG2	2.24	0.52
1:B:387:TYR:HH	2:D:131:TYR:HD2	1.55	0.52
2:C:93:GLY:HA3	2:C:169:PHE:HB2	1.92	0.52
2:C:86:ASP:HB3	2:C:89:LEU:HB2	1.90	0.52
1:B:260:LYS:O	1:B:263:GLN:HB2	2.10	0.52
1:B:300:PRO:O	1:B:301:MET:CB	2.34	0.52
1:B:278:ILE:HD12	1:B:362:ILE:HD12	1.91	0.52
1:A:307:SER:O	1:A:311:GLN:HG3	2.10	0.52
1:A:393:ASN:HD22	2:C:24:PRO:HD3	1.75	0.52
1:A:343:PRO:O	1:A:385:VAL:HG21	2.10	0.51
1:B:306:TYR:HB3	1:B:335:ASN:HD22	1.75	0.51
1:B:171:GLN:O	1:B:174:TYR:HB3	2.10	0.51
1:A:151:VAL:HA	1:A:186:ILE:O	2.10	0.51
1:B:15:ALA:HA	1:B:18:ALA:HB3	1.92	0.51
2:C:134:SER:O	2:C:138:GLU:HB2	2.09	0.51
1:B:196:LYS:HB3	1:B:371:VAL:HG21	1.93	0.51
1:B:87:VAL:HG23	1:B:97:TYR:HD2	1.75	0.51
2:C:151:LEU:HD22	2:C:151:LEU:C	2.31	0.51
1:A:86:LEU:HD12	1:A:94:GLU:HB3	1.93	0.51
1:B:318:ALA:O	1:B:322:LEU:HB2	2.10	0.51
2:D:136:PHE:CZ	2:D:141:ARG:HD3	2.45	0.51
1:A:21:ILE:HG22	1:A:22:LYS:N	2.26	0.51
2:C:111:PRO:HD3	2:C:120:ILE:HG13	1.92	0.50
2:C:121:LEU:O	2:C:170:TYR:HB3	2.11	0.50
2:D:100:TYR:CE2	2:D:154:LEU:HB3	2.45	0.50
1:A:260:LYS:H	1:A:260:LYS:CD	2.23	0.50
1:A:17:ALA:O	1:A:21:ILE:HB	2.11	0.50
1:B:17:ALA:HB1	1:B:21:ILE:HD12	1.91	0.50
1:A:101:VAL:HG22	1:A:290:HIS:HB2	1.93	0.50
1:B:55:LEU:HD21	1:B:131:GLY:HA2	1.93	0.50
1:A:306:TYR:HD2	1:A:391:TRP:HE1	1.54	0.50
2:D:82:LYS:HA	2:D:174:GLN:NE2	2.27	0.50
2:C:2:PRO:HB2	2:C:7:LEU:HD13	1.94	0.49
2:D:104:CYS:O	2:D:106:VAL:HG23	2.12	0.49
1:A:300:PRO:O	1:A:302:PRO:HD3	2.12	0.49
1:A:3:ARG:HB2	1:A:28:ILE:HG12	1.94	0.49
2:D:156:LYS:NZ	2:D:163:LEU:HD21	2.27	0.49
1:B:348:SER:HB3	2:D:56:ARG:HH22	1.77	0.49
1:A:360:SER:O	1:A:361:ALA:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ARG:HE	1:A:3:ARG:HA	1.76	0.49
1:B:207:LEU:HD21	1:B:345:TYR:CD2	2.48	0.49
1:B:13:GLY:O	1:B:16:THR:CB	2.60	0.49
1:B:5:VAL:HG21	1:B:21:ILE:CD1	2.43	0.49
1:B:65:LEU:HD13	1:B:400:PHE:HA	1.94	0.49
2:C:34:PRO:HD3	2:C:74:LYS:HD3	1.92	0.49
1:B:292:ILE:HD11	1:B:315:ALA:HB2	1.94	0.49
1:B:332:SER:O	2:D:10:ASN:ND2	2.38	0.49
1:A:250:ILE:CD1	1:A:252:LEU:HD23	2.41	0.49
1:A:50:GLY:HA3	1:A:171:GLN:HE21	1.76	0.49
2:D:12:ALA:HA	2:D:15:HIS:O	2.13	0.49
1:B:324:LYS:O	1:B:325:GLY:C	2.51	0.49
2:D:111:PRO:HD3	2:D:120:ILE:HG23	1.94	0.49
1:B:16:THR:CG2	1:B:17:ALA:N	2.60	0.49
2:D:144:GLU:HG2	4:D:902:HEM:HBD2	1.95	0.49
1:A:294:ASP:HB2	3:A:699:FAD:O2P	2.13	0.49
1:A:387:TYR:OH	2:C:131:TYR:HD2	1.95	0.49
1:A:149:THR:HA	1:A:184:LYS:O	2.13	0.49
1:B:343:PRO:O	1:B:385:VAL:HG21	2.12	0.49
2:D:100:TYR:O	2:D:150:LYS:HG2	2.12	0.48
1:B:268:THR:HG23	1:B:269:ASN:O	2.13	0.48
1:A:48:VAL:HA	1:A:53:ARG:O	2.13	0.48
2:D:18:HIS:HB2	2:D:76:GLN:HG3	1.94	0.48
1:A:82:PRO:O	1:A:84:LYS:N	2.46	0.48
2:D:96:LEU:HD23	2:D:155:LEU:HD21	1.96	0.48
1:A:318:ALA:O	1:A:322:LEU:CB	2.62	0.48
2:D:98:ASP:HA	2:D:102:GLU:HB2	1.96	0.48
2:C:107:GLU:HB3	2:C:112:LEU:HD11	1.96	0.48
1:B:124:LEU:HD22	1:B:250:ILE:HG12	1.94	0.48
1:B:260:LYS:CD	1:B:260:LYS:N	2.76	0.48
2:C:150:LYS:HD3	2:C:154:LEU:HD22	1.96	0.48
1:B:113:ILE:HG12	1:B:116:TYR:HB2	1.96	0.48
1:A:126:HIS:HB3	1:A:254:PRO:HD2	1.96	0.48
1:B:227:VAL:HG13	1:B:227:VAL:O	2.13	0.47
1:B:326:GLU:HG2	1:B:327:GLU:OE2	2.14	0.47
2:D:97:HIS:ND1	2:D:101:CYS:HB2	2.29	0.47
1:A:126:HIS:NE2	1:A:133:GLN:NE2	2.62	0.47
1:A:126:HIS:CG	1:A:126:HIS:O	2.66	0.47
1:A:279:LYS:HE2	1:A:279:LYS:HB3	1.75	0.47
1:A:35:PRO:HD2	3:A:699:FAD:N3A	2.29	0.47
2:C:147:MET:HB2	4:C:902:HEM:C4C	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:THR:HG23	1:B:312:GLY:HA2	1.95	0.47
1:A:257:ARG:HG3	1:A:263:GLN:HE22	1.78	0.47
1:B:108:LEU:HD22	1:B:126:HIS:CD2	2.48	0.47
1:A:6:VAL:O	1:A:100:CYS:HA	2.13	0.47
2:C:120:ILE:O	2:C:121:LEU:HD12	2.14	0.47
2:D:144:GLU:OE1	2:D:144:GLU:HA	2.13	0.47
2:D:148:ALA:O	2:D:152:ARG:HB3	2.15	0.47
1:B:336:THR:HG22	1:B:350:ALA:HA	1.96	0.47
1:A:42:CYS:SG	3:A:699:FAD:HM71	2.54	0.47
2:C:22:VAL:HG12	2:C:23:GLY:H	1.78	0.47
1:A:365:VAL:O	1:A:368:SER:OG	2.31	0.47
1:B:152:ILE:O	1:B:187:ILE:HA	2.15	0.47
1:A:136:ILE:HG22	1:A:140:GLN:OE1	2.15	0.47
1:B:108:LEU:HD13	1:B:126:HIS:CE1	2.49	0.47
1:B:157:ALA:CB	1:B:158:PRO:HD3	2.44	0.47
1:B:187:ILE:HG23	1:B:219:TRP:HA	1.95	0.47
1:B:297:ILE:CG2	1:B:297:ILE:O	2.62	0.47
1:B:15:ALA:CB	1:B:399:THR:HG22	2.36	0.47
1:B:277:ASP:O	1:B:281:PHE:HA	2.14	0.47
1:A:160:ARG:HG3	3:A:699:FAD:H1'1	1.95	0.46
2:D:16:GLY:HA3	2:D:20:ASN:O	2.15	0.46
2:C:148:ALA:O	2:C:152:ARG:N	2.44	0.46
2:D:143:MET:HE1	2:D:151:LEU:HD22	1.98	0.46
1:A:274:CYS:SG	1:A:295:ALA:O	2.72	0.46
1:A:176:LEU:HD12	1:A:176:LEU:HA	1.77	0.46
1:B:55:LEU:HD21	1:B:131:GLY:CA	2.44	0.46
1:B:202:LYS:HE3	1:B:206:ARG:HH12	1.79	0.46
2:D:15:HIS:HA	2:D:21:SER:OG	2.15	0.46
1:B:391:TRP:O	1:B:395:ILE:HG22	2.16	0.46
1:B:127:ALA:HA	1:B:133:GLN:HG2	1.98	0.46
1:B:267:LEU:CD1	1:B:286:HIS:HD2	2.28	0.46
2:C:31:GLN:HB2	2:C:78:TYR:HB2	1.96	0.46
1:A:16:THR:O	1:A:20:TYR:HB2	2.15	0.46
1:B:79:GLY:HA3	1:B:88:LYS:HB3	1.98	0.46
2:C:155:LEU:HD23	4:C:902:HEM:HBB1	1.96	0.46
1:B:334:LEU:HD12	1:B:352:ILE:CD1	2.44	0.46
1:B:290:HIS:CD2	1:B:319:VAL:CG2	2.92	0.46
1:A:35:PRO:HD3	1:A:76:SER:HA	1.97	0.46
1:A:89:THR:O	1:A:91:GLY:N	2.49	0.46
1:B:215:ALA:HB1	1:B:217:ILE:O	2.15	0.46
1:B:15:ALA:O	1:B:16:THR:O	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:LYS:O	1:A:23:LEU:CB	2.59	0.46
1:B:35:PRO:HD2	3:B:699:FAD:N3A	2.31	0.46
1:B:268:THR:HG23	1:B:272:GLY:HA2	1.96	0.46
1:B:336:THR:HA	1:B:349:VAL:O	2.15	0.46
2:C:97:HIS:ND1	2:C:101:CYS:HB2	2.31	0.45
1:B:282:GLU:HA	1:B:290:HIS:ND1	2.31	0.45
1:A:80:ILE:O	1:A:81:ASP:C	2.54	0.45
2:C:148:ALA:O	2:C:151:LEU:N	2.48	0.45
1:A:25:ASP:O	1:A:27:SER:N	2.49	0.45
1:B:40:TYR:CD2	1:B:131:GLY:HA3	2.50	0.45
2:C:105:HIS:CE1	2:C:119:HIS:HB2	2.52	0.45
1:B:80:ILE:HD11	1:B:100:CYS:SG	2.56	0.45
1:A:260:LYS:O	1:A:264:ILE:HG13	2.16	0.45
1:B:78:THR:HB	1:B:90:ALA:N	2.32	0.45
2:D:150:LYS:HE2	2:D:154:LEU:HD22	1.98	0.45
1:B:190:SER:C	1:B:222:GLY:HA3	2.37	0.45
2:C:145:LYS:CD	2:C:145:LYS:N	2.61	0.45
1:A:385:VAL:O	1:A:388:ALA:HB3	2.17	0.45
1:A:80:ILE:HG21	1:A:265:ALA:CB	2.47	0.45
1:B:336:THR:HG21	4:D:901:HEM:CBC	2.47	0.45
2:D:34:PRO:HA	2:D:70:ALA:HB1	1.98	0.45
1:A:101:VAL:CG1	1:A:292:ILE:HD11	2.46	0.45
1:A:132:GLU:CD	1:A:132:GLU:H	2.20	0.45
1:B:299:ASN:CB	1:B:300:PRO:HD2	2.27	0.44
3:A:699:FAD:H5'2	3:A:699:FAD:O2A	2.17	0.44
1:A:318:ALA:O	1:A:322:LEU:HB2	2.16	0.44
2:D:144:GLU:HG3	4:D:902:HEM:HMD1	2.00	0.44
1:B:336:THR:HG22	1:B:350:ALA:CB	2.47	0.44
1:A:392:TYR:O	1:A:396:VAL:HG13	2.18	0.44
1:B:319:VAL:HG12	1:B:320:VAL:N	2.33	0.44
1:B:35:PRO:HB3	1:B:76:SER:OG	2.18	0.44
1:B:247:ALA:HB3	1:B:250:ILE:HG22	1.99	0.44
1:B:267:LEU:HD11	1:B:289:ILE:HD12	1.99	0.44
1:B:194:PHE:HE1	1:B:200:PHE:CD2	2.35	0.44
1:A:383:ARG:HG2	1:A:383:ARG:HH11	1.82	0.44
1:A:107:GLU:HA	1:A:260:LYS:NZ	2.33	0.44
1:B:28:ILE:HD12	1:B:323:LEU:CD2	2.47	0.44
1:A:310:SER:O	1:A:313:LYS:HB2	2.18	0.44
2:C:144:GLU:HG2	2:C:146:LYS:CE	2.48	0.44
1:A:278:ILE:HD12	1:A:362:ILE:CD1	2.47	0.44
2:C:111:PRO:HA	2:C:118:TYR:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:5:GLU:HA	2:C:8:THR:OG1	2.17	0.44
1:B:22:LYS:HD2	1:B:22:LYS:HA	1.73	0.44
1:A:319:VAL:HG22	1:A:320:VAL:H	1.82	0.43
2:C:126:THR:HB	2:C:127:PRO:HD3	1.98	0.43
1:A:319:VAL:HG22	1:A:320:VAL:N	2.32	0.43
1:A:356:ASN:ND2	1:A:363:GLU:HB3	2.32	0.43
1:A:42:CYS:SG	3:A:699:FAD:C7M	3.06	0.43
1:A:314:VAL:O	1:A:318:ALA:HB2	2.18	0.43
1:A:274:CYS:HA	1:A:275:PRO:HD2	1.74	0.43
1:B:4:LYS:HA	1:B:29:GLU:O	2.18	0.43
2:D:95:LYS:HG3	2:D:96:LEU:H	1.84	0.43
1:A:126:HIS:H	1:A:126:HIS:CD2	2.37	0.43
1:B:75:ASP:OD2	1:B:89:THR:HG22	2.18	0.43
1:A:175:TYR:O	1:A:178:ALA:N	2.37	0.43
1:A:292:ILE:HG22	1:A:311:GLN:HB3	2.00	0.43
1:B:87:VAL:HG23	1:B:97:TYR:CD2	2.54	0.43
1:B:13:GLY:O	1:B:16:THR:OG1	2.34	0.43
1:B:18:ALA:HA	1:B:30:VAL:HG21	1.99	0.43
2:C:150:LYS:O	2:C:155:LEU:N	2.46	0.43
1:B:369:GLY:HA2	2:D:56:ARG:HB3	2.00	0.43
1:B:231:ASP:HB2	1:B:237:VAL:HG23	2.00	0.43
1:B:299:ASN:HB2	1:B:362:ILE:HB	1.99	0.43
1:B:319:VAL:O	1:B:323:LEU:HD13	2.17	0.43
2:D:31:GLN:CB	2:D:76:GLN:O	2.65	0.43
1:A:11:GLY:O	1:A:14:GLY:N	2.51	0.43
1:A:176:LEU:HB3	1:A:216:MET:CE	2.47	0.43
1:A:273:TRP:CZ2	1:A:303:LYS:HE3	2.53	0.43
2:C:100:TYR:CE1	2:C:154:LEU:HB3	2.53	0.43
2:C:133:MET:HG2	2:C:163:LEU:HD22	2.00	0.43
1:A:82:PRO:HB2	1:A:83:ASP:H	1.38	0.43
2:C:22:VAL:HG12	2:C:23:GLY:N	2.34	0.43
1:A:292:ILE:HG22	1:A:311:GLN:CB	2.49	0.43
1:B:23:LEU:O	1:B:24:ALA:C	2.57	0.43
2:C:16:GLY:HA3	2:C:20:ASN:O	2.18	0.43
2:D:103:LYS:HE3	4:D:902:HEM:HMC2	2.00	0.43
1:B:338:TYR:HE1	1:B:384:GLU:HG2	1.84	0.43
1:B:379:TRP:HH2	2:D:50:ALA:HB1	1.84	0.43
1:A:180:LYS:CD	1:A:180:LYS:N	2.81	0.43
1:B:3:ARG:CZ	1:B:323:LEU:HB3	2.49	0.43
1:A:106:ILE:HG13	1:A:106:ILE:O	2.19	0.42
1:A:154:PRO:HG3	1:A:165:PRO:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LYS:HA	1:A:29:GLU:O	2.19	0.42
1:B:278:ILE:HG23	1:B:362:ILE:HG13	2.02	0.42
2:C:78:TYR:CD2	2:C:120:ILE:HD11	2.55	0.42
1:A:114:GLU:O	1:A:230:VAL:HA	2.19	0.42
1:A:7:VAL:HA	1:A:101:VAL:O	2.19	0.42
2:C:34:PRO:HA	2:C:70:ALA:HB1	2.00	0.42
2:D:105:HIS:CE1	2:D:119:HIS:HB2	2.54	0.42
1:A:319:VAL:HG23	1:A:320:VAL:N	2.33	0.42
2:C:147:MET:HA	4:C:902:HEM:C1C	2.55	0.42
1:B:348:SER:O	1:B:371:VAL:HG23	2.20	0.42
2:D:112:LEU:HD12	2:D:118:TYR:HB3	2.02	0.42
1:B:155:PRO:HD3	1:B:253:ILE:HB	2.01	0.42
1:A:301:MET:HE2	1:A:362:ILE:HD13	2.02	0.42
1:B:356:ASN:ND2	1:B:363:GLU:HB3	2.35	0.42
1:B:343:PRO:O	1:B:385:VAL:HG11	2.19	0.42
1:A:172:VAL:HG12	1:A:176:LEU:HD22	2.00	0.42
1:B:19:LYS:HE2	1:B:398:ASP:O	2.19	0.41
1:B:17:ALA:CB	1:B:21:ILE:HG13	2.49	0.41
1:B:194:PHE:O	1:B:197:GLN:HB2	2.19	0.41
2:D:61:TYR:HB2	2:D:66:PHE:CE1	2.55	0.41
1:A:127:ALA:HB3	1:A:168:ARG:NH2	2.35	0.41
1:B:84:LYS:O	1:B:85:LYS:CB	2.60	0.41
1:B:187:ILE:HD13	1:B:187:ILE:HG21	1.83	0.41
1:B:301:MET:CE	1:B:362:ILE:HD13	2.50	0.41
1:A:21:ILE:HG22	1:A:22:LYS:H	1.85	0.41
1:A:110:TYR:HD1	1:A:116:TYR:CD2	2.39	0.41
1:B:199:GLN:N	1:B:199:GLN:OE1	2.52	0.41
1:A:301:MET:HE3	1:A:311:GLN:HG2	2.02	0.41
1:B:85:LYS:HD2	1:B:86:LEU:HD22	2.01	0.41
1:A:65:LEU:C	1:A:68:HIS:HB3	2.41	0.41
1:A:66:ARG:HD3	1:A:72:VAL:HB	2.01	0.41
2:C:135:ASP:HB3	2:C:141:ARG:HG3	2.02	0.41
1:B:152:ILE:HD11	1:B:165:PRO:HB3	2.02	0.41
1:A:113:ILE:HG23	1:A:116:TYR:HB2	2.02	0.41
2:C:129:LEU:HA	2:C:129:LEU:HD12	1.88	0.41
1:A:233:GLY:HA2	1:A:235:MET:SD	2.61	0.41
1:A:353:TYR:HB3	1:A:362:ILE:HG23	2.02	0.41
1:B:334:LEU:CB	2:D:10:ASN:HB3	2.51	0.41
1:A:156:ALA:O	1:A:157:ALA:HB3	2.21	0.41
2:C:144:GLU:HG2	2:C:146:LYS:NZ	2.35	0.41
1:A:175:TYR:O	1:A:177:LYS:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:TYR:CD1	1:B:62:TYR:N	2.88	0.41
1:A:354:ARG:HH21	1:A:366:PRO:CD	2.33	0.41
1:B:85:LYS:HG2	1:B:97:TYR:H	1.85	0.41
1:B:206:ARG:HE	1:B:345:TYR:HE2	1.69	0.41
1:B:126:HIS:O	1:B:126:HIS:CG	2.74	0.41
1:B:321:VAL:HG11	1:B:328:PRO:CA	2.44	0.41
1:A:393:ASN:ND2	2:C:24:PRO:HD3	2.34	0.41
1:A:356:ASN:ND2	1:A:363:GLU:CB	2.83	0.41
2:D:53:ILE:HA	2:D:56:ARG:HD3	2.02	0.41
1:B:324:LYS:HA	1:B:324:LYS:HD2	1.88	0.41
2:D:37:PHE:CD1	2:D:70:ALA:HB2	2.56	0.41
1:B:267:LEU:HD12	1:B:286:HIS:CD2	2.55	0.41
1:A:21:ILE:HG21	1:A:30:VAL:HG21	2.01	0.41
1:A:320:VAL:CG1	1:A:321:VAL:N	2.83	0.41
2:D:43:GLY:C	2:D:49:ILE:HG22	2.42	0.41
1:A:219:TRP:CZ3	1:A:221:PRO:HG3	2.56	0.41
2:D:20:ASN:ND2	2:D:79:GLN:H	2.19	0.41
1:A:19:LYS:HG3	1:A:20:TYR:HD1	1.87	0.40
1:B:146:ASP:OD1	1:B:180:LYS:HB3	2.21	0.40
1:B:140:GLN:HE21	1:B:249:VAL:HG13	1.87	0.40
1:B:17:ALA:CA	1:B:21:ILE:HG13	2.51	0.40
1:A:391:TRP:O	1:A:395:ILE:HG22	2.21	0.40
1:A:330:THR:HA	1:A:331:PRO:HD3	1.93	0.40
2:C:126:THR:N	2:C:127:PRO:HD2	2.36	0.40
1:B:268:THR:CG2	1:B:272:GLY:HA2	2.51	0.40
1:A:318:ALA:O	1:A:322:LEU:HB3	2.21	0.40
1:A:66:ARG:C	1:A:68:HIS:N	2.74	0.40
2:C:3:THR:HG22	2:C:5:GLU:H	1.87	0.40
2:C:155:LEU:O	2:C:158:GLU:HB2	2.21	0.40
2:D:95:LYS:HE3	2:D:96:LEU:HD12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	399/401 (100%)	330 (83%)	41 (10%)	28 (7%)	1 1
1	B	399/401 (100%)	328 (82%)	51 (13%)	20 (5%)	3 2
2	C	172/174 (99%)	144 (84%)	24 (14%)	4 (2%)	8 11
2	D	172/174 (99%)	151 (88%)	16 (9%)	5 (3%)	6 8
All	All	1142/1150 (99%)	953 (84%)	132 (12%)	57 (5%)	3 2

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	THR
1	A	82	PRO
1	A	85	LYS
1	A	90	ALA
1	A	149	THR
1	A	157	ALA
1	A	213	GLU
1	A	221	PRO
1	A	229	LYS
1	A	230	VAL
1	A	293	GLY
1	A	294	ASP
1	A	299	ASN
1	A	361	ALA
2	C	106	VAL
2	C	115	GLU
2	C	117	ASP
1	B	16	THR
1	B	81	ASP
1	B	157	ALA
1	B	233	GLY
1	B	301	MET
1	B	325	GLY
1	B	327	GLU
2	D	16	GLY
2	D	59	LYS
2	D	103	LYS
1	A	80	ILE
1	A	83	ASP
1	A	181	PRO

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Mol	Chain	Res	Type
1	A	399	THR
1	B	23	LEU
1	B	267	LEU
1	B	299	ASN
1	B	352	ILE
1	B	359	GLY
1	A	176	LEU
1	A	233	GLY
1	A	331	PRO
2	D	115	GLU
1	A	26	PRO
1	A	35	PRO
1	A	67	ALA
1	A	210	PHE
1	A	300	PRO
1	B	55	LEU
1	B	82	PRO
1	B	270	ASP
2	D	10	ASN
1	A	180	LYS
1	B	260	LYS
1	A	155	PRO
1	B	161	CYS
1	B	286	HIS
1	B	227	VAL
2	C	16	GLY
1	B	155	PRO

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	313/313 (100%)	254 (81%)	59 (19%)	2 3
1	B	313/313 (100%)	247 (79%)	66 (21%)	1 2
2	C	138/138 (100%)	119 (86%)	19 (14%)	4 7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	138/138 (100%)	116 (84%)	22 (16%)	3 5
All	All	902/902 (100%)	736 (82%)	166 (18%)	2 3

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	19	LYS
1	A	21	ILE
1	A	25	ASP
1	A	29	GLU
1	A	31	THR
1	A	34	GLU
1	A	41	THR
1	A	42	CYS
1	A	43	TYR
1	A	44	LEU
1	A	53	ARG
1	A	56	GLU
1	A	65	LEU
1	A	78	THR
1	A	84	LYS
1	A	86	LEU
1	A	88	LYS
1	A	112	LYS
1	A	113	ILE
1	A	116	TYR
1	A	123	LYS
1	A	128	TRP
1	A	132	GLU
1	A	137	LEU
1	A	139	LYS
1	A	162	PRO
1	A	176	LEU
1	A	177	LYS
1	A	180	LYS
1	A	196	LYS
1	A	207	LEU
1	A	214	ASN
1	A	221	PRO
1	A	224	ASP
1	A	237	VAL

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Mol	Chain	Res	Type
1	A	246	LYS
1	A	248	ASP
1	A	251	ASN
1	A	252	LEU
1	A	261	ILE
1	A	267	LEU
1	A	284	SER
1	A	292	ILE
1	A	294	ASP
1	A	319	VAL
1	A	321	VAL
1	A	324	LYS
1	A	330	THR
1	A	332	SER
1	A	333	TYR
1	A	336	THR
1	A	337	CYS
1	A	340	ILE
1	A	352	ILE
1	A	356	ASN
1	A	364	SER
1	A	371	VAL
1	A	383	ARG
2	C	7	LEU
2	C	15	HIS
2	C	17	THR
2	C	32	MET
2	C	42	GLU
2	C	44	PHE
2	C	76	GLN
2	C	77	THR
2	C	87	THR
2	C	89	LEU
2	C	91	ASP
2	C	129	LEU
2	C	135	ASP
2	C	136	PHE
2	C	138	GLU
2	C	145	LYS
2	C	146	LYS
2	C	151	LEU
2	C	155	LEU

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Mol	Chain	Res	Type
1	B	3	ARG
1	B	21	ILE
1	B	23	LEU
1	B	28	ILE
1	B	30	VAL
1	B	31	THR
1	B	32	LEU
1	B	36	ASN
1	B	41	THR
1	B	43	TYR
1	B	47	GLU
1	B	55	LEU
1	B	65	LEU
1	B	78	THR
1	B	80	ILE
1	B	83	ASP
1	B	85	LYS
1	B	86	LEU
1	B	104	PRO
1	B	106	ILE
1	B	108	LEU
1	B	113	ILE
1	B	117	SER
1	B	126	HIS
1	B	137	LEU
1	B	138	ARG
1	B	141	LEU
1	B	143	ASP
1	B	152	ILE
1	B	176	LEU
1	B	184	LYS
1	B	187	ILE
1	B	188	LEU
1	B	196	LYS
1	B	198	SER
1	B	214	ASN
1	B	231	ASP
1	B	248	ASP
1	B	252	LEU
1	B	257	ARG
1	B	260	LYS
1	B	268	THR

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Mol	Chain	Res	Type
1	B	270	ASP
1	B	284	SER
1	B	289	ILE
1	B	297	ILE
1	B	299	ASN
1	B	301	MET
1	B	306	TYR
1	B	309	ASN
1	B	310	SER
1	B	319	VAL
1	B	321	VAL
1	B	322	LEU
1	B	327	GLU
1	B	330	THR
1	B	332	SER
1	B	333	TYR
1	B	337	CYS
1	B	340	ILE
1	B	341	LEU
1	B	343	PRO
1	B	354	ARG
1	B	364	SER
1	B	371	VAL
1	B	399	THR
2	D	15	HIS
2	D	18	HIS
2	D	24	PRO
2	D	28	SER
2	D	79	GLN
2	D	84	SER
2	D	92	THR
2	D	96	LEU
2	D	98	ASP
2	D	102	GLU
2	D	103	LYS
2	D	114	ASP
2	D	117	ASP
2	D	121	LEU
2	D	135	ASP
2	D	139	GLU
2	D	145	LYS
2	D	146	LYS

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Mol	Chain	Res	Type
2	D	150	LYS
2	D	152	ARG
2	D	156	LYS
2	D	166	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	171	GLN
1	A	263	GLN
1	A	290	HIS
1	A	311	GLN
1	A	356	ASN
1	A	393	ASN
2	C	20	ASN
1	B	46	ASN
1	B	60	HIS
1	B	140	GLN
1	B	171	GLN
1	B	197	GLN
1	B	220	HIS
1	B	251	ASN
1	B	263	GLN
1	B	286	HIS
1	B	309	ASN
1	B	335	ASN
2	D	9	ASN
2	D	18	HIS
2	D	20	ASN
2	D	130	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

6 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	$\#\|Z\| > 2$
3	FAD	A	699	1	48,58,58	1.53	8 (16%)	54,89,89	2.62	14 (25%)
3	FAD	B	699	1	48,58,58	1.53	12 (25%)	54,89,89	2.77	13 (24%)
4	HEM	C	901	2	30,50,50	2.32	7 (23%)	24,82,82	2.67	7 (29%)
4	HEM	C	902	2	30,50,50	2.74	7 (23%)	24,82,82	2.92	9 (37%)
4	HEM	D	901	2	30,50,50	2.18	7 (23%)	24,82,82	2.69	8 (33%)
4	HEM	D	902	2	30,50,50	2.78	8 (26%)	24,82,82	2.93	10 (41%)

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	699	1	3/3/9/9	0/30/50/50	0/6/6/6
3	FAD	B	699	1	3/3/9/9	0/30/50/50	0/6/6/6
4	HEM	C	901	2	-	0/10/54/54	0/0/8/8
4	HEM	C	902	2	-	0/10/54/54	0/0/8/8
4	HEM	D	901	2	-	0/10/54/54	0/0/8/8
4	HEM	D	902	2	-	0/10/54/54	0/0/8/8

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	902	HEM	C3B-C4B	-9.63	1.43	1.51
4	C	902	HEM	C3B-C4B	-9.03	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	902	HEM	C2D-C3D	-6.31	1.35	1.54
4	C	901	HEM	C3B-C4B	-6.21	1.46	1.51
4	C	901	HEM	C2D-C3D	-6.18	1.36	1.54
4	D	902	HEM	C2D-C3D	-5.97	1.36	1.54
4	D	901	HEM	C2D-C3D	-5.93	1.36	1.54
4	C	902	HEM	C3D-C4D	-5.62	1.44	1.51
4	D	902	HEM	C2C-C1C	-5.23	1.42	1.52
4	D	901	HEM	C2C-C1C	-5.11	1.42	1.52
4	C	902	HEM	C2C-C1C	-4.62	1.43	1.52
4	D	901	HEM	C3D-C4D	-4.49	1.45	1.51
4	C	901	HEM	C3D-C4D	-4.41	1.45	1.51
4	D	902	HEM	C3D-C4D	-4.40	1.45	1.51
4	C	901	HEM	C2C-C1C	-3.99	1.45	1.52
4	D	901	HEM	C3B-C4B	-2.90	1.49	1.51
4	C	901	HEM	C2D-C1D	-2.83	1.42	1.51
3	A	699	FAD	C2'-C3'	-2.50	1.48	1.53
4	D	902	HEM	C2B-C1B	-2.45	1.43	1.51
4	D	901	HEM	C2D-C1D	-2.40	1.44	1.51
3	A	699	FAD	O2'-C2'	-2.36	1.38	1.43
3	A	699	FAD	C5'-C4'	-2.36	1.48	1.51
3	B	699	FAD	C5A-C4A	-2.32	1.35	1.40
3	B	699	FAD	C4'-C3'	-2.22	1.48	1.53
3	B	699	FAD	C2A-N1A	-2.17	1.29	1.33
4	C	902	HEM	C2B-C1B	-2.14	1.44	1.51
3	B	699	FAD	C2'-C3'	-2.13	1.49	1.53
3	A	699	FAD	C4X-N5	2.06	1.36	1.33
4	D	902	HEM	CHD-C4C	2.07	1.41	1.36
3	B	699	FAD	C8M-C8	2.13	1.55	1.51
3	B	699	FAD	C5'-C4'	2.19	1.55	1.51
3	B	699	FAD	C4X-N5	2.27	1.36	1.33
3	B	699	FAD	O4B-C1B	2.34	1.44	1.41
3	B	699	FAD	C4-C4X	2.34	1.45	1.41
3	B	699	FAD	C9A-N10	2.61	1.42	1.38
3	A	699	FAD	C9A-N10	2.61	1.42	1.38
3	A	699	FAD	C4-N3	2.99	1.38	1.33
3	B	699	FAD	C4-N3	3.35	1.39	1.33
4	C	902	HEM	CBB-CAB	3.68	1.50	1.29
4	C	901	HEM	CBC-CAC	3.87	1.51	1.29
3	A	699	FAD	O4B-C1B	3.88	1.46	1.41
4	C	901	HEM	CBB-CAB	3.89	1.51	1.29
4	D	902	HEM	CBC-CAC	4.00	1.52	1.29
4	D	901	HEM	CBC-CAC	4.03	1.52	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	901	HEM	CBB-CAB	4.03	1.52	1.29
4	D	902	HEM	CBB-CAB	4.22	1.53	1.29
4	C	902	HEM	CBC-CAC	4.42	1.54	1.29
3	A	699	FAD	C10-N10	5.06	1.45	1.39
3	B	699	FAD	C10-N10	5.27	1.45	1.39

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	902	HEM	C3B-CAB-CBB	-8.54	111.36	124.46
3	A	699	FAD	C4X-C10-N10	-7.58	116.05	120.52
4	D	902	HEM	C3B-CAB-CBB	-6.95	113.79	124.46
3	B	699	FAD	C4X-C4-N3	-6.76	114.34	123.59
3	B	699	FAD	C4X-C10-N10	-6.75	116.54	120.52
4	D	901	HEM	C3C-CAC-CBC	-6.35	114.72	124.46
3	A	699	FAD	C4X-C4-N3	-6.00	115.38	123.59
4	C	901	HEM	C3B-CAB-CBB	-5.79	115.58	124.46
4	C	901	HEM	C3C-CAC-CBC	-5.67	115.75	124.46
4	D	902	HEM	C3C-CAC-CBC	-5.41	116.16	124.46
3	B	699	FAD	C4-C4X-C10	-4.91	116.80	119.94
3	B	699	FAD	P-O3P-PA	-4.91	118.95	132.73
4	C	902	HEM	C3C-CAC-CBC	-4.88	116.97	124.46
3	B	699	FAD	C4X-N5-C5X	-4.04	112.12	116.76
3	A	699	FAD	C4-C4X-C10	-3.89	117.45	119.94
3	B	699	FAD	C6-C5X-N5	-3.57	114.36	118.96
4	D	901	HEM	C3B-CAB-CBB	-3.44	119.17	124.46
3	A	699	FAD	C4-C4X-N5	-3.25	114.78	118.72
3	A	699	FAD	C6-C5X-N5	-3.10	114.97	118.96
3	A	699	FAD	C4X-N5-C5X	-2.98	113.33	116.76
3	B	699	FAD	C1B-N9A-C4A	-2.88	122.60	126.94
4	D	902	HEM	CMA-C3A-C4A	-2.69	123.92	128.36
3	A	699	FAD	O3P-PA-O5B	-2.52	96.25	102.94
3	A	699	FAD	C4B-O4B-C1B	-2.46	107.02	109.72
3	B	699	FAD	C4-C4X-N5	-2.40	115.81	118.72
3	B	699	FAD	O3P-PA-O5B	-2.09	97.39	102.94
3	A	699	FAD	O3P-P-O5'	2.13	108.58	102.94
3	A	699	FAD	N3A-C2A-N1A	2.22	130.60	128.89
3	A	699	FAD	C1'-N10-C9A	2.36	121.51	118.86
4	D	901	HEM	C2D-C3D-C4D	2.37	105.52	101.50
4	D	902	HEM	C2D-C3D-C4D	2.44	105.64	101.50
4	C	902	HEM	C2D-C3D-C4D	2.51	105.75	101.50
4	C	902	HEM	CMD-C2D-C3D	2.56	125.66	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	902	HEM	CAA-CBA-CGA	2.59	117.49	112.75
4	D	902	HEM	CMD-C2D-C3D	2.60	125.85	114.35
4	D	902	HEM	CBD-CAD-C3D	2.60	121.12	113.55
3	B	699	FAD	O3'-C3'-C2'	2.61	115.34	108.75
3	B	699	FAD	C1'-N10-C9A	2.62	121.80	118.86
4	D	901	HEM	CAD-C3D-C4D	3.06	123.25	112.47
3	A	699	FAD	C9A-C5X-N5	3.14	126.99	122.36
4	C	901	HEM	CMD-C2D-C3D	3.32	129.03	114.35
4	D	901	HEM	CMD-C2D-C3D	3.58	130.21	114.35
3	A	699	FAD	O4'-C4'-C3'	3.63	118.14	109.02
4	C	901	HEM	CAD-C3D-C4D	3.71	125.55	112.47
3	B	699	FAD	C9A-C5X-N5	3.86	128.06	122.36
4	D	902	HEM	CAD-C3D-C4D	4.09	126.90	112.47
4	C	902	HEM	CAD-C3D-C4D	4.13	127.05	112.47
4	C	902	HEM	CMB-C2B-C3B	4.27	127.19	116.53
4	C	901	HEM	CMB-C2B-C3B	4.35	127.39	116.53
4	D	901	HEM	CMB-C2B-C3B	4.51	127.79	116.53
4	C	902	HEM	CMC-C2C-C3C	4.55	127.89	116.53
4	C	901	HEM	CMC-C2C-C3C	4.69	128.23	116.53
4	D	902	HEM	CMC-C2C-C3C	4.76	128.40	116.53
4	C	902	HEM	CAD-C3D-C2D	4.85	127.15	113.22
4	D	902	HEM	CAD-C3D-C2D	4.95	127.45	113.22
4	D	901	HEM	CMC-C2C-C3C	5.08	129.22	116.53
4	D	902	HEM	CMB-C2B-C3B	5.12	129.30	116.53
4	C	901	HEM	CAD-C3D-C2D	5.29	128.41	113.22
4	D	901	HEM	CAD-C3D-C2D	5.81	129.93	113.22
3	A	699	FAD	C4-N3-C2	12.09	125.70	115.25
3	B	699	FAD	C4-N3-C2	12.68	126.20	115.25

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	699	FAD	C4'
3	B	699	FAD	C2'
3	B	699	FAD	C3'
3	A	699	FAD	C4'
3	A	699	FAD	C2'
3	A	699	FAD	C3'

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	699	FAD	7	0
3	B	699	FAD	2	0
4	C	902	HEM	3	0
4	D	901	HEM	1	0
4	D	902	HEM	3	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

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.