



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:03 AM UTC

PDB ID : 1MMO / pdb_00001mmo
Title : CRYSTAL STRUCTURE OF A BACTERIAL NON-HAEM IRON HYDROXYLASE THAT CATALYSES THE BIOLOGICAL OXIDATION OF METHANE
Authors : Rosenzweig, A.C.; Frederick, C.A.; Lippard, S.J.; Nordlund, P.
Deposited on : 1994-02-22
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

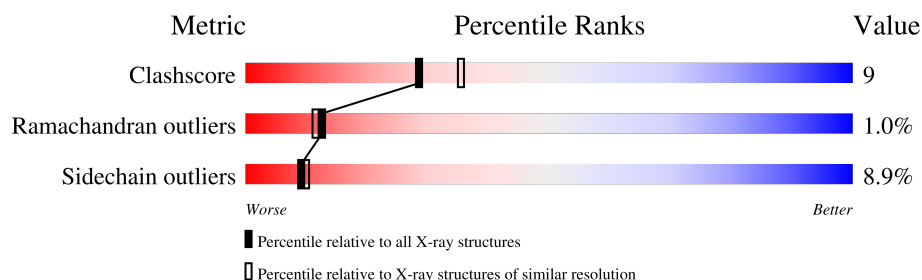
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	384	71% 22% 5% •
1	C	384	68% 25% 5% •
2	D	512	67% 25% 6% •
2	E	512	65% 27% 6% •
3	G	162	65% 27% 7% •
3	H	162	65% 30% 5% •

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23859 atoms, of which 5642 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 METHANE MONOOXYGENASE HYDROLASE (BETA CHAIN).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	384	Total	C	H	N	O	S	0	0	0
			3855	2024	705	544	574	8			
1	C	384	Total	C	H	N	O	S	0	0	0
			3855	2024	705	544	574	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	142	THR	ASP	conflict	UNP P18798
B	143	SER	GLU	conflict	UNP P18798
B	144	SER	PHE	conflict	UNP P18798
B	145	CYS	ILE	conflict	UNP P18798
C	142	THR	ASP	conflict	UNP P18798
C	143	SER	GLU	conflict	UNP P18798
C	144	SER	PHE	conflict	UNP P18798
C	145	CYS	ILE	conflict	UNP P18798

- Molecule 2 is a protein called METHANE MONOOXYGENASE HYDROLASE (ALPHA CHAIN).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	512	Total	C	H	N	O	S	0	0	0
			5122	2680	936	721	767	18			
2	E	512	Total	C	H	N	O	S	0	0	0
			5122	2680	936	721	767	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	306	ASP	ASN	conflict	UNP P22869
D	444	GLU	GLN	conflict	UNP P22869

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Chain	Residue	Modelled	Actual	Comment	Reference
E	306	ASP	ASN	conflict	UNP P22869
E	444	GLU	GLN	conflict	UNP P22869

- Molecule 3 is a protein called METHANE MONOOXYGENASE HYDROLASE (GAMMA CHAIN).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	G	162	Total	C	H	N	O	S	0	0	0
			1658	847	321	241	244	5			
3	H	162	Total	C	H	N	O	S	0	0	0
			1658	847	321	241	244	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	38	ASP	HIS	conflict	UNP P11987
G	80	LYS	ASN	conflict	UNP P11987
H	38	ASP	HIS	conflict	UNP P11987
H	80	LYS	ASN	conflict	UNP P11987

- Molecule 4 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	2	Total	Fe	0	0
			2	2		
4	E	2	Total	Fe	0	0
			2	2		

- Molecule 5 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

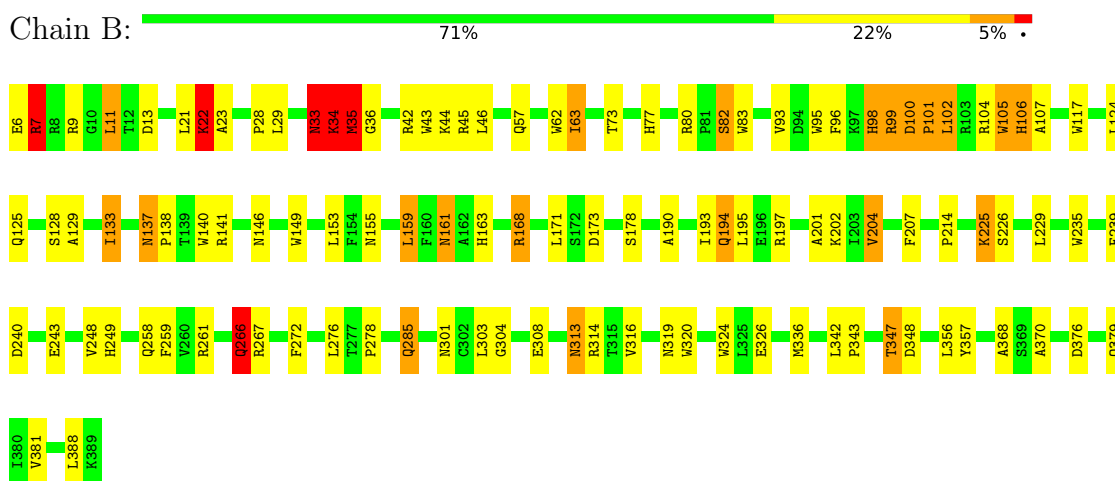
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	164	Total	H	O	0	0
			492	328	164		
6	C	142	Total	H	O	0	0
			426	284	142		
6	D	194	Total	H	O	0	0
			582	388	194		
6	E	199	Total	H	O	0	0
			597	398	199		
6	G	74	Total	H	O	0	0
			222	148	74		
6	H	86	Total	H	O	0	0
			258	172	86		

3 Residue-property plots

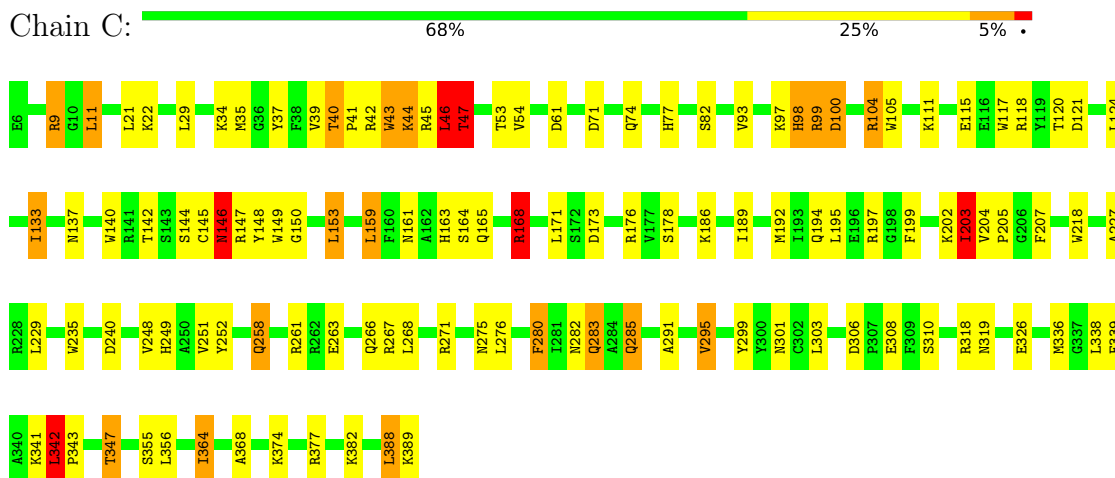
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: METHANE MONOOXYGENASE HYDROLASE (BETA CHAIN)

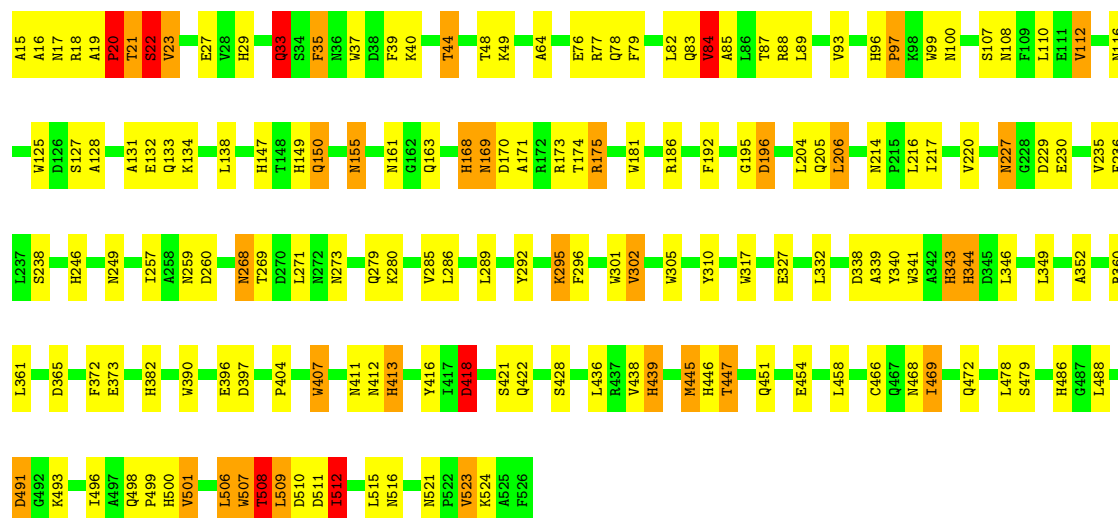


• Molecule 1: METHANE MONOOXYGENASE HYDROLASE (BETA CHAIN)



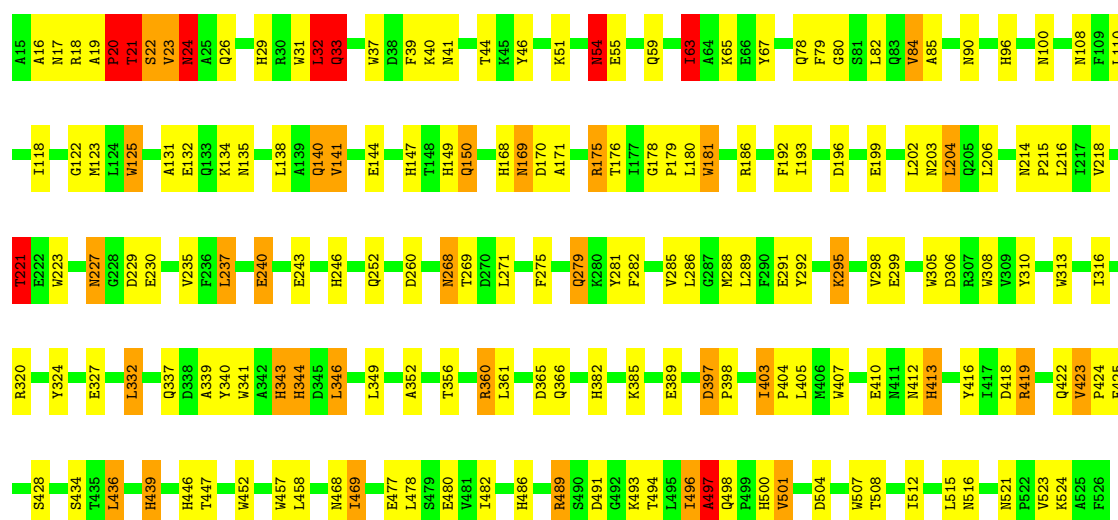
• Molecule 2: METHANE MONOOXYGENASE HYDROLASE (ALPHA CHAIN)





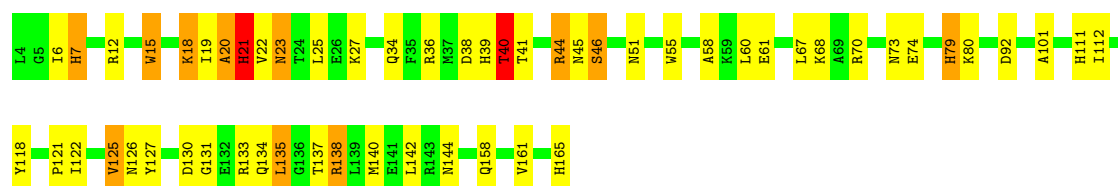
• Molecule 2: METHANE MONOOXYGENASE HYDROLASE (ALPHA CHAIN)

Chain E: 65% 27% 6%



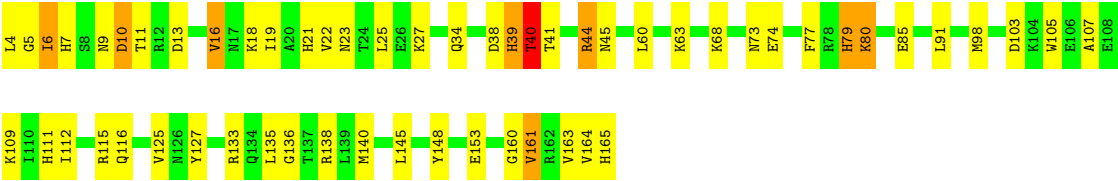
• Molecule 3: METHANE MONOOXYGENASE HYDROLASE (GAMMA CHAIN)

Chain G: 65% 27% 7%



• Molecule 3: METHANE MONOOXYGENASE HYDROLASE (GAMMA CHAIN)

Chain H: 65% 30% 5%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.60Å 110.10Å 333.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (5.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.170 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	23859	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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

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	B	0.95	5/3245 (0.2%)	1.69	71/4407 (1.6%)
1	C	0.96	7/3245 (0.2%)	1.71	69/4407 (1.6%)
2	D	1.01	15/4311 (0.3%)	1.87	105/5855 (1.8%)
2	E	1.00	14/4311 (0.3%)	1.84	108/5855 (1.8%)
3	G	1.06	8/1366 (0.6%)	1.77	39/1840 (2.1%)
3	H	1.05	9/1366 (0.7%)	1.73	22/1840 (1.2%)
All	All	1.00	58/17844 (0.3%)	1.79	414/24204 (1.7%)

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	C	0	1
2	D	0	2
2	E	0	3
All	All	0	6

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	84	VAL	CA-CB	7.69	1.65	1.54
3	H	21	HIS	CD2-NE2	-7.28	1.29	1.37
3	G	21	HIS	CD2-NE2	-7.12	1.30	1.37
2	D	343	HIS	CD2-NE2	-7.03	1.30	1.37
2	E	246	HIS	CD2-NE2	-6.98	1.30	1.37
2	E	500	HIS	CD2-NE2	-6.92	1.30	1.37
1	B	163	HIS	CD2-NE2	-6.89	1.30	1.37
2	E	149	HIS	CD2-NE2	-6.89	1.30	1.37
2	E	96	HIS	CD2-NE2	-6.86	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	246	HIS	CD2-NE2	-6.77	1.30	1.37
3	H	79	HIS	CD2-NE2	-6.67	1.30	1.37
2	E	344	HIS	CD2-NE2	-6.63	1.30	1.37
2	D	344	HIS	CD2-NE2	-6.60	1.30	1.37
2	D	382	HIS	CD2-NE2	-6.59	1.30	1.37
3	G	79	HIS	CD2-NE2	-6.54	1.30	1.37
1	C	98	HIS	CD2-NE2	-6.49	1.30	1.37
2	E	147	HIS	CD2-NE2	-6.44	1.30	1.37
2	E	446	HIS	CD2-NE2	-6.44	1.30	1.37
2	D	29	HIS	CD2-NE2	-6.39	1.30	1.37
3	H	39	HIS	CD2-NE2	-6.35	1.30	1.37
2	E	413	HIS	CD2-NE2	-6.34	1.30	1.37
1	B	106	HIS	CD2-NE2	-6.34	1.30	1.37
2	E	439	HIS	CD2-NE2	-6.32	1.30	1.37
3	G	111	HIS	CD2-NE2	-6.31	1.30	1.37
2	E	382	HIS	CD2-NE2	-6.24	1.30	1.37
2	E	343	HIS	CD2-NE2	-6.21	1.31	1.37
1	B	77	HIS	CD2-NE2	-6.20	1.31	1.37
3	G	125	VAL	CA-CB	6.18	1.63	1.54
3	H	111	HIS	CD2-NE2	-6.18	1.31	1.37
2	D	147	HIS	CD2-NE2	-6.17	1.31	1.37
1	C	77	HIS	CD2-NE2	-6.16	1.31	1.37
2	D	486	HIS	CD2-NE2	-6.16	1.31	1.37
2	D	413	HIS	CD2-NE2	-6.14	1.31	1.37
2	E	29	HIS	CD2-NE2	-6.14	1.31	1.37
3	G	39	HIS	CD2-NE2	-6.11	1.31	1.37
2	D	439	HIS	CD2-NE2	-6.10	1.31	1.37
1	B	98	HIS	CD2-NE2	-6.07	1.31	1.37
2	D	149	HIS	CD2-NE2	-6.05	1.31	1.37
3	H	7	HIS	CD2-NE2	-6.05	1.31	1.37
3	H	165	HIS	CD2-NE2	-6.03	1.31	1.37
2	E	168	HIS	CD2-NE2	-6.00	1.31	1.37
2	D	500	HIS	CD2-NE2	-5.97	1.31	1.37
2	E	486	HIS	CD2-NE2	-5.96	1.31	1.37
3	G	7	HIS	CD2-NE2	-5.92	1.31	1.37
2	D	96	HIS	CD2-NE2	-5.87	1.31	1.37
3	H	16	VAL	CA-CB	5.83	1.62	1.54
2	D	168	HIS	CD2-NE2	-5.66	1.31	1.37
1	C	163	HIS	CD2-NE2	-5.58	1.31	1.37
1	C	249	HIS	CD2-NE2	-5.55	1.31	1.37
3	H	79	HIS	CG-ND1	-5.52	1.32	1.38
1	B	249	HIS	CD2-NE2	-5.50	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	165	HIS	CG-ND1	-5.49	1.32	1.38
1	C	249	HIS	CG-ND1	-5.47	1.32	1.38
2	D	446	HIS	CD2-NE2	-5.45	1.31	1.37
3	G	165	HIS	CD2-NE2	-5.44	1.31	1.37
1	C	295	VAL	CA-CB	5.37	1.61	1.54
1	C	47	THR	CA-CB	5.17	1.62	1.53
3	G	21	HIS	CG-ND1	-5.15	1.32	1.38

All (414) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	491	ASP	CA-CB-CG	15.17	127.77	112.60
2	D	21	THR	N-CA-C	-13.62	92.76	111.96
1	C	39	VAL	N-CA-C	13.24	124.13	110.62
2	D	507	TRP	N-CA-C	12.72	128.06	112.54
1	C	168	ARG	NE-CZ-NH2	-11.87	108.52	119.20
2	E	496	ILE	N-CA-C	-11.56	94.67	109.58
3	H	112	ILE	O-C-N	-11.01	111.20	122.54
3	G	112	ILE	O-C-N	-10.52	109.42	122.57
2	D	79	PHE	O-C-N	-9.91	110.56	122.65
2	D	501	VAL	N-CA-CB	-9.91	99.24	112.22
2	D	365	ASP	CA-CB-CG	9.88	122.48	112.60
2	E	501	VAL	N-CA-CB	-9.73	99.48	112.22
2	D	84	VAL	CG1-CB-CG2	-9.63	89.61	110.80
1	C	168	ARG	NE-CZ-NH1	9.42	130.92	121.50
2	E	79	PHE	N-CA-C	-9.27	99.00	110.41
3	G	6	ILE	O-C-N	-9.22	112.70	122.57
1	B	194	GLN	OE1-CD-NE2	-9.15	113.45	122.60
2	E	418	ASP	O-C-N	-9.09	110.50	122.59
2	E	500	HIS	CB-CG-CD2	-9.06	119.42	131.20
3	H	103	ASP	CA-CB-CG	9.05	121.65	112.60
2	E	22	SER	N-CA-C	-8.87	102.38	113.55
3	H	112	ILE	N-CA-C	-8.86	100.20	110.21
2	D	175	ARG	CA-CB-CG	8.77	131.64	114.10
1	B	101	PRO	O-C-N	-8.51	112.19	122.99
2	E	339	ALA	N-CA-C	8.50	120.16	111.07
2	E	295	LYS	N-CA-C	-8.45	100.80	112.12
2	D	260	ASP	CA-CB-CG	8.43	121.03	112.60
2	E	39	PHE	CA-CB-CG	8.41	122.21	113.80
2	E	32	LEU	N-CA-C	-8.38	98.68	110.50
2	D	268	ASN	OD1-CG-ND2	-8.36	114.24	122.60
2	D	23	VAL	N-CA-C	-8.32	92.03	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	418	ASP	O-C-N	-8.28	111.58	122.59
2	E	140	GLN	CA-C-O	-8.26	111.66	120.42
2	E	268	ASN	OD1-CG-ND2	-8.22	114.38	122.60
3	H	40	THR	N-CA-CB	-8.21	97.04	111.08
1	C	342	LEU	CB-CA-C	8.17	121.11	108.61
3	H	6	ILE	O-C-N	-8.14	112.39	122.57
2	D	39	PHE	CA-CB-CG	8.11	121.91	113.80
2	E	169	ASN	OD1-CG-ND2	-8.09	114.51	122.60
2	E	24	ASN	CA-CB-CG	8.04	120.64	112.60
2	E	33	GLN	OE1-CD-NE2	-7.98	114.62	122.60
2	D	16	ALA	N-CA-C	-7.96	96.25	109.07
2	D	84	VAL	CA-CB-CG1	7.91	123.84	110.40
2	E	418	ASP	CA-CB-CG	7.91	120.50	112.60
2	D	33	GLN	OE1-CD-NE2	-7.89	114.71	122.60
1	C	388	LEU	N-CA-C	7.84	119.61	111.14
3	G	7	HIS	CA-CB-CG	7.81	121.61	113.80
2	E	412	ASN	OD1-CG-ND2	-7.80	114.80	122.60
3	G	20	ALA	N-CA-C	-7.78	99.77	110.35
2	D	21	THR	CB-CA-C	-7.78	97.12	110.88
2	D	21	THR	O-C-N	7.76	131.35	122.19
2	E	227	ASN	OD1-CG-ND2	-7.75	114.84	122.60
3	G	111	HIS	CB-CG-CD2	-7.71	121.18	131.20
2	D	516	ASN	OD1-CG-ND2	-7.65	114.95	122.60
1	B	22	LYS	CA-CB-CG	7.64	129.39	114.10
2	D	229	ASP	CA-CB-CG	7.64	120.24	112.60
2	E	491	ASP	CA-CB-CG	7.61	120.21	112.60
2	D	507	TRP	CA-C-O	-7.58	110.06	119.38
2	D	169	ASN	OD1-CG-ND2	-7.56	115.04	122.60
2	D	150	GLN	OE1-CD-NE2	-7.56	115.04	122.60
3	G	45	ASN	OD1-CG-ND2	-7.55	115.05	122.60
2	E	316	ILE	N-CA-C	7.51	117.59	110.30
1	B	35	MET	N-CA-C	-7.51	94.81	110.80
3	H	80	LYS	CB-CG-CD	-7.50	94.05	111.30
2	E	16	ALA	N-CA-C	-7.49	95.35	108.23
3	H	80	LYS	CA-CB-CG	7.48	129.06	114.10
2	E	135	ASN	OD1-CG-ND2	-7.41	115.19	122.60
2	D	339	ALA	N-CA-C	7.41	118.99	111.07
3	G	38	ASP	N-CA-C	7.38	120.39	111.82
2	E	79	PHE	O-C-N	-7.37	113.66	122.65
1	B	376	ASP	CA-CB-CG	7.37	119.97	112.60
1	B	133	ILE	CB-CA-C	-7.36	100.75	112.16
1	B	266	GLN	OE1-CD-NE2	-7.35	115.25	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	155	ASN	OD1-CG-ND2	-7.22	115.38	122.60
1	C	252	TYR	N-CA-C	7.20	118.92	111.14
1	B	163	HIS	CB-CG-CD2	-7.17	121.87	131.20
2	E	20	PRO	CA-N-CD	-7.17	101.96	112.00
2	D	507	TRP	O-C-N	-7.15	112.85	122.43
2	D	468	ASN	CA-CB-CG	7.14	119.74	112.60
1	B	101	PRO	CA-C-O	-7.10	113.48	121.43
1	C	146	ASN	OD1-CG-ND2	-7.10	115.50	122.60
1	C	342	LEU	N-CA-CB	-7.08	98.35	110.10
1	B	313	ASN	CA-CB-CG	7.04	119.64	112.60
3	G	23	ASN	OD1-CG-ND2	-7.03	115.57	122.60
3	G	92	ASP	CA-CB-CG	7.01	119.61	112.60
2	E	125	TRP	CA-CB-CG	7.00	126.89	113.60
1	C	47	THR	N-CA-CB	6.92	122.19	110.49
2	E	221	THR	CA-CB-OG1	-6.92	99.22	109.60
2	E	446	HIS	CB-CG-CD2	-6.91	122.22	131.20
2	E	96	HIS	CB-CG-CD2	-6.87	122.27	131.20
2	E	299	GLU	O-C-N	-6.87	117.04	121.85
1	C	100	ASP	CA-CB-CG	6.85	119.45	112.60
3	G	6	ILE	N-CA-C	-6.85	100.69	109.80
2	E	468	ASN	CA-CB-CG	6.83	119.43	112.60
2	E	59	GLN	OE1-CD-NE2	-6.83	115.77	122.60
2	D	446	HIS	CB-CG-CD2	-6.82	122.33	131.20
1	B	105	TRP	O-C-N	-6.80	113.54	122.59
2	D	96	HIS	CB-CG-CD2	-6.80	122.36	131.20
2	E	500	HIS	CB-CG-ND1	6.77	132.86	122.70
2	E	282	PHE	CA-CB-CG	-6.76	107.03	113.80
2	E	282	PHE	N-CA-C	6.75	118.72	111.36
2	E	170	ASP	CA-CB-CG	6.73	119.33	112.60
3	H	74	GLU	N-CA-C	6.72	118.60	111.28
2	D	79	PHE	N-CA-C	-6.71	102.16	110.41
2	E	504	ASP	CA-CB-CG	6.70	119.30	112.60
2	D	249	ASN	OD1-CG-ND2	-6.69	115.91	122.60
2	D	99	TRP	CG-CD2-CE3	6.67	140.57	133.90
3	H	34	GLN	OE1-CD-NE2	-6.67	115.92	122.60
1	C	168	ARG	CG-CD-NE	-6.58	97.52	112.00
1	C	168	ARG	CB-CG-CD	6.58	126.43	111.30
1	C	163	HIS	CB-CG-CD2	-6.58	122.65	131.20
2	D	175	ARG	NE-CZ-NH2	-6.58	113.28	119.20
1	C	118	ARG	NE-CZ-NH1	6.55	128.05	121.50
2	E	446	HIS	CB-CG-ND1	6.52	132.48	122.70
3	G	34	GLN	OE1-CD-NE2	-6.50	116.10	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	469	ILE	N-CA-CB	-6.42	101.81	110.54
2	D	21	THR	N-CA-CB	6.41	121.75	110.27
2	E	100	ASN	OD1-CG-ND2	-6.41	116.19	122.60
2	E	54	ASN	CA-CB-CG	6.41	119.01	112.60
1	C	342	LEU	CA-CB-CG	6.40	138.70	116.30
1	B	168	ARG	CB-CG-CD	6.39	126.01	111.30
2	D	373	GLU	CA-CB-CG	6.39	126.89	114.10
2	D	37	TRP	CG-CD2-CE3	6.39	140.29	133.90
3	G	51	ASN	OD1-CG-ND2	-6.39	116.21	122.60
1	B	155	ASN	N-CA-C	-6.36	104.27	111.14
1	C	118	ARG	NE-CZ-NH2	-6.36	113.48	119.20
2	E	33	GLN	N-CA-CB	6.35	121.22	110.49
1	C	35	MET	O-C-N	-6.35	114.80	122.22
2	E	418	ASP	N-CA-C	6.35	124.32	110.80
1	C	74	GLN	OE1-CD-NE2	-6.32	116.28	122.60
1	B	285	GLN	OE1-CD-NE2	-6.29	116.31	122.60
2	E	150	GLN	OE1-CD-NE2	-6.26	116.34	122.60
1	B	348	ASP	CA-CB-CG	6.25	118.85	112.60
2	E	360	ARG	NE-CZ-NH2	-6.24	113.59	119.20
1	C	168	ARG	CA-CB-CG	6.23	126.56	114.10
3	H	38	ASP	N-CA-C	6.21	120.05	112.23
2	E	21	THR	N-CA-C	-6.19	99.73	108.96
3	H	10	ASP	CA-CB-CG	6.18	118.78	112.60
1	B	7	ARG	N-CA-C	-6.17	97.65	110.80
1	B	99	ARG	NE-CZ-NH2	-6.17	113.64	119.20
2	D	411	ASN	OD1-CG-ND2	-6.17	116.43	122.60
3	G	55	TRP	CG-CD2-CE3	6.15	140.05	133.90
1	B	80	ARG	NE-CZ-NH2	-6.15	113.67	119.20
1	C	377	ARG	N-CA-C	6.14	117.97	111.28
1	B	240	ASP	CA-CB-CG	6.13	118.73	112.60
1	B	324	TRP	CG-CD2-CE3	6.13	140.03	133.90
2	E	489	ARG	CG-CD-NE	-6.13	98.51	112.00
3	G	21	HIS	N-CA-CB	6.13	120.84	110.49
2	D	20	PRO	CA-N-CD	-6.12	103.43	112.00
2	D	397	ASP	CA-CB-CG	6.11	118.71	112.60
3	H	39	HIS	CB-CG-CD2	-6.11	123.26	131.20
3	H	73	ASN	OD1-CG-ND2	-6.11	116.50	122.60
1	C	104	ARG	NE-CZ-NH2	-6.10	113.71	119.20
2	D	285	VAL	N-CA-C	6.10	116.27	110.53
2	E	37	TRP	CG-CD2-CE3	6.09	139.99	133.90
2	E	40	LYS	N-CA-C	-6.08	100.09	109.76
1	B	140	TRP	CG-CD2-CE3	6.07	139.97	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	168	ARG	CG-CD-NE	-6.07	98.65	112.00
2	D	295	LYS	N-CA-C	-6.07	104.61	112.68
2	D	382	HIS	CB-CG-CD2	-6.06	123.32	131.20
3	G	133	ARG	CG-CD-NE	-6.05	98.68	112.00
2	E	360	ARG	NE-CZ-NH1	6.05	127.55	121.50
2	E	168	HIS	CB-CG-CD2	-6.04	123.35	131.20
2	D	418	ASP	CA-CB-CG	6.04	118.64	112.60
2	D	491	ASP	N-CA-CB	6.01	120.65	110.49
1	C	207	PHE	N-CA-C	-6.01	101.39	110.28
1	B	379	GLN	CA-CB-CG	-6.00	102.11	114.10
3	G	118	TYR	N-CA-C	5.99	120.61	112.88
2	E	149	HIS	CB-CG-CD2	-5.99	123.42	131.20
2	D	447	THR	N-CA-CB	-5.99	100.67	110.43
2	D	469	ILE	N-CA-CB	-5.98	102.41	110.54
2	D	496	ILE	N-CA-C	-5.98	105.02	110.82
2	D	413	HIS	CB-CG-CD2	-5.97	123.44	131.20
2	D	64	ALA	N-CA-C	5.96	118.26	111.11
2	E	306	ASP	CA-CB-CG	-5.95	106.65	112.60
1	C	45	ARG	CA-C-O	-5.94	114.08	120.92
3	G	68	LYS	CG-CD-CE	5.94	124.97	111.30
1	B	149	TRP	CG-CD2-CE3	5.93	139.83	133.90
1	B	168	ARG	CA-CB-CG	5.93	125.95	114.10
1	C	147	ARG	CB-CG-CD	-5.92	97.68	111.30
3	G	122	ILE	N-CA-C	-5.92	104.86	110.42
1	C	306	ASP	CA-C-N	5.92	125.79	119.28
1	C	306	ASP	C-N-CA	5.92	125.79	119.28
1	B	243	GLU	N-CA-C	-5.91	104.92	111.36
2	E	365	ASP	CA-CB-CG	5.90	118.50	112.60
2	D	501	VAL	CB-CA-C	5.90	120.30	112.46
2	E	54	ASN	N-CA-C	-5.88	102.94	110.53
2	D	338	ASP	CA-CB-CG	5.88	118.48	112.60
1	C	149	TRP	N-CA-C	-5.88	104.95	111.36
3	G	7	HIS	O-C-N	-5.88	114.77	122.59
2	D	174	THR	CA-C-O	5.84	126.56	119.38
1	B	225	LYS	N-CA-C	-5.83	102.84	110.53
1	C	137	ASN	CA-C-N	5.82	125.51	119.05
1	C	137	ASN	C-N-CA	5.82	125.51	119.05
1	B	95	TRP	CG-CD2-CE3	5.82	139.72	133.90
1	B	117	TRP	CB-CG-CD1	-5.82	118.18	126.90
2	D	227	ASN	CA-CB-CG	-5.81	106.79	112.60
2	D	445	MET	CA-CB-CG	-5.81	102.48	114.10
2	D	500	HIS	CB-CG-CD2	-5.80	123.66	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	39	HIS	CB-CG-CD2	-5.80	123.67	131.20
1	C	61	ASP	CA-CB-CG	5.79	118.39	112.60
3	G	45	ASN	CB-CG-ND2	5.77	125.06	116.40
1	B	101	PRO	N-CA-C	-5.74	101.99	111.11
2	E	240	GLU	CA-CB-CG	5.74	125.57	114.10
1	C	301	ASN	OD1-CG-ND2	-5.73	116.87	122.60
2	E	468	ASN	OD1-CG-ND2	-5.73	116.87	122.60
3	G	111	HIS	CB-CG-ND1	5.72	131.29	122.70
2	D	170	ASP	CA-CB-CG	5.72	118.32	112.60
3	G	79	HIS	CB-CG-CD2	-5.71	123.77	131.20
1	C	146	ASN	CB-CG-ND2	5.70	124.95	116.40
2	D	382	HIS	CB-CG-ND1	5.70	131.25	122.70
3	H	111	HIS	CB-CG-CD2	-5.70	123.79	131.20
3	H	13	ASP	CA-CB-CG	5.69	118.29	112.60
2	E	221	THR	N-CA-CB	-5.68	101.75	110.16
1	C	240	ASP	CA-CB-CG	5.68	118.28	112.60
2	D	96	HIS	CB-CG-ND1	5.67	131.21	122.70
2	D	413	HIS	CB-CG-ND1	5.67	131.21	122.70
1	C	98	HIS	CB-CG-CD2	-5.67	123.83	131.20
3	H	23	ASN	OD1-CG-ND2	-5.67	116.94	122.60
1	B	368	ALA	N-CA-C	5.66	117.45	111.28
2	E	84	VAL	CA-CB-CG2	-5.65	100.79	110.40
1	C	43	TRP	CG-CD2-CE3	5.65	139.55	133.90
2	E	497	ALA	N-CA-CB	5.64	120.03	110.49
1	B	106	HIS	CA-CB-CG	-5.63	108.17	113.80
2	E	279	GLN	OE1-CD-NE2	-5.63	116.97	122.60
1	C	227	ALA	N-CA-C	-5.63	105.06	111.14
2	D	35	PHE	CA-CB-CG	5.62	119.42	113.80
2	E	85	ALA	N-CA-C	5.62	117.86	111.11
2	E	425	PHE	CA-CB-CG	5.62	119.42	113.80
1	B	98	HIS	CB-CG-CD2	-5.61	123.90	131.20
3	G	46	SER	CA-CB-OG	5.61	122.33	111.10
1	B	43	TRP	CE2-CD2-CG	-5.58	100.51	107.20
2	E	397	ASP	CA-CB-CG	5.56	118.16	112.60
1	C	77	HIS	CB-CG-CD2	-5.56	123.97	131.20
2	D	192	PHE	CA-CB-CG	5.56	119.36	113.80
2	E	175	ARG	CB-CG-CD	5.56	124.09	111.30
1	C	382	LYS	CA-CB-CG	-5.55	103.00	114.10
2	D	76	GLU	CA-CB-CG	5.54	125.19	114.10
3	G	55	TRP	CB-CG-CD1	-5.54	118.58	126.90
2	E	17	ASN	O-C-N	-5.54	115.23	122.59
1	B	133	ILE	N-CA-CB	5.53	120.11	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	343	HIS	CA-CB-CG	5.53	119.33	113.80
2	E	178	GLY	CA-C-N	5.52	125.35	119.28
2	E	178	GLY	C-N-CA	5.52	125.35	119.28
2	D	259	ASN	OD1-CG-ND2	-5.52	117.08	122.60
1	C	104	ARG	NE-CZ-NH1	5.51	127.01	121.50
3	G	20	ALA	O-C-N	-5.51	116.03	122.81
2	D	175	ARG	CB-CG-CD	-5.51	98.63	111.30
1	C	168	ARG	CD-NE-CZ	5.51	132.11	124.40
2	E	478	LEU	N-CA-C	5.50	117.99	111.33
2	D	340	TYR	N-CA-C	5.50	120.44	111.37
2	E	482	ILE	CB-CA-C	-5.49	104.85	111.88
3	H	45	ASN	OD1-CG-ND2	-5.49	117.11	122.60
2	D	205	GLN	OE1-CD-NE2	-5.49	117.11	122.60
2	D	407	TRP	CB-CG-CD1	-5.49	118.67	126.90
1	B	140	TRP	CE2-CD2-CG	-5.48	100.62	107.20
2	D	99	TRP	CB-CG-CD1	-5.48	118.67	126.90
2	E	344	HIS	CB-CG-CD2	-5.48	124.07	131.20
3	G	73	ASN	CA-CB-CG	5.47	118.07	112.60
2	D	372	PHE	CA-C-N	5.46	127.54	120.44
2	D	372	PHE	C-N-CA	5.46	127.54	120.44
1	B	149	TRP	CB-CG-CD1	-5.46	118.71	126.90
1	B	100	ASP	CA-CB-CG	5.46	118.06	112.60
2	D	161	ASN	OD1-CG-ND2	-5.46	117.14	122.60
1	B	324	TRP	CB-CG-CD1	-5.45	118.72	126.90
2	E	84	VAL	CA-CB-CG1	5.45	119.67	110.40
1	B	9	ARG	NE-CZ-NH2	-5.45	114.30	119.20
2	D	472	GLN	OE1-CD-NE2	-5.44	117.16	122.60
1	B	161	ASN	OD1-CG-ND2	-5.43	117.17	122.60
2	E	37	TRP	CB-CG-CD1	-5.43	118.75	126.90
1	C	140	TRP	CG-CD2-CE3	5.42	139.32	133.90
1	C	285	GLN	OE1-CD-NE2	-5.41	117.19	122.60
2	E	17	ASN	OD1-CG-ND2	-5.39	117.21	122.60
2	E	181	TRP	CG-CD2-CE3	5.38	139.28	133.90
3	G	158	GLN	OE1-CD-NE2	-5.38	117.22	122.60
1	B	168	ARG	NE-CZ-NH2	-5.38	114.36	119.20
2	E	243	GLU	N-CA-C	5.37	118.93	112.38
3	H	7	HIS	O-C-N	-5.37	115.45	122.59
2	E	24	ASN	CA-C-O	5.37	128.18	120.51
3	G	6	ILE	CA-C-O	-5.35	116.08	121.59
1	C	71	ASP	CA-CB-CG	5.35	117.95	112.60
2	D	168	HIS	CA-CB-CG	5.34	119.14	113.80
2	E	452	TRP	CG-CD2-CE3	5.34	139.24	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	249	HIS	N-CA-C	5.34	119.89	112.90
1	B	13	ASP	CA-C-N	5.32	125.39	119.32
1	B	13	ASP	C-N-CA	5.32	125.39	119.32
2	E	31	TRP	CE2-CD2-CG	-5.32	100.81	107.20
2	E	181	TRP	CE2-CD2-CG	-5.32	100.82	107.20
2	E	423	VAL	CA-C-N	5.32	125.26	119.78
2	E	423	VAL	C-N-CA	5.32	125.26	119.78
1	B	266	GLN	CG-CD-NE2	5.32	124.37	116.40
1	C	388	LEU	CA-C-O	-5.32	115.22	120.70
2	E	340	TYR	N-CA-C	5.31	117.48	111.11
2	D	227	ASN	OD1-CG-ND2	-5.30	117.30	122.60
2	E	469	ILE	CA-CB-CG1	-5.30	101.39	110.40
3	G	144	ASN	OD1-CG-ND2	-5.30	117.30	122.60
2	D	214	ASN	OD1-CG-ND2	-5.29	117.31	122.60
3	G	74	GLU	N-CA-C	5.29	117.80	111.71
2	D	84	VAL	CA-CB-CG2	-5.29	101.41	110.40
2	D	512	ILE	CB-CG1-CD1	5.29	124.90	113.80
3	H	161	VAL	CA-CB-CG2	-5.29	101.42	110.40
2	D	40	LYS	CB-CG-CD	-5.27	99.17	111.30
2	E	199	GLU	N-CA-C	-5.27	105.43	111.07
1	B	155	ASN	CA-CB-CG	5.27	117.87	112.60
2	E	203	ASN	OD1-CG-ND2	-5.26	117.34	122.60
1	C	164	SER	N-CA-C	5.26	117.01	111.28
3	G	40	THR	N-CA-CB	-5.26	101.80	111.37
3	H	153	GLU	CB-CG-CD	5.26	121.54	112.60
2	D	421	SER	N-CA-C	5.24	118.93	112.54
3	G	67	LEU	CA-C-O	-5.24	115.00	120.55
1	C	97	LYS	N-CA-CB	-5.23	102.17	110.28
1	C	43	TRP	CB-CG-CD1	-5.23	119.06	126.90
1	B	82	SER	O-C-N	-5.23	115.57	122.57
2	D	17	ASN	N-CA-C	5.23	121.93	110.80
1	B	117	TRP	CG-CD2-CE3	5.22	139.12	133.90
2	D	499	PRO	CB-CA-C	5.22	115.84	110.00
1	C	258	GLN	OE1-CD-NE2	-5.21	117.39	122.60
2	D	269	THR	CA-CB-OG1	-5.21	101.79	109.60
3	G	80	LYS	CB-CG-CD	-5.21	99.32	111.30
1	B	43	TRP	CG-CD2-CE3	5.21	139.11	133.90
2	E	140	GLN	OE1-CD-NE2	-5.21	117.39	122.60
1	B	36	GLY	N-CA-C	-5.21	108.07	115.30
1	B	324	TRP	CE2-CD2-CG	-5.21	100.95	107.20
2	D	29	HIS	CB-CG-CD2	-5.20	124.44	131.20
1	B	149	TRP	CE2-CD2-CG	-5.20	100.96	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	364	ILE	N-CA-C	-5.20	105.64	110.53
1	B	259	PHE	CA-CB-CG	-5.20	108.60	113.80
2	D	344	HIS	CB-CG-CD2	-5.20	124.45	131.20
2	E	260	ASP	CA-C-N	5.19	125.49	119.47
2	E	260	ASP	C-N-CA	5.19	125.49	119.47
2	D	37	TRP	CB-CG-CD1	-5.19	119.11	126.90
2	D	438	VAL	N-CA-C	-5.19	100.65	108.12
2	E	37	TRP	CE2-CD2-CG	-5.19	100.97	107.20
1	C	203	ILE	N-CA-CB	-5.19	100.76	111.76
2	E	305	TRP	CB-CG-CD1	-5.19	119.12	126.90
3	H	21	HIS	CB-CG-CD2	-5.19	124.45	131.20
1	C	282	ASN	OD1-CG-ND2	-5.19	117.41	122.60
2	E	324	TYR	N-CA-C	-5.17	106.28	112.59
1	B	43	TRP	CD1-CG-CD2	5.17	114.57	106.30
1	C	46	LEU	CA-C-N	5.17	131.41	121.54
1	C	46	LEU	C-N-CA	5.17	131.41	121.54
2	D	273	ASN	OD1-CG-ND2	-5.17	117.43	122.60
1	B	107	ALA	CA-C-O	-5.16	113.83	118.79
2	E	229	ASP	CA-CB-CG	5.16	117.76	112.60
3	H	133	ARG	CB-CG-CD	-5.16	99.43	111.30
1	C	165	GLN	OE1-CD-NE2	-5.16	117.44	122.60
2	D	301	TRP	CE2-CD2-CG	-5.16	101.01	107.20
1	B	106	HIS	CA-C-O	-5.15	113.14	120.51
1	B	105	TRP	CG-CD2-CE3	5.15	139.05	133.90
1	B	204	VAL	CA-C-N	5.15	125.44	119.93
1	B	204	VAL	C-N-CA	5.15	125.44	119.93
2	E	366	GLN	OE1-CD-NE2	-5.15	117.45	122.60
2	E	486	HIS	CB-CG-CD2	-5.15	124.51	131.20
2	D	301	TRP	CB-CG-CD1	-5.14	119.18	126.90
2	D	508	THR	N-CA-C	5.14	121.76	110.80
3	G	130	ASP	N-CA-C	-5.14	105.37	111.69
1	B	105	TRP	CB-CG-CD1	-5.13	119.20	126.90
1	C	37	TYR	N-CA-C	5.13	119.02	112.34
1	B	43	TRP	CG-CD1-NE1	-5.13	103.53	110.20
2	D	99	TRP	CE2-CD2-CG	-5.13	101.05	107.20
1	B	301	ASN	OD1-CG-ND2	-5.12	117.47	122.60
2	E	141	VAL	CB-CA-C	-5.12	105.32	111.88
2	D	343	HIS	CB-CG-CD2	-5.12	124.54	131.20
2	E	341	TRP	CG-CD2-CE3	5.12	139.02	133.90
2	E	63	ILE	N-CA-C	-5.12	100.96	108.85
1	B	57	GLN	OE1-CD-NE2	-5.12	117.48	122.60
2	E	260	ASP	CA-CB-CG	5.12	117.72	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	33	ASN	OD1-CG-ND2	-5.11	117.49	122.60
1	C	9	ARG	CA-CB-CG	-5.11	103.87	114.10
1	C	218	TRP	CB-CG-CD1	-5.11	119.23	126.90
1	B	43	TRP	CB-CG-CD1	-5.11	119.23	126.90
3	G	21	HIS	CB-CG-CD2	-5.11	124.56	131.20
1	C	275	ASN	OD1-CG-ND2	-5.11	117.49	122.60
3	G	20	ALA	CA-C-O	-5.11	116.14	121.55
1	B	320	TRP	CG-CD1-NE1	-5.10	103.57	110.20
2	E	343	HIS	CB-CG-CD2	-5.10	124.57	131.20
2	E	31	TRP	CB-CG-CD1	-5.10	119.26	126.90
2	D	341	TRP	CB-CG-CD1	-5.09	119.26	126.90
1	C	319	ASN	CA-CB-CG	5.09	117.69	112.60
1	C	283	GLN	OE1-CD-NE2	-5.09	117.51	122.60
1	B	62	TRP	CE2-CD2-CG	-5.08	101.10	107.20
2	E	26	GLN	OE1-CD-NE2	-5.08	117.52	122.60
1	C	35	MET	N-CA-C	5.08	117.55	111.71
2	E	59	GLN	CG-CD-NE2	5.08	124.02	116.40
2	E	313	TRP	CE2-CD2-CG	-5.08	101.11	107.20
1	C	149	TRP	CE2-CD2-CG	-5.07	101.11	107.20
2	D	27	GLU	CA-CB-CG	-5.07	103.96	114.10
2	D	87	THR	CA-CB-OG1	-5.06	102.01	109.60
2	D	100	ASN	OD1-CG-ND2	-5.06	117.54	122.60
2	E	122	GLY	N-CA-C	-5.06	106.30	112.77
1	C	99	ARG	NE-CZ-NH1	5.05	126.55	121.50
1	C	266	GLN	OE1-CD-NE2	-5.04	117.56	122.60
1	B	63	ILE	N-CA-C	-5.04	99.91	107.37
2	D	301	TRP	CG-CD2-CE3	5.04	138.94	133.90
1	C	105	TRP	CE2-CD2-CG	-5.04	101.16	107.20
2	D	83	GLN	CA-C-O	-5.04	114.65	120.24
2	D	173	ARG	O-C-N	-5.04	116.21	122.25
1	C	280	PHE	CA-CB-CG	-5.03	108.77	113.80
3	G	15	TRP	CE2-CD2-CG	-5.03	101.17	107.20
2	D	116	ASN	OD1-CG-ND2	-5.03	117.57	122.60
2	D	396	GLU	CA-CB-CG	5.03	124.16	114.10
2	D	23	VAL	CA-CB-CG1	-5.02	101.86	110.40
2	D	446	HIS	CB-CG-ND1	5.02	130.23	122.70
2	E	413	HIS	CB-CG-CD2	-5.02	124.68	131.20
2	D	305	TRP	CB-CG-CD1	-5.02	119.37	126.90
1	B	95	TRP	CE2-CD2-CG	-5.01	101.18	107.20
1	C	140	TRP	CE2-CD2-CG	-5.01	101.18	107.20
2	E	419	ARG	O-C-N	-5.01	115.92	122.59
1	C	318	ARG	CB-CG-CD	-5.01	99.77	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	235	VAL	N-CA-C	5.01	115.68	110.82
1	B	137	ASN	CA-C-N	5.01	124.79	119.28
1	B	137	ASN	C-N-CA	5.01	124.79	119.28
2	E	419	ARG	NE-CZ-NH1	5.00	126.50	121.50
3	G	134	GLN	OE1-CD-NE2	-5.00	117.60	122.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	299	TYR	Sidechain
2	D	19	ALA	Peptide
2	D	22	SER	Mainchain
2	E	19	ALA	Peptide
2	E	24	ASN	Mainchain
2	E	67	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3150	705	2998	57	0
1	C	3150	705	2998	55	0
2	D	4186	936	3990	77	0
2	E	4186	936	3990	92	0
3	G	1337	321	1323	24	0
3	H	1337	321	1323	29	1
4	D	2	0	0	0	0
4	E	2	0	0	0	0
5	D	4	0	3	0	0
5	E	4	0	3	0	0
6	B	164	328	0	19	1
6	C	142	284	0	5	0
6	D	194	388	0	10	1
6	E	199	398	0	25	1
6	G	74	148	0	5	0
6	H	86	172	0	15	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	18217	5642	16628	298	3

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 9.

All (298) 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)
2:D:196:ASP:HB2	3:G:140:MET:HE1	1.43	0.97
2:D:171:ALA:O	2:D:175:ARG:HB2	1.77	0.84
2:E:44:THR:HB	6:E:640:HOH:O	1.84	0.78
2:E:507:TRP:HB3	6:E:700:HOH:O	1.83	0.77
1:C:267:ARG:HH22	1:C:347:THR:HG21	1.50	0.77
2:D:44:THR:HG23	2:D:127:SER:HA	1.68	0.75
2:E:63:ILE:HG21	6:E:670:HOH:O	1.86	0.75
2:E:403:ILE:HG21	6:E:721:HOH:O	1.87	0.75
2:D:416:TYR:HB3	2:D:447:THR:HG21	1.70	0.73
2:D:78:GLN:HE22	2:D:150:GLN:HE21	1.35	0.72
1:C:9:ARG:HD3	6:E:636:HOH:O	1.89	0.71
2:E:422:GLN:HA	6:E:638:HOH:O	1.89	0.71
2:E:237:LEU:HD13	6:E:693:HOH:O	1.89	0.71
1:B:159:LEU:HD13	6:B:524:HOH:O	1.91	0.71
1:B:370:ALA:HB2	6:B:422:HOH:O	1.89	0.70
1:B:190:ALA:HA	6:B:550:HOH:O	1.90	0.70
2:E:416:TYR:HB3	2:E:447:THR:HG21	1.73	0.70
6:B:474:HOH:O	2:D:35:PHE:HB2	1.92	0.70
2:E:286:LEU:HD13	6:E:696:HOH:O	1.93	0.68
2:E:216:LEU:HB2	6:E:696:HOH:O	1.94	0.68
2:E:403:ILE:HD13	2:E:515:LEU:HD11	1.75	0.66
2:E:44:THR:HG22	2:E:46:TYR:H	1.60	0.66
2:D:89:LEU:HD13	6:E:636:HOH:O	1.93	0.66
2:E:118:ILE:HA	6:E:681:HOH:O	1.96	0.66
1:C:194:GLN:HE22	1:C:197:ARG:HH11	1.41	0.66
2:E:171:ALA:O	2:E:175:ARG:HG2	1.96	0.66
2:E:227:ASN:HD21	2:E:295:LYS:H	1.43	0.66
2:D:108:ASN:HD21	2:D:175:ARG:HE	1.42	0.66
2:D:352:ALA:HA	2:D:404:PRO:HB2	1.77	0.65
1:B:193:ILE:HB	6:B:550:HOH:O	1.95	0.65
2:D:206:LEU:HD13	2:D:317:TRP:HE1	1.59	0.65
1:B:261:ARG:HE	1:B:285:GLN:HE22	1.45	0.64
1:B:267:ARG:HH22	1:B:347:THR:HG21	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:105:TRP:O	3:H:109:LYS:HD3	1.96	0.64
2:D:77:ARG:HB3	2:E:84:VAL:HG21	1.80	0.64
2:E:202:LEU:HA	2:E:206:LEU:HB2	1.81	0.63
2:E:419:ARG:N	6:E:638:HOH:O	2.32	0.63
2:E:33:GLN:HA	2:E:131:ALA:HB3	1.80	0.62
1:C:124:LEU:HD12	2:E:21:THR:HG22	1.82	0.62
1:C:261:ARG:HE	1:C:285:GLN:HE22	1.48	0.62
2:D:155:ASN:HD22	2:D:168:HIS:HD2	1.48	0.62
1:B:258:GLN:HE21	1:B:261:ARG:HH21	1.47	0.62
3:H:145:LEU:HD22	6:H:244:HOH:O	2.00	0.61
2:D:479:SER:HB2	2:D:509:LEU:HD22	1.80	0.61
1:C:192:MET:HE2	1:C:283:GLN:HE22	1.66	0.61
3:H:39:HIS:HD2	6:H:188:HOH:O	1.83	0.61
2:D:78:GLN:NE2	2:D:150:GLN:HE21	1.99	0.61
1:B:194:GLN:HE22	1:B:197:ARG:HH11	1.49	0.60
2:E:24:ASN:HA	6:E:616:HOH:O	2.01	0.60
2:E:352:ALA:HA	2:E:404:PRO:HB2	1.83	0.60
2:E:18:ARG:O	2:E:20:PRO:HD3	2.01	0.59
1:C:117:TRP:HH2	2:E:23:VAL:O	1.84	0.59
1:C:195:LEU:HD11	2:E:23:VAL:HA	1.84	0.59
2:E:457:TRP:HZ3	6:H:248:HOH:O	1.86	0.59
1:C:186:LYS:HD3	6:C:524:HOH:O	2.02	0.59
3:H:68:LYS:HB3	6:H:229:HOH:O	2.01	0.59
1:B:124:LEU:HD12	2:D:21:THR:HG23	1.85	0.58
2:E:269:THR:HG21	6:H:178:HOH:O	2.03	0.58
1:C:124:LEU:HB2	2:E:21:THR:HG23	1.86	0.58
2:E:22:SER:O	2:E:24:ASN:N	2.37	0.57
1:C:339:PHE:HA	1:C:342:LEU:HD13	1.86	0.57
2:E:227:ASN:ND2	2:E:295:LYS:H	2.01	0.57
2:D:506:LEU:HD12	6:D:588:HOH:O	2.03	0.57
3:G:19:ILE:O	3:G:22:VAL:HG22	2.04	0.57
2:E:141:VAL:HA	6:E:681:HOH:O	2.02	0.57
3:H:77:PHE:HE1	6:H:229:HOH:O	1.87	0.57
1:C:192:MET:HE3	1:C:280:PHE:CE1	2.40	0.57
1:C:46:LEU:O	1:C:47:THR:HG23	2.05	0.56
1:C:338:LEU:HD12	1:C:341:LYS:HD2	1.88	0.56
1:C:336:MET:HB3	1:C:388:LEU:HA	1.88	0.56
2:D:268:ASN:HD21	2:D:327:GLU:H	1.53	0.56
2:D:508:THR:N	6:D:666:HOH:O	2.37	0.55
2:E:292:TYR:OH	2:E:344:HIS:HD2	1.88	0.55
1:B:153:LEU:HA	6:B:550:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:THR:N	6:C:467:HOH:O	2.40	0.55
2:E:439:HIS:HB3	3:H:161:VAL:CG2	2.36	0.55
2:E:436:LEU:HD13	6:H:199:HOH:O	2.07	0.55
1:C:144:SER:HA	1:C:148:TYR:HD2	1.71	0.54
2:E:175:ARG:HD3	2:E:181:TRP:CZ2	2.42	0.54
3:H:4:LEU:HB3	6:H:185:HOH:O	2.07	0.54
1:B:159:LEU:HG	1:B:248:VAL:HG13	1.89	0.54
3:H:19:ILE:HA	6:H:221:HOH:O	2.06	0.54
1:B:304:GLY:HA2	6:B:546:HOH:O	2.07	0.54
2:D:21:THR:O	2:D:23:VAL:HG23	2.08	0.53
2:D:422:GLN:HA	6:D:582:HOH:O	2.08	0.53
2:E:360:ARG:HG2	2:E:498:GLN:HB2	1.90	0.53
1:C:53:THR:HG23	6:C:487:HOH:O	2.09	0.53
3:H:136:GLY:N	6:H:226:HOH:O	2.41	0.53
3:H:5:GLY:HA2	3:H:9:ASN:HB3	1.90	0.53
2:D:302:VAL:HB	6:D:699:HOH:O	2.07	0.53
2:D:84:VAL:HG13	2:D:88:ARG:HH21	1.74	0.53
2:E:489:ARG:NE	6:E:664:HOH:O	2.41	0.53
1:B:313:ASN:HB2	6:B:546:HOH:O	2.09	0.53
2:E:175:ARG:HD3	2:E:181:TRP:CE2	2.44	0.52
2:D:360:ARG:HG2	2:D:498:GLN:HB2	1.90	0.52
3:G:41:THR:O	3:G:44:ARG:HD2	2.09	0.52
2:E:21:THR:HG22	2:E:23:VAL:HG13	1.92	0.52
1:C:41:PRO:HB3	1:C:46:LEU:HA	1.92	0.52
2:D:85:ALA:O	2:D:89:LEU:HD23	2.10	0.52
2:E:439:HIS:HD2	3:H:163:VAL:HA	1.75	0.52
1:B:194:GLN:HE22	1:B:197:ARG:NH1	2.06	0.52
1:C:202:LYS:HD2	6:E:628:HOH:O	2.10	0.52
3:G:22:VAL:HG21	6:G:230:HOH:O	2.09	0.51
1:C:199:PHE:HA	6:E:628:HOH:O	2.10	0.51
2:D:227:ASN:HD21	2:D:296:PHE:H	1.57	0.51
2:E:33:GLN:HA	2:E:33:GLN:HE21	1.74	0.51
2:E:108:ASN:HD21	2:E:175:ARG:HE	1.59	0.51
1:B:73:THR:HA	2:D:466:CYS:HB2	1.93	0.51
2:E:308:TRP:HZ3	6:E:696:HOH:O	1.93	0.51
3:G:18:LYS:HD3	6:G:215:HOH:O	2.10	0.51
3:G:40:THR:HG21	6:G:174:HOH:O	2.10	0.51
2:E:33:GLN:NE2	2:E:132:GLU:H	2.09	0.51
1:C:11:LEU:HD12	2:E:230:GLU:HG3	1.93	0.51
1:B:82:SER:HA	6:B:485:HOH:O	2.09	0.51
1:B:314:ARG:HG3	6:B:546:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:479:SER:HB3	2:D:512:ILE:HG22	1.93	0.51
2:E:413:HIS:HD2	2:E:428:SER:OG	1.94	0.51
1:B:201:ALA:HA	1:B:207:PHE:HB3	1.93	0.50
2:D:33:GLN:HE21	2:D:131:ALA:HB3	1.75	0.50
2:E:439:HIS:HB3	3:H:161:VAL:HG21	1.92	0.50
2:E:477:GLU:O	2:E:480:GLU:HG2	2.10	0.50
2:D:292:TYR:OH	2:D:344:HIS:HD2	1.95	0.50
1:B:42:ARG:HB2	1:B:99:ARG:HG3	1.93	0.50
1:B:128:SER:HB2	2:D:20:PRO:HD2	1.93	0.50
2:E:288:MET:SD	2:E:346:LEU:HD13	2.52	0.50
3:G:15:TRP:HA	3:G:18:LYS:HG2	1.92	0.50
3:H:161:VAL:HB	6:H:248:HOH:O	2.11	0.50
2:D:112:VAL:HG21	2:D:181:TRP:HH2	1.76	0.50
2:E:214:ASN:HB3	2:E:215:PRO:HD3	1.94	0.50
1:B:101:PRO:O	1:B:102:LEU:HB2	2.11	0.50
1:C:203:ILE:HG22	1:C:204:VAL:HG23	1.92	0.50
1:C:291:ALA:O	1:C:295:VAL:HG13	2.12	0.49
2:D:175:ARG:HG2	2:D:181:TRP:CD2	2.47	0.49
1:B:106:HIS:N	6:B:424:HOH:O	2.45	0.49
2:D:507:TRP:O	2:D:511:ASP:HB2	2.12	0.49
1:B:266:GLN:HE22	1:B:278:PRO:HA	1.76	0.49
3:G:58:ALA:HB2	6:G:229:HOH:O	2.13	0.49
2:D:77:ARG:HA	2:E:80:GLY:HA2	1.95	0.49
3:G:140:MET:HE3	6:G:166:HOH:O	2.12	0.49
1:C:117:TRP:CH2	2:E:23:VAL:O	2.65	0.49
2:D:493:LYS:HZ1	2:D:510:ASP:H	1.59	0.49
1:C:42:ARG:HB2	1:C:99:ARG:HG3	1.95	0.48
1:C:258:GLN:HE21	1:C:261:ARG:HH21	1.61	0.48
2:D:48:THR:O	3:G:137:THR:HG23	2.12	0.48
1:C:54:VAL:HG13	6:C:436:HOH:O	2.13	0.48
2:D:89:LEU:HD22	6:E:636:HOH:O	2.13	0.48
2:E:269:THR:HG22	3:H:148:TYR:CE2	2.48	0.48
2:E:434:SER:HA	6:E:662:HOH:O	2.14	0.48
1:C:159:LEU:HG	1:C:248:VAL:HG13	1.95	0.48
2:D:216:LEU:O	2:D:220:VAL:HG23	2.13	0.48
2:E:23:VAL:HG23	2:E:24:ASN:H	1.78	0.48
3:G:61:GLU:HG2	3:G:121:PRO:HD3	1.96	0.48
2:D:44:THR:CG2	2:D:127:SER:HA	2.43	0.48
1:B:98:HIS:HE1	1:B:178:SER:OG	1.97	0.48
1:B:124:LEU:HD11	1:B:195:LEU:HD21	1.96	0.48
1:B:146:ASN:O	1:B:214:PRO:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:TYR:CZ	1:B:381:VAL:HG21	2.49	0.48
1:C:261:ARG:NE	1:C:285:GLN:HE22	2.12	0.48
3:G:101:ALA:HB3	3:G:138:ARG:HH12	1.78	0.48
3:G:138:ARG:HG3	3:G:138:ARG:HH11	1.79	0.48
2:E:78:GLN:HE21	2:E:235:VAL:HA	1.79	0.48
3:H:22:VAL:O	3:H:63:LYS:HE3	2.14	0.48
2:E:78:GLN:HE22	2:E:150:GLN:HE21	1.60	0.47
2:D:196:ASP:N	6:D:640:HOH:O	2.46	0.47
1:C:161:ASN:HB3	1:C:235:TRP:CE2	2.48	0.47
1:B:202:LYS:HZ2	2:D:22:SER:C	2.21	0.47
1:C:189:ILE:HB	6:C:524:HOH:O	2.12	0.47
1:B:28:PRO:HA	2:D:163:GLN:O	2.15	0.47
1:B:33:ASN:HD22	1:B:33:ASN:H	1.63	0.47
1:B:124:LEU:HD12	2:D:21:THR:CG2	2.45	0.47
2:E:54:ASN:O	2:E:55:GLU:HB2	2.15	0.47
3:G:44:ARG:HG3	3:G:46:SER:O	2.14	0.47
1:B:225:LYS:HA	6:B:503:HOH:O	2.14	0.47
1:C:100:ASP:OD2	1:C:104:ARG:HD3	2.14	0.47
1:C:192:MET:HE3	1:C:280:PHE:CD1	2.50	0.47
2:E:21:THR:HB	2:E:23:VAL:HG22	1.97	0.47
1:B:6:GLU:N	6:B:538:HOH:O	2.48	0.46
2:D:521:ASN:HB3	2:D:524:LYS:HD3	1.97	0.46
1:B:11:LEU:HD12	2:D:230:GLU:HG3	1.96	0.46
2:E:108:ASN:ND2	2:E:175:ARG:HH21	2.13	0.46
3:H:98:MET:HE1	3:H:107:ALA:O	2.15	0.46
1:B:22:LYS:HE2	1:B:23:ALA:N	2.31	0.46
1:C:120:THR:HG21	1:C:192:MET:HE1	1.98	0.46
2:D:390:TRP:HE1	2:D:407:TRP:CG	2.34	0.46
3:G:40:THR:HG22	3:G:41:THR:HG23	1.98	0.46
1:B:100:ASP:OD2	1:B:104:ARG:HD3	2.15	0.46
1:B:129:ALA:O	2:D:15:ALA:N	2.49	0.46
1:B:239:PHE:HB2	3:G:126:ASN:HA	1.98	0.46
1:C:98:HIS:HE1	1:C:178:SER:OG	1.99	0.46
2:E:223:TRP:CE2	2:E:298:VAL:HB	2.51	0.46
3:H:116:GLN:HG3	6:H:203:HOH:O	2.15	0.46
2:E:179:PRO:HD2	6:E:632:HOH:O	2.16	0.46
1:B:161:ASN:HB3	1:B:235:TRP:CE2	2.51	0.46
1:B:336:MET:HB3	1:B:388:LEU:HA	1.97	0.46
2:D:227:ASN:HD21	2:D:295:LYS:H	1.63	0.46
2:D:493:LYS:HD2	2:D:493:LYS:HA	1.76	0.46
2:D:84:VAL:HG13	2:D:88:ARG:NH2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:108:ASN:ND2	2:D:175:ARG:HH21	2.13	0.45
2:D:439:HIS:HE1	2:D:454:GLU:OE2	1.99	0.45
1:B:6:GLU:O	1:B:7:ARG:HB3	2.15	0.45
1:C:82:SER:HB3	2:E:193:ILE:HD11	1.99	0.45
2:E:51:LYS:HD2	2:E:51:LYS:N	2.31	0.45
1:C:342:LEU:HA	1:C:343:PRO:HD3	1.91	0.45
2:D:413:HIS:HD2	2:D:428:SER:OG	2.00	0.45
3:H:79:HIS:HD2	3:H:127:TYR:OH	1.99	0.45
2:D:493:LYS:HE3	2:D:508:THR:HG23	1.99	0.45
2:D:33:GLN:NE2	2:D:132:GLU:H	2.15	0.45
2:D:418:ASP:C	6:D:582:HOH:O	2.59	0.45
2:E:140:GLN:O	2:E:144:GLU:HG2	2.17	0.45
2:E:385:LYS:O	2:E:389:GLU:HG2	2.18	0.44
1:B:161:ASN:HD21	2:D:134:LYS:HD3	1.82	0.44
1:C:364:ILE:HA	1:C:368:ALA:HB3	1.99	0.44
2:D:493:LYS:CE	2:D:508:THR:HG23	2.46	0.44
2:E:175:ARG:HG3	2:E:176:THR:N	2.32	0.44
1:B:42:ARG:CB	1:B:99:ARG:HG3	2.47	0.44
1:C:111:LYS:O	1:C:115:GLU:HG3	2.17	0.44
3:H:41:THR:O	3:H:44:ARG:HD2	2.17	0.44
2:D:493:LYS:NZ	2:D:510:ASP:H	2.16	0.44
2:E:275:PHE:CZ	2:E:332:LEU:HD23	2.52	0.44
3:H:40:THR:HG22	3:H:41:THR:HG23	2.00	0.44
1:B:225:LYS:O	1:B:226:SER:HB2	2.17	0.44
3:G:138:ARG:NH1	3:G:142:LEU:HD11	2.33	0.44
1:C:146:ASN:ND2	1:C:197:ARG:HH21	2.15	0.43
1:C:168:ARG:HD3	2:E:123:MET:SD	2.58	0.43
2:E:407:TRP:HA	2:E:410:GLU:HG2	1.99	0.43
2:D:21:THR:O	2:D:22:SER:C	2.62	0.43
2:D:498:GLN:NE2	6:D:588:HOH:O	2.51	0.43
2:E:291:GLU:HB2	6:E:726:HOH:O	2.19	0.43
3:G:79:HIS:HD2	3:G:127:TYR:OH	2.01	0.43
3:H:115:ARG:HB2	6:H:203:HOH:O	2.19	0.43
2:D:33:GLN:HA	2:D:131:ALA:HB3	2.00	0.43
2:D:49:LYS:HD3	3:G:140:MET:HB3	2.00	0.43
2:D:445:MET:HE3	2:D:523:VAL:HG13	2.00	0.43
2:E:423:VAL:HA	2:E:424:PRO:HD3	1.90	0.43
1:B:96:PHE:O	1:B:99:ARG:NH2	2.52	0.43
1:C:161:ASN:HD21	2:E:134:LYS:HD3	1.83	0.43
2:D:44:THR:HB	6:D:690:HOH:O	2.18	0.43
1:C:42:ARG:CB	1:C:99:ARG:HG3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:257:ILE:HB	6:D:673:HOH:O	2.19	0.43
2:E:32:LEU:O	2:E:33:GLN:CB	2.67	0.43
1:C:194:GLN:HE22	1:C:197:ARG:NH1	2.13	0.42
2:E:496:ILE:O	2:E:497:ALA:HB3	2.19	0.42
3:G:7:HIS:HA	3:G:12:ARG:NH1	2.34	0.42
2:D:108:ASN:HD21	2:D:175:ARG:HH21	1.68	0.42
2:E:494:THR:HA	2:E:508:THR:HA	2.00	0.42
6:B:474:HOH:O	2:D:131:ALA:CB	2.68	0.42
1:C:268:LEU:HD23	1:C:271:ARG:HD2	2.00	0.42
2:E:268:ASN:ND2	2:E:327:GLU:H	2.17	0.42
3:G:131:GLY:O	3:G:135:LEU:HB2	2.20	0.42
1:C:263:GLU:HB3	1:C:355:SER:HB2	2.01	0.42
1:C:204:VAL:HA	1:C:205:PRO:HD2	1.80	0.42
2:E:22:SER:HB2	6:E:628:HOH:O	2.20	0.42
2:E:218:VAL:O	2:E:221:THR:HB	2.20	0.42
2:E:512:ILE:HG12	6:E:700:HOH:O	2.19	0.42
2:D:343:HIS:CD2	2:D:343:HIS:H	2.38	0.42
2:E:268:ASN:HD21	2:E:327:GLU:H	1.67	0.42
3:H:160:GLY:HA2	6:H:235:HOH:O	2.20	0.42
1:C:117:TRP:CE3	2:E:65:LYS:HD3	2.55	0.42
1:B:128:SER:CB	2:D:20:PRO:HD2	2.49	0.42
1:C:150:GLY:O	1:C:153:LEU:HB3	2.20	0.42
2:D:108:ASN:HD21	2:D:175:ARG:NE	2.11	0.42
3:G:36:ARG:O	3:G:40:THR:HB	2.20	0.42
3:H:19:ILE:HG12	3:H:60:LEU:HD13	2.00	0.42
1:B:272:PHE:HZ	6:B:531:HOH:O	2.03	0.42
2:D:217:ILE:HG23	2:D:236:PHE:HB3	2.02	0.42
2:E:21:THR:CG2	2:E:23:VAL:HG13	2.48	0.42
2:E:196:ASP:HB2	3:H:140:MET:SD	2.60	0.41
1:B:125:GLN:HG3	2:D:21:THR:OG1	2.20	0.41
2:D:422:GLN:N	6:D:582:HOH:O	2.46	0.41
1:C:40:THR:HA	1:C:41:PRO:HD3	1.72	0.41
1:C:192:MET:HE3	1:C:280:PHE:HE1	1.83	0.41
2:E:439:HIS:HB3	3:H:161:VAL:HG22	2.02	0.41
1:B:316:VAL:O	1:B:319:ASN:HB3	2.20	0.41
1:B:267:ARG:HH22	1:B:347:THR:CG2	2.31	0.41
1:C:133:ILE:HG12	1:C:203:ILE:HG23	2.02	0.41
2:D:128:ALA:HB1	2:D:133:GLN:HB3	2.03	0.41
1:C:121:ASP:HA	2:E:21:THR:HG21	2.03	0.41
2:E:281:TYR:CZ	2:E:285:VAL:HG21	2.55	0.41
2:E:397:ASP:HA	2:E:398:PRO:HD2	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ARG:HD2	1:B:204:VAL:HG21	2.02	0.41
1:B:195:LEU:HG	2:D:23:VAL:HG11	2.02	0.41
2:E:269:THR:HG22	3:H:148:TYR:HE2	1.86	0.41
2:E:286:LEU:HB3	6:E:580:HOH:O	2.20	0.41
2:E:521:ASN:HB3	2:E:524:LYS:HG3	2.03	0.41
2:E:343:HIS:H	2:E:343:HIS:CD2	2.39	0.41
3:H:98:MET:O	3:H:138:ARG:NH1	2.54	0.41
1:B:63:ILE:HD12	6:B:400:HOH:O	2.20	0.40
1:B:137:ASN:HA	1:B:138:PRO:HD3	1.96	0.40
1:B:314:ARG:N	6:B:546:HOH:O	2.53	0.40
3:G:20:ALA:O	3:G:21:HIS:CB	2.69	0.40
1:C:43:TRP:O	1:C:44:LYS:HB2	2.21	0.40
3:H:80:LYS:HB2	3:H:85:GLU:O	2.22	0.40
1:B:105:TRP:N	6:B:424:HOH:O	2.54	0.40
6:B:418:HOH:O	2:D:195:GLY:HA2	2.22	0.40
3:G:138:ARG:HH11	3:G:138:ARG:CG	2.35	0.40
3:H:10:ASP:HB2	6:H:190:HOH:O	2.21	0.40
1:B:34:LYS:HB3	1:B:35:MET:H	1.75	0.40
2:E:192:PHE:CE1	2:E:204:LEU:HA	2.57	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:27:LYS:HZ1	6:H:249:HOH:H1[4_465]	1.28	0.32
6:B:521:HOH:O	6:H:169:HOH:H1[1_545]	1.52	0.08
6:D:672:HOH:O	6:E:673:HOH:H2[3_645]	1.60	0.00

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	B	382/384 (100%)	359 (94%)	19 (5%)	4 (1%)	12	11
1	C	382/384 (100%)	368 (96%)	10 (3%)	4 (1%)	12	11
2	D	510/512 (100%)	481 (94%)	22 (4%)	7 (1%)	9	7
2	E	510/512 (100%)	482 (94%)	23 (4%)	5 (1%)	12	11
3	G	160/162 (99%)	156 (98%)	3 (2%)	1 (1%)	21	23
3	H	160/162 (99%)	156 (98%)	3 (2%)	1 (1%)	21	23
All	All	2104/2116 (99%)	2002 (95%)	80 (4%)	22 (1%)	12	11

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	35	MET
1	C	46	LEU
1	C	47	THR
2	D	22	SER
2	D	196	ASP
2	D	508	THR
2	E	23	VAL
2	E	33	GLN
3	H	6	ILE
1	B	34	LYS
2	D	418	ASP
2	D	491	ASP
1	B	7	ARG
1	B	83	TRP
2	E	41	ASN
3	G	21	HIS
1	C	40	THR
2	D	20	PRO
2	E	497	ALA
1	C	251	VAL
2	E	20	PRO
2	D	97	PRO

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	B	318/318 (100%)	291 (92%)	27 (8%)	10	11
1	C	318/318 (100%)	289 (91%)	29 (9%)	9	9
2	D	432/432 (100%)	391 (90%)	41 (10%)	8	8
2	E	432/432 (100%)	393 (91%)	39 (9%)	9	9
3	G	140/140 (100%)	128 (91%)	12 (9%)	10	10
3	H	140/140 (100%)	130 (93%)	10 (7%)	13	16
All	All	1780/1780 (100%)	1622 (91%)	158 (9%)	9	10

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	7	ARG
1	B	11	LEU
1	B	21	LEU
1	B	22	LYS
1	B	29	LEU
1	B	33	ASN
1	B	34	LYS
1	B	44	LYS
1	B	45	ARG
1	B	46	LEU
1	B	93	VAL
1	B	102	LEU
1	B	133	ILE
1	B	159	LEU
1	B	168	ARG
1	B	171	LEU
1	B	173	ASP
1	B	229	LEU
1	B	266	GLN
1	B	276	LEU
1	B	303	LEU
1	B	308	GLU
1	B	326	GLU
1	B	342	LEU
1	B	343	PRO
1	B	347	THR
1	B	356	LEU
1	C	11	LEU

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Mol	Chain	Res	Type
1	C	21	LEU
1	C	22	LYS
1	C	29	LEU
1	C	34	LYS
1	C	44	LYS
1	C	93	VAL
1	C	133	ILE
1	C	142	THR
1	C	145	CYS
1	C	146	ASN
1	C	153	LEU
1	C	159	LEU
1	C	168	ARG
1	C	171	LEU
1	C	173	ASP
1	C	176	ARG
1	C	203	ILE
1	C	229	LEU
1	C	276	LEU
1	C	303	LEU
1	C	308	GLU
1	C	310	SER
1	C	326	GLU
1	C	342	LEU
1	C	347	THR
1	C	356	LEU
1	C	374	LYS
1	C	389	LYS
2	D	18	ARG
2	D	33	GLN
2	D	44	THR
2	D	82	LEU
2	D	84	VAL
2	D	93	VAL
2	D	97	PRO
2	D	107	SER
2	D	110	LEU
2	D	112	VAL
2	D	125	TRP
2	D	138	LEU
2	D	169	ASN
2	D	186	ARG

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Mol	Chain	Res	Type
2	D	204	LEU
2	D	206	LEU
2	D	238	SER
2	D	271	LEU
2	D	279	GLN
2	D	280	LYS
2	D	286	LEU
2	D	289	LEU
2	D	302	VAL
2	D	310	TYR
2	D	332	LEU
2	D	346	LEU
2	D	349	LEU
2	D	361	LEU
2	D	412	ASN
2	D	436	LEU
2	D	451	GLN
2	D	458	LEU
2	D	469	ILE
2	D	478	LEU
2	D	488	LEU
2	D	501	VAL
2	D	506	LEU
2	D	509	LEU
2	D	512	ILE
2	D	515	LEU
2	D	523	VAL
2	E	21	THR
2	E	24	ASN
2	E	32	LEU
2	E	33	GLN
2	E	54	ASN
2	E	63	ILE
2	E	82	LEU
2	E	90	ASN
2	E	110	LEU
2	E	125	TRP
2	E	138	LEU
2	E	169	ASN
2	E	180	LEU
2	E	186	ARG
2	E	204	LEU

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Mol	Chain	Res	Type
2	E	221	THR
2	E	237	LEU
2	E	240	GLU
2	E	252	GLN
2	E	271	LEU
2	E	279	GLN
2	E	289	LEU
2	E	310	TYR
2	E	320	ARG
2	E	332	LEU
2	E	337	GLN
2	E	346	LEU
2	E	349	LEU
2	E	356	THR
2	E	361	LEU
2	E	403	ILE
2	E	405	LEU
2	E	436	LEU
2	E	458	LEU
2	E	469	ILE
2	E	493	LYS
2	E	501	VAL
2	E	516	ASN
2	E	523	VAL
3	G	18	LYS
3	G	23	ASN
3	G	25	LEU
3	G	27	LYS
3	G	40	THR
3	G	44	ARG
3	G	60	LEU
3	G	70	ARG
3	G	125	VAL
3	G	135	LEU
3	G	138	ARG
3	G	161	VAL
3	H	11	THR
3	H	16	VAL
3	H	18	LYS
3	H	25	LEU
3	H	40	THR
3	H	44	ARG

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Mol	Chain	Res	Type
3	H	91	LEU
3	H	125	VAL
3	H	135	LEU
3	H	164	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	33	ASN
1	B	98	HIS
1	B	146	ASN
1	B	161	ASN
1	B	194	GLN
1	B	220	ASN
1	B	258	GLN
1	B	266	GLN
1	B	283	GLN
1	B	285	GLN
1	C	98	HIS
1	C	146	ASN
1	C	155	ASN
1	C	161	ASN
1	C	194	GLN
1	C	258	GLN
1	C	283	GLN
1	C	285	GLN
1	C	301	ASN
2	D	33	GLN
2	D	41	ASN
2	D	59	GLN
2	D	78	GLN
2	D	90	ASN
2	D	108	ASN
2	D	133	GLN
2	D	161	ASN
2	D	163	GLN
2	D	168	HIS
2	D	169	ASN
2	D	227	ASN
2	D	268	ASN
2	D	273	ASN
2	D	279	GLN

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Mol	Chain	Res	Type
2	D	343	HIS
2	D	344	HIS
2	D	422	GLN
2	D	439	HIS
2	D	486	HIS
2	E	33	GLN
2	E	59	GLN
2	E	78	GLN
2	E	90	ASN
2	E	108	ASN
2	E	133	GLN
2	E	161	ASN
2	E	169	ASN
2	E	227	ASN
2	E	249	ASN
2	E	268	ASN
2	E	273	ASN
2	E	278	GLN
2	E	279	GLN
2	E	337	GLN
2	E	344	HIS
2	E	413	HIS
2	E	422	GLN
2	E	439	HIS
3	G	7	HIS
3	G	45	ASN
3	G	79	HIS
3	G	116	GLN
3	H	7	HIS
3	H	39	HIS
3	H	79	HIS
3	H	158	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	ACY	D	1	4	3,3,3	1.18	0	3,3,3	0.64	0
5	ACY	E	527	4	3,3,3	1.16	0	3,3,3	0.88	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.