



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:29 AM UTC

PDB ID : 1L0N / pdb_0000110n
Title : native structure of bovine mitochondrial cytochrome bc1 complex
Authors : Gao, X.; Wen, X.; Yu, C.A.; Esser, L.; Tsao, S.; Quinn, B.; Zhang, L.; Yu, L.; Xia, D.
Deposited on : 2002-02-11
Resolution : 2.60 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

<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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

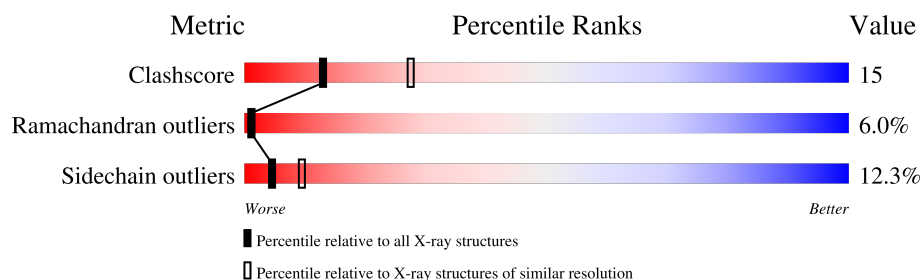
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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	A	446	70% 24% 7%
2	B	439	64% 25% 7% . .
3	C	379	69% 22% 8% ..
4	D	241	49% 33% 16% .
5	E	196	44% 40% 12% .
6	F	110	61% 25% 7% . 5%
7	G	81	60% 20% 9% . 7%
8	H	78	47% 32% 9% . 10%

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Mol	Chain	Length	Quality of chain
9	I	78	14%23%31%5%27%
10	J	62	53%27%11%• 6%
11	K	56	52%16%9%11%12%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 16577 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 UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX CORE PROTEIN I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	0	0
			3458	2161	609	668	20			

- Molecule 2 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX CORE PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	0	0
			3172	1993	562	610	7			

- Molecule 3 is a protein called Cytochrome B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	377	Total	C	N	O	S	0	0	0
			2996	2009	470	499	18			

- Molecule 4 is a protein called Cytochrome c1, heme protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1919	1225	330	349	15			

- Molecule 5 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1519	957	263	291	8			

- Molecule 6 is a protein called Ubiquinol-cytochrome C reductase complex 14 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	105	Total	C	N	O	S	0	0	0
			911	576	165	168	2			

- Molecule 7 is a protein called Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	75	Total	C	N	O	S	0	0	0
			628	410	118	99	1			

- Molecule 8 is a protein called Ubiquinol-cytochrome C reductase complex 11 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	70	Total	C	N	O	S	0	0	0
			575	347	102	121	5			

- Molecule 9 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE 8 KDA PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	57	Total	C	N	O	S	0	0	0
			406	253	77	74	2			

- Molecule 10 is a protein called Ubiquinol-cytochrome C reductase complex 7.2 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	58	Total	C	N	O	S	0	0	0
			473	311	83	79				

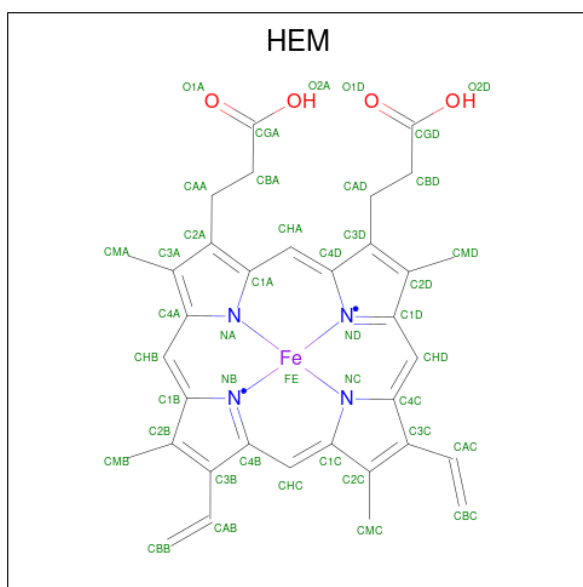
- Molecule 11 is a protein called cytochrome b-c1 complex 6.4K protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	0	0
			387	251	71	64	1			

There is a discrepancy between the modelled and reference sequences:

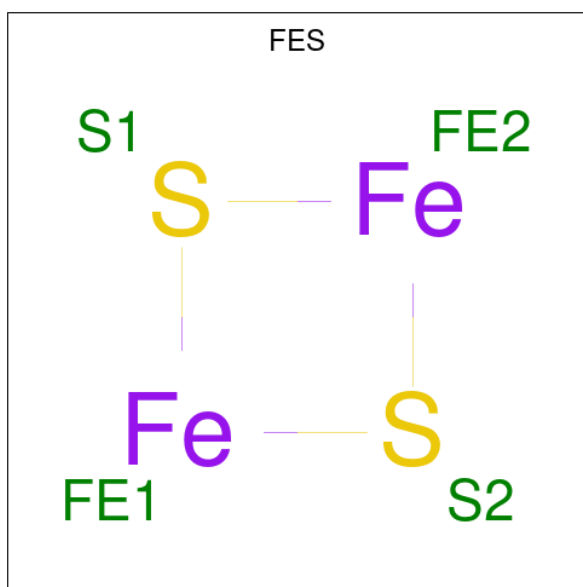
Chain	Residue	Modelled	Actual	Comment	Reference
K	47	THR	TYR	conflict	UNP P07552

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



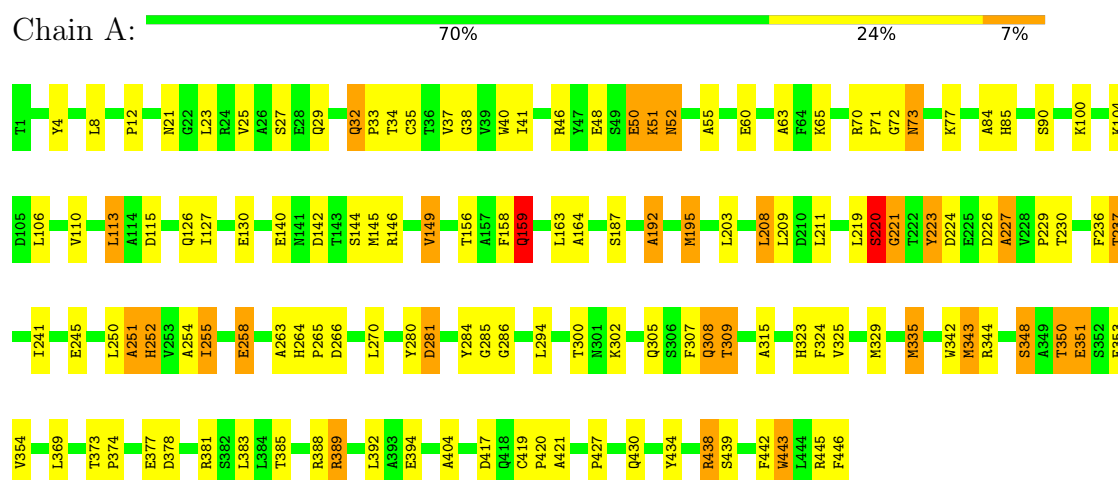
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	E	1	Total	Fe	S	0	0
			4	2	2		

3 Residue-property plots

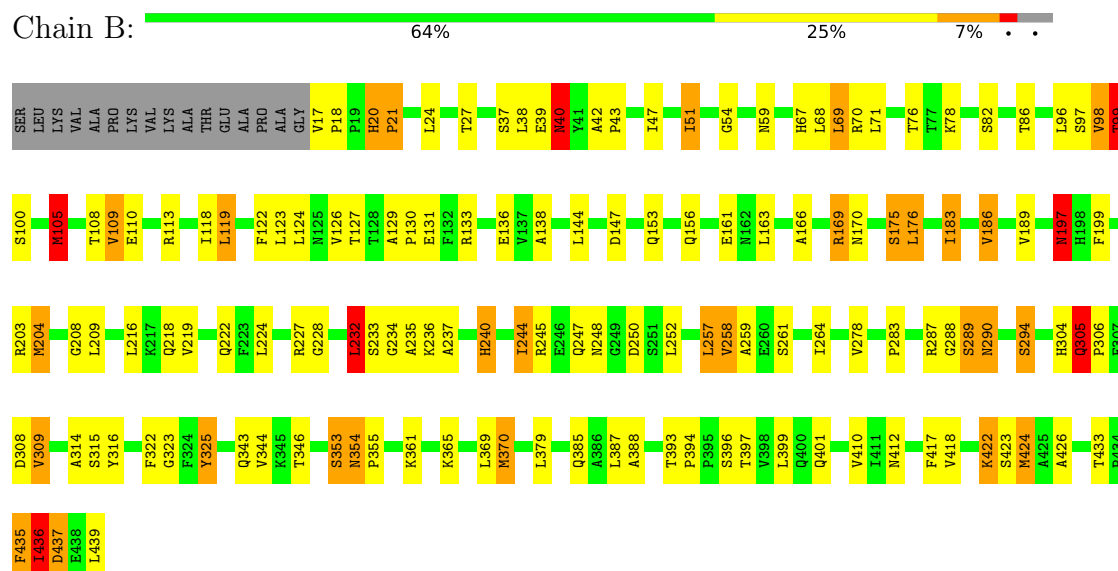
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX CORE PROTEIN I

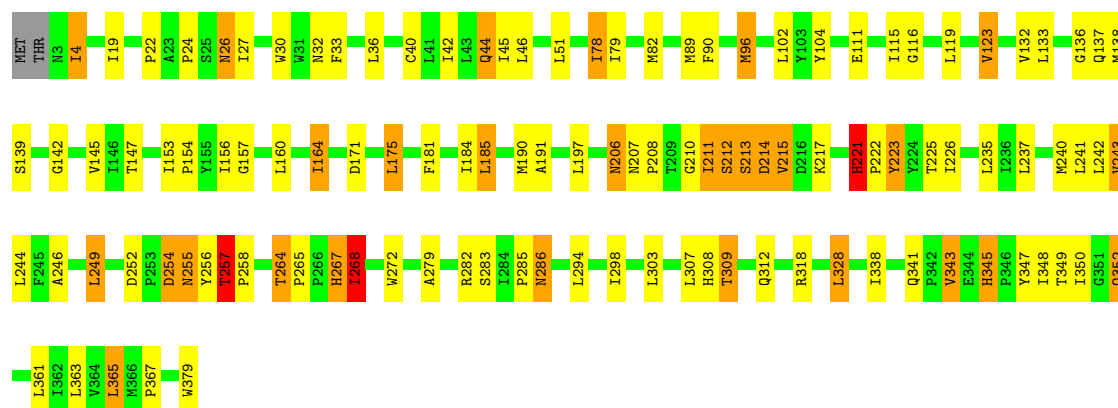


- Molecule 2: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX CORE PROTEIN 2



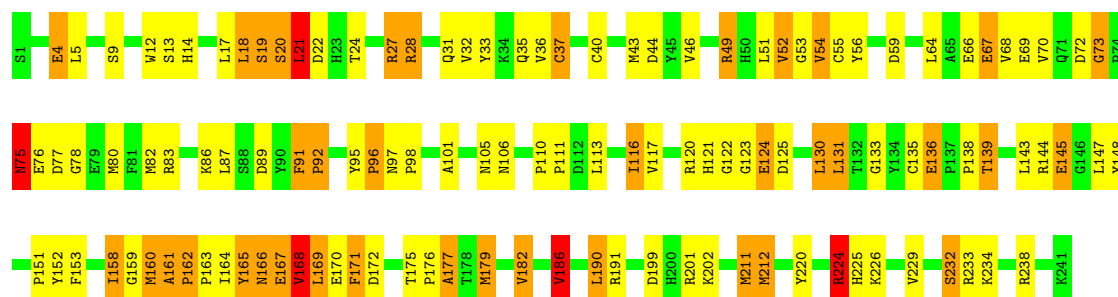
- Molecule 3: Cytochrome B

Chain C:  69% 22% 8% ..

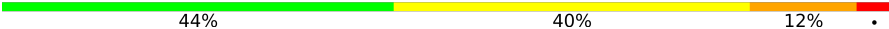


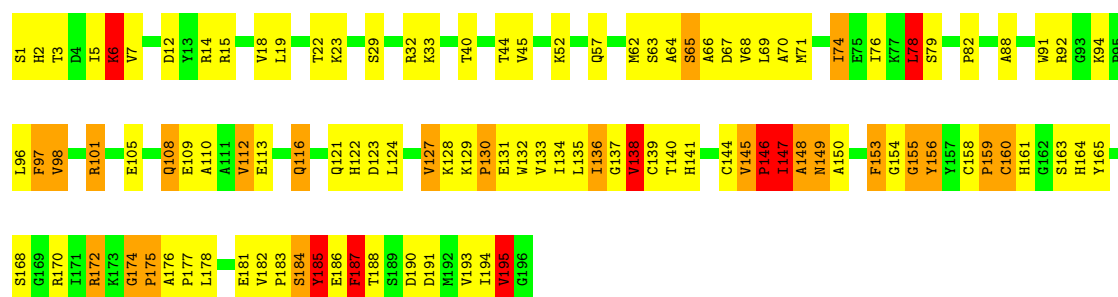
- Molecule 4: Cytochrome c1, heme protein

Chain D:  49% 33% 16% .



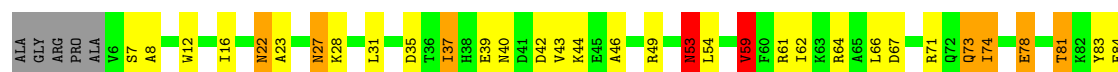
- Molecule 5: UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT

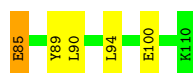
Chain E:  44% 40% 12% .



- Molecule 6: Ubiquinol-cytochrome C reductase complex 14 kDa protein

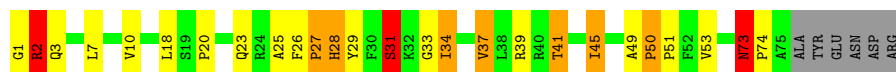
Chain F:  61% 25% 7% . 5%





- Molecule 7: Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C

Chain G: 60% 20% 9% 7%



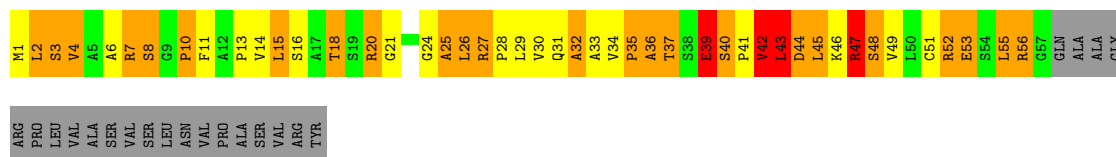
- Molecule 8: Ubiquinol-cytochrome C reductase complex 11 kDa protein

Chain H: 47% 32% 9% 10%



- Molecule 9: UBIQUINOL-CYTOCHROME C REDUCTASE 8 KDA PROTEIN

Chain I: 14% 23% 31% 5% 27%



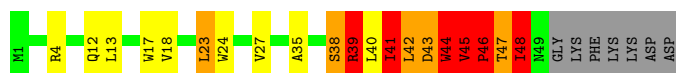
- Molecule 10: Ubiquinol-cytochrome C reductase complex 7.2 kDa protein

Chain J: 53% 27% 11% 6%



- Molecule 11: cytochrome b-c1 complex 6.4K protein

Chain K: 52% 16% 9% 11% 12%



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	153.83Å 153.83Å 596.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.99 – 2.60	Depositor
% Data completeness (in resolution range)	100.0 (28.99-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.261 , 0.297	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16577	wwPDB-VP
Average B, all atoms (Å ²)	43.0	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, FES

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.27	15/3531 (0.4%)	1.14	21/4792 (0.4%)
2	B	1.59	36/3232 (1.1%)	1.27	22/4386 (0.5%)
3	C	1.19	11/3093 (0.4%)	1.18	15/4232 (0.4%)
4	D	1.05	4/1978 (0.2%)	1.48	30/2684 (1.1%)
5	E	1.09	4/1553 (0.3%)	1.36	24/2100 (1.1%)
6	F	1.26	2/930 (0.2%)	1.20	5/1246 (0.4%)
7	G	1.37	4/649 (0.6%)	1.24	6/878 (0.7%)
8	H	0.92	0/580	1.28	5/777 (0.6%)
9	I	1.68	4/411 (1.0%)	1.94	12/558 (2.2%)
10	J	1.12	1/485 (0.2%)	1.08	1/655 (0.2%)
11	K	1.11	2/397 (0.5%)	1.31	7/544 (1.3%)
All	All	1.28	83/16839 (0.5%)	1.28	148/22852 (0.6%)

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
3	C	0	1
4	D	1	0
All	All	1	1

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	34	ILE	CA-CB	14.34	1.61	1.54
2	B	424	MET	SD-CE	-10.62	1.53	1.79
9	I	25	ALA	CA-CB	-9.64	1.37	1.53
4	D	92	PRO	CB-CG	-9.59	1.13	1.51
9	I	43	LEU	N-CA	-9.08	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	177	ALA	CA-CB	-9.04	1.41	1.52
5	E	5	ILE	CA-C	-8.41	1.45	1.53
1	A	335	MET	SD-CE	-8.30	1.58	1.79
2	B	86	THR	CA-CB	-7.83	1.41	1.53
6	F	46	ALA	CA-CB	-7.69	1.41	1.53
7	G	3	GLN	N-CA	7.69	1.56	1.46
1	A	324	PHE	CA-C	-7.54	1.43	1.52
2	B	105	MET	SD-CE	-7.46	1.60	1.79
2	B	309	VAL	CA-C	-7.37	1.43	1.52
11	K	45	VAL	CA-C	7.36	1.60	1.52
2	B	278	VAL	CA-CB	-7.25	1.45	1.54
1	A	309	THR	CA-CB	-7.17	1.42	1.53
4	D	232	SER	CA-C	-7.16	1.44	1.52
2	B	436	ILE	N-CA	7.15	1.55	1.46
3	C	26	ASN	CB-CG	-7.13	1.34	1.52
2	B	309	VAL	CA-CB	-7.04	1.45	1.55
2	B	370	MET	SD-CE	-6.95	1.62	1.79
1	A	250	LEU	N-CA	6.89	1.54	1.46
2	B	314	ALA	CA-C	-6.62	1.44	1.52
5	E	62	MET	SD-CE	-6.50	1.63	1.79
2	B	170	ASN	N-CA	-6.45	1.37	1.46
2	B	259	ALA	CA-CB	-6.36	1.42	1.53
9	I	42	VAL	CA-C	-6.35	1.44	1.52
3	C	318	ARG	CA-C	6.34	1.59	1.52
2	B	237	ALA	CA-CB	-6.31	1.45	1.53
1	A	254	ALA	CA-CB	-6.24	1.43	1.53
2	B	27	THR	CA-CB	-6.23	1.42	1.53
3	C	257	THR	CA-CB	6.19	1.63	1.53
2	B	133	ARG	C-O	6.19	1.31	1.23
2	B	426	ALA	CA-CB	-6.19	1.43	1.53
2	B	244	ILE	CA-CB	-6.18	1.46	1.54
1	A	251	ALA	CA-C	-6.15	1.44	1.52
2	B	96	LEU	CA-C	-6.12	1.45	1.52
2	B	412	ASN	CA-C	6.08	1.60	1.52
2	B	183	ILE	CA-CB	-6.01	1.44	1.53
1	A	300	THR	CB-CG2	-6.00	1.32	1.52
9	I	10	PRO	C-O	-5.97	1.16	1.23
2	B	131	GLU	CA-C	5.94	1.60	1.52
11	K	45	VAL	CA-CB	5.93	1.61	1.54
10	J	41	ALA	C-O	-5.92	1.17	1.24
1	A	84	ALA	CA-CB	-5.89	1.43	1.53
7	G	73	ASN	CA-C	5.87	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	211	ILE	CA-CB	-5.84	1.46	1.54
2	B	127	THR	CA-C	-5.80	1.44	1.52
2	B	170	ASN	CA-C	-5.80	1.45	1.52
1	A	258	GLU	CA-C	-5.76	1.45	1.52
1	A	237	THR	CA-CB	-5.76	1.44	1.53
2	B	204	MET	SD-CE	-5.74	1.65	1.79
3	C	214	ASP	C-O	-5.74	1.16	1.24
1	A	106	LEU	CA-C	5.59	1.59	1.52
3	C	308	HIS	CA-CB	-5.59	1.44	1.53
6	F	23	ALA	CA-CB	-5.54	1.44	1.53
2	B	138	ALA	CA-CB	-5.51	1.44	1.53
1	A	252	HIS	C-O	5.49	1.30	1.24
2	B	97	SER	CA-C	-5.49	1.46	1.52
1	A	302	LYS	CA-C	-5.48	1.46	1.53
1	A	385	THR	CA-CB	-5.45	1.45	1.53
2	B	51	ILE	CA-CB	-5.45	1.47	1.54
2	B	147	ASP	CA-CB	-5.43	1.45	1.53
2	B	108	THR	C-O	5.41	1.30	1.23
2	B	325	TYR	CA-C	5.40	1.59	1.52
2	B	175	SER	CA-CB	-5.39	1.45	1.53
3	C	115	ILE	CA-CB	-5.36	1.47	1.54
3	C	19	ILE	CA-CB	-5.26	1.47	1.54
5	E	63	SER	CA-C	5.25	1.57	1.52
2	B	169	ARG	CA-C	-5.22	1.45	1.52
1	A	281	ASP	CB-CG	-5.21	1.39	1.52
2	B	47	ILE	CA-CB	-5.20	1.48	1.54
4	D	233	ARG	CA-C	-5.18	1.45	1.52
2	B	197	ASN	CB-CG	-5.18	1.39	1.52
2	B	203	ARG	CA-C	-5.16	1.46	1.52
3	C	27	ILE	CA-CB	-5.16	1.48	1.54
3	C	89	MET	SD-CE	-5.14	1.66	1.79
3	C	211	ILE	N-CA	-5.13	1.40	1.46
2	B	99	THR	CA-C	-5.09	1.46	1.52
2	B	410	VAL	CA-CB	-5.08	1.48	1.54
7	G	3	GLN	C-O	-5.07	1.17	1.24
5	E	185	TYR	CA-C	5.06	1.59	1.52

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	91	PHE	C-N-CD	-23.89	68.03	120.60
3	C	221	HIS	O-C-N	-16.20	102.69	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	42	VAL	O-C-N	15.53	141.98	122.57
2	B	234	GLY	N-CA-C	14.99	128.86	111.63
4	D	91	PHE	CA-C-N	13.58	159.59	127.00
4	D	91	PHE	C-N-CA	13.58	159.59	127.00
4	D	168	VAL	O-C-N	13.26	139.15	122.57
8	H	53	ASP	N-CA-C	11.79	127.18	113.15
5	E	78	LEU	N-CA-C	10.72	126.69	113.50
2	B	235	ALA	N-CA-C	-10.57	99.98	113.72
9	I	44	ASP	N-CA-C	-10.38	95.15	110.52
4	D	92	PRO	CA-N-CD	-10.23	97.18	111.50
2	B	305	GLN	O-C-N	-9.72	110.14	121.32
2	B	304	HIS	O-C-N	9.59	135.47	123.01
3	C	171	ASP	N-CA-C	9.32	116.42	108.78
9	I	36	ALA	N-CA-C	9.32	124.57	109.94
9	I	26	LEU	N-CA-C	9.16	124.39	109.72
5	E	187	PHE	CB-CA-C	-8.91	103.26	114.40
4	D	4	GLU	N-CA-C	8.59	119.98	108.38
6	F	85	GLU	N-CA-C	-8.53	92.64	110.80
4	D	167	GLU	O-C-N	8.40	131.78	123.04
5	E	2	HIS	N-CA-C	-8.32	103.14	113.20
9	I	32	ALA	N-CA-C	-8.07	102.68	114.39
5	E	66	ALA	N-CA-C	-8.05	101.31	112.25
4	D	145	GLU	O-C-N	8.04	133.27	122.82
4	D	171	PHE	N-CA-C	8.03	127.91	110.80
2	B	305	GLN	N-CA-C	8.02	127.53	109.81
1	A	51	LYS	N-CA-C	-8.01	95.51	108.41
4	D	167	GLU	N-CA-C	7.96	119.10	107.88
3	C	243	VAL	N-CA-C	7.94	120.97	111.05
4	D	135	CYS	N-CA-C	7.83	121.66	109.52
3	C	157	GLY	N-CA-C	7.78	122.06	112.64
9	I	7	ARG	N-CA-C	-7.65	102.81	113.37
5	E	79	SER	N-CA-C	-7.39	104.27	113.28
5	E	5	ILE	N-CA-C	7.37	117.84	107.37
1	A	285	GLY	N-CA-C	-7.29	101.11	112.85
3	C	345	HIS	N-CA-C	7.27	125.88	109.81
5	E	23	LYS	N-CA-C	7.20	120.68	109.52
2	B	435	PHE	N-CA-C	7.15	121.71	112.92
1	A	351	GLU	N-CA-C	7.05	119.86	111.33
8	H	27	LEU	N-CA-C	7.00	125.72	110.80
5	E	63	SER	N-CA-C	6.97	121.67	112.13
1	A	220	SER	N-CA-C	6.96	125.62	110.80
11	K	47	THR	N-CA-C	6.94	120.23	107.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	225	THR	N-CA-C	-6.92	103.67	111.14
8	H	66	ASP	N-CA-C	6.92	118.82	111.28
4	D	24	THR	N-CA-C	-6.91	103.53	112.23
7	G	34	ILE	N-CA-CB	6.87	115.12	110.52
2	B	304	HIS	CA-C-N	6.80	138.41	121.80
2	B	304	HIS	C-N-CA	6.80	138.41	121.80
9	I	35	PRO	N-CA-C	-6.72	98.63	112.47
1	A	192	ALA	N-CA-C	6.65	124.51	109.81
11	K	48	ILE	N-CA-C	6.59	123.04	109.34
5	E	108	GLN	N-CA-C	-6.58	105.07	113.23
4	D	167	GLU	CA-C-N	6.54	133.74	121.97
4	D	167	GLU	C-N-CA	6.54	133.74	121.97
4	D	69	GLU	N-CA-C	6.53	118.88	109.14
3	C	185	LEU	N-CA-C	6.51	121.60	112.75
10	J	4	THR	N-CA-C	6.51	124.66	110.80
1	A	443	TRP	N-CA-C	6.50	120.10	109.24
4	D	232	SER	N-CA-C	-6.50	98.14	108.73
5	E	98	VAL	N-CA-C	6.48	115.94	106.55
4	D	186	VAL	CB-CA-C	-6.47	103.68	111.97
11	K	42	LEU	N-CA-C	6.39	124.41	110.80
5	E	168	SER	N-CA-C	-6.34	104.78	114.16
4	D	139	THR	N-CA-C	6.33	118.93	109.25
9	I	52	ARG	N-CA-C	6.30	119.28	109.52
3	C	272	TRP	N-CA-C	6.27	119.78	111.75
6	F	59	VAL	N-CA-CB	6.26	119.06	110.54
9	I	24	GLY	N-CA-C	6.12	127.68	113.18
11	K	4	ARG	N-CA-C	-6.11	105.79	113.18
5	E	174	GLY	N-CA-C	6.05	124.68	112.34
9	I	42	VAL	N-CA-CB	6.00	121.14	111.23
1	A	48	GLU	N-CA-C	6.00	119.72	110.42
7	G	34	ILE	N-CA-C	5.99	120.15	112.67
6	F	59	VAL	N-CA-C	5.98	116.72	110.62
1	A	266	ASP	N-CA-C	5.96	120.06	113.21
4	D	37	CYS	N-CA-C	5.92	117.82	111.36
3	C	347	TYR	N-CA-C	5.88	119.28	111.75
9	I	42	VAL	CB-CA-C	5.88	120.93	111.29
1	A	159	GLN	N-CA-C	5.83	123.21	110.80
4	D	177	ALA	N-CA-C	5.80	118.88	107.98
5	E	70	ALA	N-CA-C	5.75	121.55	113.56
1	A	46	ARG	N-CA-C	-5.70	106.17	113.01
5	E	110	ALA	N-CA-C	-5.67	106.41	113.15
5	E	127	VAL	N-CA-C	5.65	117.00	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	78	LYS	N-CA-C	-5.64	102.05	110.23
11	K	45	VAL	CB-CA-C	5.62	121.59	111.36
5	E	150	ALA	N-CA-C	5.61	119.43	112.47
2	B	197	ASN	N-CA-C	5.61	120.40	113.50
2	B	232	LEU	N-CA-C	5.60	117.98	109.63
2	B	309	VAL	CB-CA-C	-5.60	101.10	111.18
2	B	40	ASN	N-CA-C	-5.59	100.17	109.46
7	G	1	GLY	O-C-N	5.59	131.95	123.00
3	C	142	GLY	N-CA-C	-5.58	105.62	112.77
11	K	39	ARG	N-CA-C	-5.58	105.51	112.93
9	I	33	ALA	N-CA-C	-5.55	106.00	112.89
4	D	91	PHE	CA-C-O	-5.54	115.06	119.71
1	A	445	ARG	CB-CA-C	-5.53	102.16	110.90
2	B	78	LYS	CA-C-N	-5.53	114.38	122.46
2	B	78	LYS	C-N-CA	-5.53	114.38	122.46
1	A	421	ALA	N-CA-C	-5.52	99.73	108.73
1	A	389	ARG	CA-C-N	-5.50	118.86	122.60
1	A	389	ARG	C-N-CA	-5.50	118.86	122.60
2	B	305	GLN	CA-CB-CG	-5.48	103.14	114.10
5	E	92	ARG	N-CA-C	-5.46	106.56	113.23
1	A	305	GLN	N-CA-C	-5.45	107.17	113.88
8	H	47	ARG	N-CA-C	5.45	115.22	108.19
1	A	389	ARG	N-CA-C	-5.41	99.58	108.41
3	C	223	TYR	N-CA-C	5.41	122.32	110.80
4	D	212	MET	N-CA-C	-5.40	105.39	111.28
4	D	19	SER	N-CA-C	5.40	116.25	107.23
6	F	39	GLU	N-CA-C	5.37	117.91	108.56
4	D	21	LEU	N-CA-C	-5.36	99.39	110.80
4	D	168	VAL	CB-CA-C	5.30	119.99	111.29
3	C	213	SER	N-CA-C	5.29	119.71	112.88
4	D	75	ASN	N-CA-C	-5.28	102.47	110.28
5	E	101	ARG	N-CA-C	5.27	117.41	108.02
7	G	49	ALA	N-CA-C	5.27	121.45	109.81
8	H	10	GLU	N-CA-C	-5.26	106.92	113.55
3	C	206	ASN	N-CA-C	-5.26	102.20	110.36
4	D	28	ARG	N-CA-C	-5.25	105.63	111.36
1	A	263	ALA	N-CA-C	5.25	117.69	111.33
4	D	145	GLU	N-CA-C	5.24	116.80	108.67
7	G	2	ARG	O-C-N	-5.23	115.64	122.59
5	E	74	ILE	N-CA-C	5.22	120.19	109.34
4	D	224	ARG	NE-CZ-NH2	5.20	123.88	119.20
7	G	50	PRO	N-CA-C	5.18	117.02	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	145	VAL	CA-C-N	5.18	126.31	119.84
5	E	145	VAL	C-N-CA	5.18	126.31	119.84
2	B	422	LYS	N-CA-C	5.17	118.08	110.59
2	B	437	ASP	CB-CA-C	-5.14	102.21	110.74
2	B	261	SER	CB-CA-C	-5.13	109.05	116.54
2	B	176	LEU	N-CA-C	-5.13	106.97	113.18
6	F	53	ASN	N-CA-C	5.12	117.27	111.02
1	A	50	GLU	N-CA-C	-5.11	99.91	110.80
5	E	146	PRO	N-CA-C	5.11	122.99	112.47
5	E	164	HIS	N-CA-C	5.10	117.28	109.07
1	A	348	SER	N-CA-C	5.10	119.06	111.87
4	D	144	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	A	55	ALA	N-CA-C	5.09	117.22	111.11
1	A	63	ALA	N-CA-C	5.08	117.48	111.33
5	E	130	PRO	N-CA-C	5.08	122.93	112.47
11	K	46	PRO	N-CA-C	5.06	122.89	112.47
2	B	394	PRO	O-C-N	5.04	123.63	121.31
3	C	268	ILE	N-CA-C	5.04	119.82	109.34
2	B	435	PHE	CB-CA-C	-5.04	102.05	110.56
3	C	22	PRO	CA-C-O	-5.01	115.06	120.92

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	171	PHE	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	221	HIS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3458	0	3356	79	0
2	B	3172	0	3152	92	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2996	0	3058	61	0
4	D	1919	0	1867	90	0
5	E	1519	0	1505	73	0
6	F	911	0	904	25	0
7	G	628	0	636	19	0
8	H	575	0	550	15	0
9	I	406	0	437	65	0
10	J	473	0	484	26	0
11	K	387	0	400	20	0
12	C	86	0	60	3	0
12	D	43	0	30	7	0
13	E	4	0	0	1	0
All	All	16577	0	16439	495	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 15.

All (495) 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:B:305:GLN:NE2	2:B:305:GLN:HA	1.52	1.10
5:E:52:LYS:HE2	11:K:35:ALA:HA	1.22	1.10
7:G:73:ASN:HB3	7:G:74:PRO:HD3	1.28	1.08
4:D:167:GLU:HG2	4:D:169:LEU:HD23	1.08	1.05
4:D:167:GLU:HG2	4:D:169:LEU:CD2	1.86	1.05
11:K:43:ASP:O	11:K:44:TRP:HB2	1.56	1.03
2:B:305:GLN:HA	2:B:305:GLN:HE21	1.02	1.00
2:B:76:THR:HG22	2:B:82:SER:H	1.26	0.98
1:A:325:VAL:HG21	9:I:43:LEU:HD12	1.46	0.97
3:C:214:ASP:OD2	7:G:2:ARG:NH2	1.98	0.96
3:C:221:HIS:O	3:C:222:PRO:C	1.99	0.95
2:B:385:GLN:HE22	2:B:393:THR:H	1.13	0.92
12:C:381:HEM:HBA1	12:C:381:HEM:HH A	1.51	0.91
2:B:305:GLN:HE21	2:B:305:GLN:CA	1.83	0.89
3:C:78:ILE:HD12	5:E:57:GLN:HE22	1.35	0.89
3:C:221:HIS:O	3:C:223:TYR:N	2.06	0.88
7:G:27:PRO:O	7:G:29:TYR:N	2.08	0.87
9:I:34:VAL:HB	9:I:35:PRO:HD3	1.57	0.86
2:B:99:THR:HB	9:I:14:VAL:HG22	1.55	0.86
1:A:144:SER:HA	9:I:42:VAL:HB	1.56	0.85
1:A:51:LYS:O	1:A:52:ASN:HB2	1.73	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:2:ALA:O	10:J:4:THR:N	2.07	0.85
5:E:183:PRO:C	5:E:185:TYR:H	1.83	0.84
11:K:38:SER:HB3	11:K:43:ASP:HA	1.60	0.83
2:B:325:TYR:CD2	9:I:28:PRO:HD2	2.14	0.83
2:B:305:GLN:NE2	2:B:305:GLN:CA	2.39	0.82
10:J:2:ALA:HB1	10:J:3:PRO:HD2	1.62	0.81
5:E:52:LYS:HE2	11:K:35:ALA:CA	2.07	0.81
9:I:47:ARG:HG2	9:I:48:SER:H	1.46	0.80
5:E:137:GLY:HA3	5:E:145:VAL:HG13	1.62	0.80
1:A:60:GLU:OE2	2:B:287:ARG:NH2	2.15	0.78
7:G:73:ASN:HB3	7:G:74:PRO:CD	2.09	0.78
4:D:131:LEU:HD22	4:D:164:ILE:HD11	1.66	0.78
1:A:252:HIS:HD2	1:A:323:HIS:HE1	1.32	0.78
3:C:343:VAL:HG13	3:C:343:VAL:O	1.82	0.77
11:K:45:VAL:HG12	11:K:46:PRO:HD3	1.66	0.77
2:B:305:GLN:HB3	2:B:306:PRO:HD3	1.66	0.77
1:A:252:HIS:HE1	9:I:43:LEU:HB2	1.50	0.76
3:C:211:ILE:O	3:C:212:SER:HB2	1.84	0.75
2:B:245:ARG:NH2	2:B:433:THR:O	2.18	0.75
2:B:40:ASN:O	2:B:40:ASN:ND2	2.18	0.75
6:F:27:ASN:OD1	6:F:27:ASN:N	2.18	0.73
1:A:348:SER:HB3	11:K:17:TRP:HE1	1.53	0.73
4:D:164:ILE:O	4:D:166:ASN:N	2.20	0.73
9:I:6:ALA:C	9:I:8:SER:H	1.95	0.73
4:D:37:CYS:SG	12:D:242:HEM:HMC3	2.29	0.73
2:B:325:TYR:HB3	9:I:28:PRO:CD	2.18	0.73
7:G:73:ASN:CB	7:G:74:PRO:HD3	2.14	0.73
6:F:31:LEU:O	6:F:81:THR:HG21	1.88	0.73
10:J:10:TYR:HA	10:J:14:PHE:HB2	1.69	0.72
9:I:4:VAL:HG12	9:I:10:PRO:HG2	1.71	0.72
2:B:385:GLN:HE22	2:B:393:THR:N	1.86	0.72
4:D:167:GLU:CG	4:D:169:LEU:HD23	2.04	0.71
2:B:325:TYR:HB3	9:I:28:PRO:HD3	1.71	0.71
2:B:305:GLN:O	2:B:306:PRO:C	2.23	0.71
9:I:47:ARG:HG2	9:I:48:SER:N	2.05	0.71
1:A:252:HIS:CD2	1:A:323:HIS:HE1	2.09	0.70
2:B:308:ASP:HB2	9:I:32:ALA:HB2	1.74	0.70
2:B:305:GLN:HB3	2:B:306:PRO:CD	2.22	0.70
9:I:47:ARG:CG	9:I:48:SER:H	2.03	0.70
1:A:255:ILE:HD13	1:A:335:MET:HE1	1.72	0.70
4:D:166:ASN:O	4:D:167:GLU:HG3	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:20:SER:O	4:D:21:LEU:HB2	1.93	0.69
1:A:378:ASP:OD2	1:A:389:ARG:NH1	2.26	0.69
9:I:41:PRO:O	9:I:42:VAL:HG23	1.92	0.69
10:J:2:ALA:HB1	10:J:3:PRO:CD	2.23	0.69
2:B:169:ARG:HD3	2:B:240:HIS:HB3	1.74	0.68
3:C:343:VAL:O	3:C:343:VAL:CG1	2.41	0.68
2:B:76:THR:HG22	2:B:82:SER:N	2.06	0.68
5:E:132:TRP:HB3	5:E:187:PHE:HZ	1.58	0.68
2:B:176:LEU:HD21	9:I:13:PRO:HD3	1.76	0.67
4:D:27:ARG:NH2	10:J:58:LYS:HD3	2.11	0.66
8:H:11:GLU:O	8:H:12:GLU:HB2	1.95	0.66
4:D:97:ASN:HB2	4:D:98:PRO:CD	2.26	0.66
5:E:76:ILE:HB	5:E:193:VAL:HG13	1.77	0.66
1:A:252:HIS:CE1	9:I:43:LEU:HB2	2.31	0.66
1:A:146:ARG:H	9:I:42:VAL:HG12	1.61	0.65
2:B:435:PHE:O	2:B:436:ILE:HB	1.95	0.65
5:E:52:LYS:CE	11:K:35:ALA:HA	2.14	0.65
2:B:385:GLN:NE2	2:B:393:THR:H	1.91	0.65
9:I:43:LEU:HD22	9:I:46:LYS:HD3	1.77	0.65
3:C:78:ILE:HD12	5:E:57:GLN:NE2	2.09	0.65
10:J:46:ILE:O	10:J:46:ILE:HG23	1.97	0.65
6:F:37:ILE:HD12	6:F:43:VAL:HG21	1.79	0.65
5:E:183:PRO:C	5:E:185:TYR:N	2.54	0.64
5:E:139:CYS:HB2	5:E:158:CYS:SG	2.37	0.64
3:C:24:PRO:C	3:C:26:ASN:H	2.04	0.64
4:D:49:ARG:HG3	4:D:87:LEU:O	1.96	0.64
11:K:39:ARG:HG3	11:K:40:LEU:N	2.11	0.64
11:K:45:VAL:CG1	11:K:46:PRO:HD3	2.28	0.64
9:I:2:LEU:O	9:I:3:SER:HB3	1.98	0.63
4:D:138:PRO:HG3	8:H:58:LEU:HD22	1.81	0.63
7:G:28:HIS:HB3	7:G:31:SER:HB2	1.80	0.63
9:I:6:ALA:C	9:I:8:SER:N	2.57	0.63
1:A:145:MET:O	1:A:149:VAL:HG23	2.00	0.62
1:A:146:ARG:H	9:I:42:VAL:CG1	2.13	0.62
3:C:240:MET:HE2	3:C:240:MET:HA	1.81	0.62
2:B:315:SER:O	9:I:4:VAL:HG13	1.99	0.62
2:B:68:LEU:HD13	2:B:144:LEU:HD11	1.82	0.61
2:B:100:SER:O	9:I:13:PRO:HD2	2.01	0.61
3:C:181:PHE:HA	3:C:184:ILE:HG22	1.82	0.61
3:C:206:ASN:HD21	3:C:210:GLY:HA2	1.66	0.61
3:C:285:PRO:O	3:C:286:ASN:HB2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:56:TYR:HA	10:J:58:LYS:HZ1	1.66	0.60
6:F:28:LYS:HB3	6:F:74:ILE:HG12	1.83	0.60
9:I:46:LYS:HG2	9:I:47:ARG:N	2.17	0.60
10:J:41:ALA:O	10:J:44:GLU:HG2	2.02	0.60
3:C:211:ILE:HG21	6:F:62:ILE:HD12	1.84	0.60
4:D:121:HIS:C	4:D:123:GLY:H	2.09	0.60
3:C:145:VAL:HG21	3:C:268:ILE:HG21	1.84	0.60
4:D:75:ASN:O	4:D:77:ASP:N	2.35	0.60
4:D:147:LEU:HA	4:D:158:ILE:O	2.02	0.60
3:C:138:MET:HE1	3:C:268:ILE:HA	1.83	0.59
5:E:140:THR:HG21	5:E:178:LEU:HB2	1.84	0.59
2:B:290:ASN:OD1	9:I:31:GLN:NE2	2.35	0.59
9:I:15:LEU:HD13	9:I:16:SER:H	1.65	0.59
1:A:27:SER:HB3	1:A:208:LEU:HD12	1.84	0.59
2:B:354:ASN:H	2:B:355:PRO:HD2	1.68	0.59
4:D:97:ASN:HB2	4:D:98:PRO:HD3	1.84	0.59
5:E:113:GLU:HB3	5:E:116:GLN:HG3	1.85	0.59
5:E:112:VAL:HG13	5:E:113:GLU:N	2.16	0.59
1:A:34:THR:HG21	2:B:370:MET:HG3	1.85	0.59
1:A:149:VAL:HG21	1:A:252:HIS:HB3	1.82	0.59
2:B:283:PRO:HG3	9:I:31:GLN:HG3	1.85	0.59
5:E:156:TYR:HB3	5:E:165:TYR:HB2	1.85	0.59
2:B:204:MET:HE1	2:B:224:LEU:HD22	1.84	0.59
5:E:170:ARG:HD2	5:E:172:ARG:HH21	1.68	0.59
5:E:128:LYS:HB3	5:E:185:TYR:HE2	1.67	0.59
8:H:25:GLU:OE1	8:H:34:ARG:NH1	2.36	0.58
3:C:206:ASN:ND2	3:C:207:ASN:H	2.01	0.58
5:E:148:ALA:O	5:E:149:ASN:HB2	2.03	0.58
2:B:197:ASN:C	2:B:197:ASN:HD22	2.12	0.58
3:C:309:THR:HG21	3:C:367:PRO:O	2.04	0.58
4:D:158:ILE:HG23	4:D:159:GLY:N	2.18	0.58
12:D:242:HEM:HMC2	12:D:242:HEM:HBC2	1.85	0.58
5:E:129:LYS:N	5:E:185:TYR:OH	2.37	0.58
6:F:83:TYR:CE1	6:F:84:GLU:HG3	2.37	0.57
9:I:34:VAL:HB	9:I:35:PRO:CD	2.30	0.57
9:I:44:ASP:O	9:I:46:LYS:HB2	2.04	0.57
2:B:290:ASN:HD22	2:B:290:ASN:N	2.01	0.57
3:C:282:ARG:NH2	3:C:341:GLN:O	2.37	0.57
2:B:40:ASN:HD22	2:B:40:ASN:C	2.08	0.57
8:H:37:LEU:HD11	8:H:58:LEU:HA	1.87	0.57
2:B:153:GLN:NE2	9:I:46:LYS:HG3	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ILE:HD13	1:A:335:MET:CE	2.34	0.57
4:D:19:SER:H	4:D:202:LYS:HD3	1.70	0.57
10:J:2:ALA:C	10:J:4:THR:H	2.07	0.57
2:B:166:ALA:HB2	2:B:244:ILE:HG13	1.86	0.57
5:E:153:PHE:CD1	5:E:172:ARG:HD3	2.40	0.56
2:B:129:ALA:N	2:B:130:PRO:HD3	2.19	0.56
8:H:73:LEU:O	8:H:75:ASN:N	2.38	0.56
4:D:224:ARG:HB3	7:G:25:ALA:HB1	1.87	0.56
1:A:41:ILE:HG12	1:A:195:MET:HB3	1.86	0.56
5:E:187:PHE:N	5:E:187:PHE:CD2	2.74	0.56
8:H:12:GLU:OE2	8:H:12:GLU:HA	2.05	0.56
5:E:187:PHE:N	5:E:187:PHE:HD2	2.03	0.56
1:A:309:THR:O	9:I:52:ARG:NH1	2.39	0.56
1:A:343:MET:HE2	1:A:343:MET:HA	1.87	0.56
1:A:100:LYS:HD3	2:B:370:MET:HE3	1.87	0.56
5:E:18:VAL:HG12	5:E:18:VAL:O	2.06	0.56
1:A:388:ARG:NH2	1:A:394:GLU:OE2	2.39	0.55
4:D:167:GLU:OE2	4:D:169:LEU:HG	2.07	0.55
1:A:140:GLU:OE2	9:I:36:ALA:HB1	2.05	0.55
6:F:27:ASN:HA	6:F:81:THR:HG23	1.87	0.55
1:A:348:SER:HB3	11:K:17:TRP:NE1	2.21	0.55
4:D:121:HIS:O	4:D:123:GLY:N	2.38	0.55
4:D:168:VAL:O	4:D:168:VAL:CG1	2.54	0.55
4:D:151:PRO:O	4:D:152:TYR:HB2	2.07	0.55
6:F:53:ASN:N	6:F:53:ASN:HD22	2.05	0.55
4:D:165:TYR:O	4:D:167:GLU:N	2.37	0.54
9:I:39:GLU:O	9:I:40:SER:HB3	2.07	0.54
4:D:169:LEU:HD21	4:D:177:ALA:HB3	1.88	0.54
9:I:18:THR:OG1	9:I:53:GLU:OE2	2.17	0.54
10:J:19:THR:O	10:J:23:THR:HG23	2.07	0.54
3:C:30:TRP:HZ3	3:C:96:MET:HG3	1.73	0.54
4:D:14:HIS:HB3	4:D:21:LEU:HA	1.89	0.54
5:E:96:LEU:HD21	5:E:195:VAL:HG11	1.90	0.54
11:K:39:ARG:HG3	11:K:40:LEU:H	1.71	0.54
3:C:244:LEU:O	4:D:201:ARG:NE	2.40	0.54
4:D:169:LEU:HD11	4:D:177:ALA:HB3	1.89	0.54
9:I:44:ASP:O	9:I:45:LEU:C	2.50	0.54
11:K:43:ASP:O	11:K:44:TRP:CB	2.43	0.54
4:D:161:ALA:O	4:D:163:PRO:HD3	2.08	0.53
8:H:25:GLU:HG3	8:H:61:PHE:HZ	1.73	0.53
2:B:37:SER:HB3	2:B:216:LEU:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:33:PHE:CZ	3:C:96:MET:HG2	2.43	0.53
5:E:98:VAL:HG22	5:E:134:ILE:HG23	1.90	0.53
3:C:136:GLY:H	3:C:139:SER:HB2	1.73	0.53
4:D:12:TRP:NE1	4:D:125:ASP:OD2	2.26	0.53
5:E:64:ALA:O	5:E:65:SER:OG	2.22	0.53
1:A:294:LEU:HG	1:A:307:PHE:CE1	2.44	0.53
4:D:40:CYS:SG	12:D:242:HEM:HMB3	2.48	0.53
4:D:160:MET:O	4:D:161:ALA:CB	2.56	0.53
5:E:123:ASP:O	5:E:127:VAL:HG12	2.08	0.53
4:D:168:VAL:O	4:D:168:VAL:HG12	2.08	0.53
9:I:46:LYS:HG2	9:I:47:ARG:H	1.74	0.53
4:D:52:VAL:HG12	4:D:53:GLY:N	2.24	0.53
2:B:161:GLU:OE1	2:B:175:SER:OG	2.14	0.53
3:C:222:PRO:HB3	4:D:226:LYS:HD3	1.91	0.53
2:B:70:ARG:HG3	2:B:98:VAL:HG22	1.91	0.53
2:B:156:GLN:HG2	9:I:27:ARG:CD	2.39	0.52
11:K:45:VAL:CB	11:K:46:PRO:HD3	2.39	0.52
1:A:351:GLU:H	11:K:12:GLN:NE2	2.07	0.52
5:E:15:ARG:HH11	5:E:32:ARG:HG2	1.75	0.52
2:B:388:ALA:HB3	9:I:2:LEU:HD13	1.92	0.52
4:D:72:ASP:OD1	4:D:73:GLY:N	2.40	0.52
1:A:85:HIS:ND1	2:B:370:MET:HE1	2.25	0.52
2:B:71:LEU:HD23	9:I:15:LEU:HG	1.91	0.52
4:D:133:GLY:HA2	8:H:21:ARG:HH22	1.75	0.52
2:B:305:GLN:HE21	2:B:305:GLN:C	2.16	0.52
5:E:138:VAL:O	5:E:139:CYS:HB3	2.09	0.52
4:D:211:MET:HA	4:D:211:MET:HE2	1.91	0.52
9:I:20:ARG:NH1	9:I:48:SER:OG	2.43	0.52
1:A:237:THR:OG1	5:E:14:ARG:NH2	2.43	0.52
4:D:160:MET:HG3	12:D:242:HEM:C1B	2.45	0.52
5:E:127:VAL:HB	5:E:133:VAL:HB	1.92	0.52
5:E:136:ILE:HD13	5:E:137:GLY:H	1.74	0.52
4:D:165:TYR:C	4:D:167:GLU:H	2.18	0.52
5:E:101:ARG:HH22	5:E:109:GLU:HG3	1.75	0.52
3:C:137:GLN:HE21	3:C:265:PRO:HG3	1.74	0.51
5:E:153:PHE:HD2	5:E:153:PHE:N	2.08	0.51
7:G:18:LEU:HB3	7:G:23:GLN:NE2	2.26	0.51
4:D:49:ARG:HA	4:D:52:VAL:HG23	1.91	0.51
7:G:27:PRO:O	7:G:28:HIS:C	2.54	0.51
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.45	0.51
5:E:141:HIS:HB2	5:E:176:ALA:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:28:ARG:O	4:D:32:VAL:HG23	2.11	0.51
4:D:31:GLN:NE2	4:D:172:ASP:OD1	2.43	0.51
5:E:127:VAL:HG23	5:E:185:TYR:CE1	2.46	0.51
4:D:160:MET:HG3	12:D:242:HEM:NB	2.26	0.51
2:B:294:SER:CB	2:B:343:GLN:HE21	2.24	0.51
6:F:22:ASN:HA	6:F:27:ASN:HD21	1.76	0.51
9:I:51:CYS:SG	9:I:52:ARG:N	2.85	0.51
6:F:49:ARG:NH2	6:F:100:GLU:OE2	2.41	0.50
2:B:288:GLY:O	2:B:290:ASN:ND2	2.44	0.50
5:E:101:ARG:HG3	5:E:131:GLU:C	2.37	0.50
1:A:281:ASP:HB3	1:A:284:TYR:CE1	2.45	0.50
9:I:11:PHE:HZ	9:I:27:ARG:HH21	1.58	0.50
9:I:55:LEU:O	9:I:56:ARG:HB2	2.10	0.50
1:A:354:VAL:HG21	1:A:404:ALA:HA	1.94	0.50
3:C:246:ALA:HB1	3:C:249:LEU:HB2	1.94	0.50
1:A:378:ASP:OD1	9:I:56:ARG:NH1	2.45	0.49
4:D:56:TYR:HA	10:J:58:LYS:NZ	2.27	0.49
3:C:119:LEU:O	3:C:123:VAL:HG12	2.12	0.49
4:D:161:ALA:C	4:D:163:PRO:HD3	2.38	0.49
5:E:122:HIS:HD2	5:E:124:LEU:HB2	1.76	0.49
1:A:284:TYR:HE1	9:I:20:ARG:HG2	1.76	0.49
1:A:369:LEU:HD12	1:A:392:LEU:HD21	1.94	0.49
3:C:343:VAL:HG22	3:C:348:ILE:HG12	1.94	0.49
1:A:34:THR:HG22	1:A:35:CYS:N	2.28	0.49
2:B:124:LEU:HD11	2:B:219:VAL:HG13	1.95	0.49
2:B:369:LEU:HD11	2:B:399:LEU:HD11	1.95	0.49
5:E:184:SER:C	5:E:186:GLU:H	2.20	0.49
3:C:147:THR:HG23	3:C:164:ILE:HD11	1.94	0.49
5:E:129:LYS:O	5:E:131:GLU:N	2.46	0.49
10:J:2:ALA:CB	10:J:3:PRO:CD	2.91	0.49
2:B:264:ILE:HG12	9:I:2:LEU:HD23	1.95	0.48
5:E:145:VAL:O	5:E:147:ILE:N	2.45	0.48
5:E:153:PHE:N	5:E:153:PHE:CD2	2.80	0.48
7:G:41:THR:O	7:G:45:ILE:HG12	2.13	0.48
2:B:436:ILE:O	2:B:437:ASP:C	2.55	0.48
1:A:65:LYS:HE3	1:A:130:GLU:OE1	2.13	0.48
2:B:69:LEU:HD13	2:B:105:MET:HE1	1.95	0.48
4:D:160:MET:O	4:D:161:ALA:HB2	2.13	0.48
5:E:132:TRP:CB	5:E:187:PHE:HZ	2.24	0.48
4:D:163:PRO:C	4:D:164:ILE:HG13	2.38	0.48
7:G:34:ILE:HA	7:G:37:VAL:HG13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:10:PRO:O	9:I:25:ALA:CB	2.61	0.48
5:E:183:PRO:O	5:E:185:TYR:N	2.47	0.48
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.96	0.48
6:F:12:TRP:O	6:F:16:ILE:HG12	2.13	0.48
10:J:2:ALA:CB	10:J:3:PRO:HD2	2.38	0.48
9:I:21:GLY:O	9:I:47:ARG:NH2	2.46	0.48
9:I:46:LYS:CG	9:I:47:ARG:H	2.25	0.48
1:A:446:PHE:OXT	10:J:17:THR:HB	2.13	0.47
1:A:29:GLN:HG2	2:B:18:PRO:HG3	1.96	0.47
1:A:70:ARG:NH1	1:A:115:ASP:OD2	2.44	0.47
2:B:76:THR:HG23	2:B:136:GLU:OE1	2.14	0.47
1:A:417:ASP:OD1	1:A:438:ARG:NH2	2.47	0.47
4:D:101:ALA:HB1	4:D:110:PRO:HD2	1.96	0.47
8:H:13:LEU:HD23	8:H:13:LEU:HA	1.60	0.47
2:B:325:TYR:CG	9:I:28:PRO:HD2	2.48	0.47
4:D:220:TYR:CE2	4:D:224:ARG:HD3	2.49	0.47
1:A:219:LEU:O	1:A:221:GLY:N	2.48	0.47
4:D:229:VAL:HG22	7:G:20:PRO:HD3	1.95	0.47
6:F:78:GLU:H	6:F:78:GLU:HG3	1.51	0.47
10:J:49:GLY:O	10:J:50:LYS:C	2.57	0.47
2:B:68:LEU:HD23	2:B:186:VAL:HG22	1.97	0.47
4:D:211:MET:HA	4:D:211:MET:CE	2.45	0.47
6:F:67:ASP:OD1	6:F:71:ARG:NH2	2.47	0.47
3:C:279:ALA:O	3:C:283:SER:OG	2.31	0.47
6:F:7:SER:OG	6:F:8:ALA:N	2.48	0.47
6:F:35:ASP:OD2	6:F:89:TYR:OH	2.29	0.47
2:B:258:VAL:HG12	2:B:423:SER:HB2	1.97	0.46
5:E:40:THR:O	5:E:44:THR:HG23	2.15	0.46
5:E:153:PHE:O	5:E:155:GLY:N	2.48	0.46
4:D:52:VAL:O	4:D:53:GLY:C	2.57	0.46
5:E:163:SER:HB2	5:E:175:PRO:HB2	1.97	0.46
1:A:420:PRO:HD2	1:A:434:TYR:OH	2.15	0.46
4:D:120:ARG:HE	12:D:242:HEM:CGD	2.29	0.46
10:J:46:ILE:O	10:J:46:ILE:CG2	2.63	0.46
2:B:418:VAL:O	2:B:422:LYS:NZ	2.48	0.46
3:C:156:ILE:HG22	3:C:160:LEU:HG	1.96	0.46
3:C:190:MET:O	3:C:191:ALA:C	2.58	0.46
5:E:6:LYS:H	5:E:6:LYS:HD3	1.80	0.46
2:B:250:ASP:C	2:B:252:LEU:H	2.23	0.46
1:A:73:ASN:HD21	1:A:77:LYS:HE3	1.81	0.46
1:A:252:HIS:CD2	1:A:323:HIS:CE1	2.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:ASP:OD1	9:I:56:ARG:CZ	2.64	0.46
2:B:67:HIS:O	2:B:68:LEU:C	2.58	0.46
9:I:2:LEU:H	9:I:2:LEU:HG	1.61	0.46
3:C:254:ASP:OD2	3:C:255:ASN:N	2.39	0.46
6:F:61:ARG:O	6:F:62:ILE:C	2.59	0.46
8:H:11:GLU:O	8:H:12:GLU:CB	2.63	0.46
4:D:56:TYR:CE1	4:D:64:LEU:HD11	2.51	0.45
5:E:136:ILE:HG21	5:E:181:GLU:HB3	1.99	0.45
2:B:122:PHE:O	2:B:126:VAL:HG23	2.15	0.45
11:K:38:SER:CB	11:K:43:ASP:HA	2.37	0.45
6:F:53:ASN:ND2	6:F:54:LEU:H	2.15	0.45
5:E:156:TYR:HB3	5:E:165:TYR:CB	2.46	0.45
12:C:381:HEM:HBA1	12:C:381:HEM:CHA	2.29	0.45
1:A:264:HIS:HA	1:A:265:PRO:HD3	1.86	0.45
1:A:294:LEU:HG	1:A:307:PHE:CZ	2.52	0.45
1:A:378:ASP:OD2	9:I:56:ARG:NH2	2.49	0.45
2:B:109:VAL:HG22	2:B:119:LEU:HD13	1.98	0.45
3:C:4:ILE:H	3:C:4:ILE:HG12	1.51	0.45
3:C:185:LEU:HD23	3:C:185:LEU:HA	1.81	0.45
5:E:128:LYS:HB3	5:E:185:TYR:CE2	2.50	0.45
1:A:307:PHE:C	1:A:307:PHE:CD2	2.94	0.45
2:B:393:THR:HG21	2:B:401:GLN:HE22	1.82	0.45
4:D:136:GLU:H	4:D:136:GLU:CD	2.22	0.45
4:D:164:ILE:HG22	4:D:179:MET:HB2	1.97	0.45
1:A:350:THR:O	1:A:353:GLU:HG2	2.16	0.44
4:D:43:MET:HE3	4:D:46:VAL:HB	1.99	0.44
4:D:56:TYR:CD1	4:D:64:LEU:HD11	2.52	0.44
9:I:26:LEU:C	9:I:27:ARG:HG3	2.42	0.44
2:B:435:PHE:O	2:B:436:ILE:CB	2.61	0.44
1:A:270:LEU:HD23	1:A:270:LEU:HA	1.85	0.44
1:A:38:GLY:HA2	1:A:113:LEU:HD21	1.99	0.44
2:B:294:SER:HB3	2:B:343:GLN:HE21	1.83	0.44
2:B:385:GLN:HG2	9:I:2:LEU:HD12	1.99	0.44
4:D:51:LEU:HD11	4:D:91:PHE:HZ	1.82	0.44
1:A:146:ARG:HH12	1:A:308:GLN:NE2	2.16	0.44
5:E:161:HIS:CD2	5:E:161:HIS:N	2.83	0.44
8:H:40:CYS:O	8:H:44:VAL:HG23	2.16	0.44
2:B:290:ASN:OD1	9:I:31:GLN:CD	2.61	0.44
3:C:82:MET:HG2	3:C:240:MET:HE1	1.99	0.44
8:H:17:LEU:HG	8:H:21:ARG:HD2	2.00	0.44
10:J:48:GLU:C	10:J:50:LYS:N	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:132:VAL:HA	3:C:139:SER:HB3	2.00	0.44
9:I:39:GLU:O	9:I:40:SER:CB	2.66	0.44
4:D:167:GLU:CG	4:D:169:LEU:CD2	2.76	0.44
5:E:141:HIS:HB3	13:E:197:FES:S1	2.57	0.44
4:D:165:TYR:C	4:D:167:GLU:N	2.76	0.44
3:C:36:LEU:HD22	3:C:235:LEU:HB2	2.00	0.43
4:D:27:ARG:CZ	10:J:58:LYS:HD3	2.48	0.43
10:J:41:ALA:O	10:J:42:ILE:C	2.59	0.43
1:A:142:ASP:OD1	5:E:1:SER:HB3	2.19	0.43
1:A:329:MET:HE3	1:A:329:MET:HB3	1.83	0.43
2:B:325:TYR:HB3	9:I:28:PRO:HD2	1.97	0.43
5:E:145:VAL:HA	5:E:146:PRO:HD2	1.67	0.43
9:I:55:LEU:HB3	9:I:56:ARG:H	1.24	0.43
1:A:373:THR:HB	1:A:374:PRO:HD3	1.98	0.43
2:B:67:HIS:O	2:B:70:ARG:N	2.51	0.43
3:C:116:GLY:C	12:C:381:HEM:HBC2	2.42	0.43
1:A:158:PHE:O	1:A:164:ALA:HB2	2.18	0.43
3:C:237:LEU:HD13	4:D:212:MET:HG2	2.01	0.43
3:C:328:LEU:HD23	3:C:328:LEU:HA	1.87	0.43
4:D:27:ARG:HB2	4:D:55:CYS:HB2	2.01	0.43
4:D:33:TYR:HA	4:D:37:CYS:HB2	2.00	0.43
1:A:220:SER:O	1:A:221:GLY:C	2.61	0.43
2:B:39:GLU:OE2	2:B:113:ARG:NH2	2.50	0.43
4:D:32:VAL:HG11	4:D:186:VAL:HG22	2.01	0.43
8:H:37:LEU:O	8:H:41:ASP:HB2	2.18	0.43
5:E:19:LEU:HD23	5:E:19:LEU:HA	1.89	0.43
5:E:29:SER:O	5:E:33:LYS:HG2	2.18	0.43
5:E:45:VAL:HG13	10:J:28:ALA:HA	2.01	0.43
11:K:23:LEU:HD12	11:K:23:LEU:HA	1.79	0.43
10:J:18:SER:HA	11:K:24:TRP:CZ3	2.53	0.43
1:A:110:VAL:HG11	1:A:211:LEU:HB3	2.00	0.43
1:A:280:TYR:CG	1:A:281:ASP:N	2.87	0.43
2:B:322:PHE:CG	2:B:323:GLY:N	2.86	0.43
8:H:73:LEU:HB3	8:H:74:PHE:H	1.65	0.43
1:A:252:HIS:HD2	1:A:323:HIS:CE1	2.23	0.42
3:C:241:LEU:HD12	3:C:241:LEU:HA	1.89	0.42
2:B:59:ASN:OD1	2:B:59:ASN:C	2.62	0.42
2:B:68:LEU:HD12	2:B:68:LEU:HA	1.62	0.42
2:B:361:LYS:O	2:B:365:LYS:HG3	2.19	0.42
5:E:122:HIS:CD2	5:E:124:LEU:HB2	2.54	0.42
2:B:24:LEU:C	2:B:24:LEU:HD23	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:289:SER:O	2:B:290:ASN:HB2	2.20	0.42
4:D:148:TYR:HB2	4:D:158:ILE:HG22	2.01	0.42
5:E:97:PHE:CZ	5:E:145:VAL:HG12	2.55	0.42
5:E:190:ASP:OD2	5:E:191:ASP:N	2.50	0.42
1:A:187:SER:O	1:A:223:TYR:OH	2.33	0.42
3:C:78:ILE:H	3:C:78:ILE:HG12	1.54	0.42
5:E:94:LYS:HB3	5:E:136:ILE:HD11	2.00	0.42
1:A:219:LEU:HB3	1:A:220:SER:H	1.73	0.42
1:A:442:PHE:CD2	1:A:442:PHE:C	2.97	0.42
3:C:40:CYS:HB3	3:C:90:PHE:CD2	2.55	0.42
4:D:95:TYR:HA	4:D:96:PRO:HD2	1.87	0.42
5:E:65:SER:C	5:E:67:ASP:H	2.28	0.42
2:B:70:ARG:HH11	2:B:70:ARG:HD3	1.70	0.42
2:B:208:GLY:HA3	2:B:216:LEU:HD11	2.01	0.42
3:C:338:ILE:HD13	3:C:338:ILE:HA	1.86	0.42
1:A:4:TYR:CZ	1:A:8:LEU:HD11	2.54	0.42
2:B:354:ASN:H	2:B:355:PRO:CD	2.30	0.42
3:C:136:GLY:N	3:C:139:SER:HB2	2.35	0.42
4:D:225:HIS:CE1	7:G:20:PRO:HB2	2.54	0.42
1:A:419:CYS:HA	1:A:420:PRO:HD3	1.87	0.42
2:B:232:LEU:HB2	2:B:233:SER:H	1.64	0.42
2:B:257:LEU:HD11	2:B:439:LEU:HD13	2.01	0.42
4:D:169:LEU:HD22	4:D:169:LEU:HA	1.79	0.42
5:E:88:ALA:HB2	5:E:97:PHE:CD1	2.55	0.42
6:F:64:ARG:HH11	6:F:64:ARG:HB3	1.85	0.42
10:J:48:GLU:C	10:J:50:LYS:H	2.26	0.42
1:A:209:LEU:HA	1:A:209:LEU:HD23	1.79	0.42
1:A:255:ILE:HG12	1:A:342:TRP:HH2	1.85	0.42
3:C:133:LEU:HA	3:C:175:LEU:HD21	2.00	0.42
4:D:66:GLU:O	4:D:67:GLU:C	2.63	0.42
4:D:182:VAL:O	4:D:186:VAL:HG23	2.20	0.42
6:F:90:LEU:HD23	6:F:90:LEU:HA	1.85	0.42
3:C:44:GLN:HE21	3:C:44:GLN:HB3	1.60	0.41
3:C:51:LEU:HD13	3:C:79:ILE:HG22	2.01	0.41
3:C:215:VAL:HG21	6:F:59:VAL:HB	2.02	0.41
5:E:159:PRO:O	5:E:160:CYS:HB2	2.19	0.41
5:E:177:PRO:HB2	5:E:178:LEU:HD12	2.02	0.41
2:B:316:TYR:OH	9:I:10:PRO:HB3	2.20	0.41
4:D:124:GLU:OE2	4:D:191:ARG:HD2	2.20	0.41
10:J:18:SER:HA	11:K:24:TRP:HZ3	1.85	0.41
5:E:136:ILE:HD13	5:E:137:GLY:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:187:PHE:HB3	5:E:188:THR:H	1.63	0.41
8:H:25:GLU:O	8:H:30:CYS:HB2	2.20	0.41
2:B:51:ILE:HD13	2:B:199:PHE:CD2	2.55	0.41
2:B:126:VAL:O	2:B:130:PRO:HG3	2.20	0.41
3:C:32:ASN:N	3:C:32:ASN:HD22	2.17	0.41
3:C:104:TYR:CD2	3:C:208:PRO:HA	2.55	0.41
7:G:26:PHE:C	7:G:27:PRO:O	2.63	0.41
1:A:255:ILE:HG21	1:A:335:MET:HE1	2.03	0.41
4:D:54:VAL:HG12	4:D:55:CYS:N	2.35	0.41
10:J:43:TYR:O	10:J:46:ILE:HG22	2.21	0.41
10:J:47:ASN:HA	10:J:50:LYS:HD2	2.01	0.41
1:A:12:PRO:HG3	2:B:18:PRO:HA	2.01	0.41
1:A:236:PHE:CG	1:A:258:GLU:HB2	2.55	0.41
2:B:20:HIS:HA	2:B:21:PRO:HD3	1.90	0.41
2:B:176:LEU:CD2	9:I:13:PRO:HD3	2.48	0.41
2:B:344:VAL:HG11	2:B:417:PHE:CD2	2.56	0.41
3:C:153:ILE:HA	3:C:154:PRO:HD3	1.83	0.41
3:C:283:SER:HB3	3:C:352:GLN:HA	2.01	0.41
4:D:70:VAL:HG21	4:D:89:ASP:OD2	2.21	0.41
4:D:162:PRO:O	4:D:164:ILE:N	2.50	0.41
6:F:73:GLN:HE21	6:F:74:ILE:H	1.69	0.41
5:E:135:LEU:HD13	5:E:156:TYR:HE1	1.86	0.41
5:E:137:GLY:CA	5:E:145:VAL:HG13	2.43	0.41
1:A:32:GLN:HA	1:A:33:PRO:HD3	1.95	0.41
1:A:156:THR:O	1:A:159:GLN:HG3	2.20	0.41
3:C:160:LEU:HD23	3:C:160:LEU:HA	1.92	0.41
4:D:31:GLN:O	4:D:35:GLN:HG3	2.20	0.41
4:D:130:LEU:HD21	4:D:153:PHE:HB2	2.03	0.41
11:K:39:ARG:C	11:K:41:ILE:H	2.28	0.41
1:A:227:ALA:O	1:A:229:PRO:HD3	2.20	0.41
2:B:71:LEU:CD2	9:I:15:LEU:HG	2.51	0.41
3:C:24:PRO:C	3:C:26:ASN:N	2.71	0.41
3:C:217:LYS:HG3	7:G:7:LEU:HD13	2.03	0.41
3:C:267:HIS:HB3	3:C:268:ILE:H	1.55	0.41
4:D:56:TYR:N	4:D:56:TYR:CD2	2.89	0.41
6:F:40:ASN:OD1	6:F:40:ASN:C	2.64	0.41
9:I:36:ALA:HB1	9:I:37:THR:H	1.69	0.41
11:K:24:TRP:O	11:K:27:VAL:HB	2.21	0.41
1:A:251:ALA:CA	1:A:427:PRO:HD2	2.51	0.41
2:B:42:ALA:HA	2:B:43:PRO:HD3	1.97	0.41
4:D:37:CYS:SG	12:D:242:HEM:CMC	3.05	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:78:LEU:HG	5:E:193:VAL:HG11	2.03	0.41
6:F:59:VAL:HG21	7:G:10:VAL:HG13	2.03	0.41
4:D:14:HIS:HE2	4:D:124:GLU:CD	2.28	0.40
4:D:199:ASP:N	4:D:199:ASP:OD1	2.51	0.40
3:C:361:LEU:HA	3:C:365:LEU:HB2	2.03	0.40
4:D:164:ILE:O	4:D:165:TYR:C	2.65	0.40
6:F:40:ASN:OD1	6:F:42:ASP:N	2.51	0.40
2:B:218:GLN:HG3	2:B:222:GLN:OE1	2.21	0.40
3:C:256:TYR:O	3:C:257:THR:OG1	2.35	0.40
4:D:110:PRO:HA	4:D:111:PRO:HD3	1.91	0.40
5:E:135:LEU:HD13	5:E:156:TYR:CE1	2.56	0.40
5:E:184:SER:O	5:E:186:GLU:N	2.47	0.40
9:I:1:MET:HE2	9:I:7:ARG:HE	1.86	0.40
1:A:344:ARG:O	1:A:348:SER:N	2.47	0.40
6:F:66:LEU:HA	6:F:66:LEU:HD23	1.89	0.40
1:A:34:THR:HG22	1:A:35:CYS:H	1.87	0.40
1:A:163:LEU:HA	1:A:163:LEU:HD12	1.72	0.40
3:C:33:PHE:HA	3:C:36:LEU:HB2	2.02	0.40
4:D:22:ASP:HA	10:J:48:GLU:CD	2.47	0.40
4:D:44:ASP:OD1	4:D:44:ASP:N	2.50	0.40
4:D:117:VAL:CG2	4:D:190:LEU:HB3	2.51	0.40
4:D:229:VAL:CG2	7:G:20:PRO:HD3	2.51	0.40
7:G:29:TYR:O	7:G:33:GLY:HA3	2.22	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	444/446 (100%)	407 (92%)	23 (5%)	14 (3%)	3 5
2	B	421/439 (96%)	391 (93%)	22 (5%)	8 (2%)	6 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	375/379 (99%)	335 (89%)	28 (8%)	12 (3%)	3	5
4	D	239/241 (99%)	177 (74%)	36 (15%)	26 (11%)	0	0
5	E	194/196 (99%)	127 (66%)	43 (22%)	24 (12%)	0	0
6	F	103/110 (94%)	96 (93%)	6 (6%)	1 (1%)	12	28
7	G	73/81 (90%)	62 (85%)	6 (8%)	5 (7%)	1	1
8	H	68/78 (87%)	50 (74%)	9 (13%)	9 (13%)	0	0
9	I	55/78 (70%)	26 (47%)	15 (27%)	14 (26%)	0	0
10	J	56/62 (90%)	43 (77%)	7 (12%)	6 (11%)	0	0
11	K	47/56 (84%)	32 (68%)	9 (19%)	6 (13%)	0	0
All	All	2075/2166 (96%)	1746 (84%)	204 (10%)	125 (6%)	1	1

All (125) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	GLN
1	A	220	SER
1	A	227	ALA
2	B	305	GLN
3	C	212	SER
3	C	221	HIS
3	C	268	ILE
3	C	286	ASN
4	D	18	LEU
4	D	20	SER
4	D	21	LEU
4	D	52	VAL
4	D	54	VAL
4	D	67	GLU
4	D	76	GLU
4	D	92	PRO
4	D	105	ASN
4	D	161	ALA
4	D	165	TYR
4	D	166	ASN
4	D	168	VAL
4	D	171	PHE
5	E	65	SER
5	E	69	LEU
5	E	71	MET

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Mol	Chain	Res	Type
5	E	82	PRO
5	E	97	PHE
5	E	130	PRO
5	E	146	PRO
5	E	147	ILE
5	E	149	ASN
5	E	154	GLY
5	E	156	TYR
5	E	159	PRO
5	E	185	TYR
7	G	28	HIS
7	G	73	ASN
8	H	11	GLU
8	H	12	GLU
8	H	27	LEU
8	H	28	GLU
8	H	73	LEU
8	H	74	PHE
9	I	29	LEU
9	I	37	THR
9	I	39	GLU
9	I	40	SER
9	I	45	LEU
9	I	47	ARG
9	I	53	GLU
9	I	56	ARG
10	J	2	ALA
10	J	3	PRO
10	J	4	THR
11	K	41	ILE
11	K	44	TRP
11	K	48	ILE
1	A	50	GLU
1	A	52	ASN
1	A	72	GLY
2	B	21	PRO
3	C	255	ASN
3	C	267	HIS
4	D	17	LEU
4	D	73	GLY
4	D	96	PRO
4	D	106	ASN

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Mol	Chain	Res	Type
4	D	131	LEU
4	D	143	LEU
5	E	6	LYS
5	E	74	ILE
8	H	26	GLN
9	I	3	SER
9	I	55	LEU
10	J	50	LYS
1	A	223	TYR
1	A	224	ASP
1	A	286	GLY
2	B	228	GLY
2	B	236	LYS
2	B	353	SER
2	B	354	ASN
3	C	254	ASP
3	C	257	THR
4	D	122	GLY
4	D	160	MET
5	E	184	SER
7	G	31	SER
9	I	8	SER
9	I	48	SER
1	A	21	ASN
1	A	192	ALA
1	A	221	GLY
1	A	315	ALA
2	B	54	GLY
3	C	258	PRO
4	D	162	PRO
5	E	160	CYS
6	F	85	GLU
7	G	2	ARG
8	H	46	SER
9	I	2	LEU
9	I	4	VAL
11	K	38	SER
4	D	116	ILE
7	G	27	PRO
8	H	49	GLN
10	J	44	GLU
10	J	46	ILE

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Mol	Chain	Res	Type
11	K	45	VAL
2	B	436	ILE
3	C	264	THR
5	E	148	ALA
11	K	46	PRO
1	A	71	PRO
3	C	252	ASP
5	E	138	VAL
5	E	174	GLY
5	E	175	PRO
5	E	155	GLY
5	E	194	ILE
4	D	78	GLY
4	D	176	PRO
3	C	345	HIS
5	E	195	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/370 (100%)	342 (92%)	28 (8%)	12	27
2	B	332/343 (97%)	294 (89%)	38 (11%)	5	11
3	C	325/327 (99%)	291 (90%)	34 (10%)	6	14
4	D	206/206 (100%)	169 (82%)	37 (18%)	2	3
5	E	168/168 (100%)	145 (86%)	23 (14%)	3	7
6	F	96/98 (98%)	85 (88%)	11 (12%)	5	11
7	G	66/71 (93%)	60 (91%)	6 (9%)	9	19
8	H	67/74 (90%)	56 (84%)	11 (16%)	2	4
9	I	44/60 (73%)	34 (77%)	10 (23%)	1	1
10	J	48/52 (92%)	41 (85%)	7 (15%)	3	6
11	K	40/46 (87%)	29 (72%)	11 (28%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1762/1815 (97%)	1546 (88%)	216 (12%)	4 9

All (216) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	25	VAL
1	A	32	GLN
1	A	37	VAL
1	A	73	ASN
1	A	90	SER
1	A	104	LYS
1	A	113	LEU
1	A	126	GLN
1	A	127	ILE
1	A	149	VAL
1	A	195	MET
1	A	203	LEU
1	A	208	LEU
1	A	226	ASP
1	A	230	THR
1	A	241	ILE
1	A	245	GLU
1	A	255	ILE
1	A	308	GLN
1	A	343	MET
1	A	350	THR
1	A	381	ARG
1	A	383	LEU
1	A	430	GLN
1	A	438	ARG
1	A	439	SER
1	A	443	TRP
2	B	17	VAL
2	B	20	HIS
2	B	38	LEU
2	B	40	ASN
2	B	69	LEU
2	B	98	VAL
2	B	99	THR
2	B	105	MET
2	B	109	VAL

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Mol	Chain	Res	Type
2	B	110	GLU
2	B	118	ILE
2	B	119	LEU
2	B	123	LEU
2	B	163	LEU
2	B	183	ILE
2	B	186	VAL
2	B	189	VAL
2	B	197	ASN
2	B	209	LEU
2	B	227	ARG
2	B	232	LEU
2	B	240	HIS
2	B	247	GLN
2	B	248	ASN
2	B	257	LEU
2	B	258	VAL
2	B	289	SER
2	B	290	ASN
2	B	294	SER
2	B	305	GLN
2	B	309	VAL
2	B	346	THR
2	B	353	SER
2	B	379	LEU
2	B	387	LEU
2	B	396	SER
2	B	397	THR
2	B	424	MET
3	C	4	ILE
3	C	42	ILE
3	C	44	GLN
3	C	45	ILE
3	C	46	LEU
3	C	78	ILE
3	C	96	MET
3	C	102	LEU
3	C	111	GLU
3	C	123	VAL
3	C	164	ILE
3	C	175	LEU
3	C	197	LEU

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Mol	Chain	Res	Type
3	C	213	SER
3	C	215	VAL
3	C	226	ILE
3	C	242	LEU
3	C	243	VAL
3	C	249	LEU
3	C	264	THR
3	C	294	LEU
3	C	298	ILE
3	C	303	LEU
3	C	307	LEU
3	C	309	THR
3	C	312	GLN
3	C	328	LEU
3	C	343	VAL
3	C	349	THR
3	C	350	ILE
3	C	352	GLN
3	C	363	LEU
3	C	365	LEU
3	C	379	TRP
4	D	4	GLU
4	D	5	LEU
4	D	9	SER
4	D	13	SER
4	D	18	LEU
4	D	21	LEU
4	D	27	ARG
4	D	36	VAL
4	D	49	ARG
4	D	59	ASP
4	D	68	VAL
4	D	75	ASN
4	D	80	MET
4	D	82	MET
4	D	83	ARG
4	D	86	LYS
4	D	113	LEU
4	D	116	ILE
4	D	124	GLU
4	D	130	LEU
4	D	136	GLU

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Mol	Chain	Res	Type
4	D	139	THR
4	D	145	GLU
4	D	158	ILE
4	D	168	VAL
4	D	169	LEU
4	D	170	GLU
4	D	175	THR
4	D	179	MET
4	D	182	VAL
4	D	186	VAL
4	D	190	LEU
4	D	211	MET
4	D	224	ARG
4	D	232	SER
4	D	234	LYS
4	D	238	ARG
5	E	3	THR
5	E	6	LYS
5	E	7	VAL
5	E	12	ASP
5	E	22	THR
5	E	68	VAL
5	E	78	LEU
5	E	91	TRP
5	E	105	GLU
5	E	108	GLN
5	E	112	VAL
5	E	116	GLN
5	E	121	GLN
5	E	136	ILE
5	E	138	VAL
5	E	144	CYS
5	E	147	ILE
5	E	153	PHE
5	E	172	ARG
5	E	182	VAL
5	E	185	TYR
5	E	187	PHE
5	E	195	VAL
6	F	22	ASN
6	F	27	ASN
6	F	37	ILE

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Mol	Chain	Res	Type
6	F	44	LYS
6	F	53	ASN
6	F	59	VAL
6	F	73	GLN
6	F	74	ILE
6	F	78	GLU
6	F	81	THR
6	F	94	LEU
7	G	31	SER
7	G	37	VAL
7	G	39	ARG
7	G	41	THR
7	G	45	ILE
7	G	53	VAL
8	H	10	GLU
8	H	12	GLU
8	H	13	LEU
8	H	14	VAL
8	H	37	LEU
8	H	51	GLU
8	H	54	CYS
8	H	55	THR
8	H	65	ARG
8	H	68	CYS
8	H	71	HIS
9	I	15	LEU
9	I	18	THR
9	I	20	ARG
9	I	27	ARG
9	I	30	VAL
9	I	39	GLU
9	I	42	VAL
9	I	43	LEU
9	I	47	ARG
9	I	49	VAL
10	J	4	THR
10	J	6	THR
10	J	13	LEU
10	J	33	ARG
10	J	37	GLN
10	J	48	GLU
10	J	54	HIS

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Mol	Chain	Res	Type
11	K	13	LEU
11	K	18	VAL
11	K	23	LEU
11	K	39	ARG
11	K	41	ILE
11	K	42	LEU
11	K	43	ASP
11	K	44	TRP
11	K	45	VAL
11	K	47	THR
11	K	48	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	52	ASN
1	A	73	ASN
1	A	119	ASN
1	A	139	GLN
1	A	141	ASN
1	A	173	ASN
1	A	252	HIS
1	A	271	GLN
1	A	274	ASN
1	A	305	GLN
1	A	311	ASN
1	A	323	HIS
1	A	359	ASN
1	A	418	GLN
2	B	143	GLN
2	B	153	GLN
2	B	162	ASN
2	B	170	ASN
2	B	174	ASN
2	B	197	ASN
2	B	248	ASN
2	B	270	ASN
2	B	276	GLN
2	B	284	HIS
2	B	305	GLN
2	B	342	ASN

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Mol	Chain	Res	Type
2	B	343	GLN
2	B	351	ASN
2	B	362	ASN
2	B	385	GLN
2	B	401	GLN
3	C	8	HIS
3	C	32	ASN
3	C	114	ASN
3	C	137	GLN
3	C	206	ASN
3	C	312	GLN
3	C	341	GLN
3	C	352	GLN
4	D	35	GLN
4	D	75	ASN
4	D	97	ASN
4	D	106	ASN
4	D	121	HIS
4	D	181	GLN
4	D	225	HIS
5	E	53	ASN
5	E	57	GLN
5	E	108	GLN
5	E	161	HIS
6	F	38	HIS
6	F	53	ASN
8	H	23	GLN
10	J	54	HIS
11	K	12	GLN
11	K	16	ASN

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](#)

4 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
12	HEM	D	242	4	50,50,50	2.01	8 (16%)	67,82,82	1.38	8 (11%)
12	HEM	C	382	3	50,50,50	1.98	9 (18%)	67,82,82	1.29	5 (7%)
13	FES	E	197	5	0,4,4	-	-	-	-	-
12	HEM	C	381	3	50,50,50	1.73	10 (20%)	67,82,82	1.44	8 (11%)

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
12	HEM	D	242	4	-	4/14/54/54	-
12	HEM	C	382	3	-	8/14/54/54	-
13	FES	E	197	5	-	-	0/1/1/1
12	HEM	C	381	3	-	6/14/54/54	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	242	HEM	FE-ND	8.62	2.21	1.94
12	C	382	HEM	C3D-C2D	7.73	1.53	1.36
12	D	242	HEM	C3D-C2D	6.96	1.51	1.36
12	C	382	HEM	FE-NB	6.39	2.14	1.94
12	C	381	HEM	FE-NB	5.88	2.13	1.94
12	C	381	HEM	C3D-C2D	5.03	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	382	HEM	FE-ND	4.40	2.08	1.94
12	C	382	HEM	FE-NA	3.44	2.06	1.95
12	C	381	HEM	CAB-C3B	2.85	1.55	1.47
12	C	381	HEM	CMB-C2B	2.67	1.56	1.50
12	C	382	HEM	CMB-C2B	2.65	1.56	1.50
12	C	382	HEM	CAB-C3B	2.56	1.54	1.47
12	D	242	HEM	CAC-C3C	2.53	1.54	1.47
12	D	242	HEM	CAB-C3B	2.48	1.54	1.47
12	C	381	HEM	CHC-C4B	-2.46	1.33	1.39
12	C	381	HEM	FE-ND	2.38	2.02	1.94
12	C	382	HEM	CMD-C2D	2.33	1.55	1.50
12	C	381	HEM	CMD-C2D	2.26	1.55	1.50
12	C	382	HEM	C3C-C2C	-2.17	1.32	1.37
12	C	381	HEM	O2A-CGA	-2.15	1.23	1.30
12	C	381	HEM	C1B-NB	-2.10	1.36	1.40
12	D	242	HEM	C1C-NC	-2.10	1.35	1.39
12	D	242	HEM	CMB-C2B	2.09	1.55	1.50
12	D	242	HEM	C1B-NB	-2.08	1.36	1.40
12	D	242	HEM	C2A-C3A	-2.08	1.33	1.38
12	C	382	HEM	FE-NC	2.07	2.02	1.95
12	C	381	HEM	CAC-C3C	2.05	1.52	1.47

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	382	HEM	C4D-ND-C1D	5.24	111.41	105.21
12	C	381	HEM	C4D-ND-C1D	4.65	110.71	105.21
12	D	242	HEM	C4D-ND-C1D	4.59	110.64	105.21
12	D	242	HEM	CAD-C3D-C4D	3.84	131.38	124.70
12	C	381	HEM	CHD-C4C-NC	3.21	127.95	124.45
12	C	381	HEM	CMD-C2D-C1D	3.15	129.95	125.03
12	D	242	HEM	CAD-CBD-CGD	-3.06	105.54	113.67
12	C	381	HEM	CAD-C3D-C4D	2.96	129.86	124.70
12	D	242	HEM	CAA-CBA-CGA	-2.94	105.86	113.67
12	C	382	HEM	C4C-C3C-C2C	2.82	109.26	106.81
12	C	381	HEM	CBD-CAD-C3D	-2.60	105.36	112.53
12	C	381	HEM	CAA-CBA-CGA	-2.54	106.92	113.67
12	D	242	HEM	C1B-NB-C4B	2.50	108.16	105.21
12	C	381	HEM	C1C-CHC-C4B	-2.32	121.09	126.02
12	C	382	HEM	C1B-NB-C4B	2.25	107.88	105.21
12	D	242	HEM	CHD-C4C-NC	2.25	126.91	124.45
12	C	382	HEM	C3B-C4B-NB	-2.20	107.89	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	242	HEM	CAD-C3D-C2D	-2.16	123.82	127.87
12	C	382	HEM	CBC-CAC-C3C	-2.10	117.05	127.53
12	D	242	HEM	CHA-C1A-NA	2.09	127.66	123.86
12	C	381	HEM	C2A-C1A-NA	-2.00	107.93	110.15

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	C	381	HEM	C1A-C2A-CAA-CBA
12	C	382	HEM	C2B-C3B-CAB-CBB
12	C	382	HEM	C2C-C3C-CAC-CBC
12	C	382	HEM	C3D-CAD-CBD-CGD
12	D	242	HEM	C2B-C3B-CAB-CBB
12	C	381	HEM	C3A-C2A-CAA-CBA
12	D	242	HEM	C2D-C3D-CAD-CBD
12	D	242	HEM	C4D-C3D-CAD-CBD
12	C	381	HEM	C4C-C3C-CAC-CBC
12	C	382	HEM	C4B-C3B-CAB-CBB
12	C	382	HEM	C4C-C3C-CAC-CBC
12	C	381	HEM	C2C-C3C-CAC-CBC
12	D	242	HEM	C4B-C3B-CAB-CBB
12	C	381	HEM	CAA-CBA-CGA-O1A
12	C	381	HEM	CAA-CBA-CGA-O2A
12	C	382	HEM	C2A-CAA-CBA-CGA
12	C	382	HEM	CAD-CBD-CGD-O2D
12	C	382	HEM	CAD-CBD-CGD-O1D

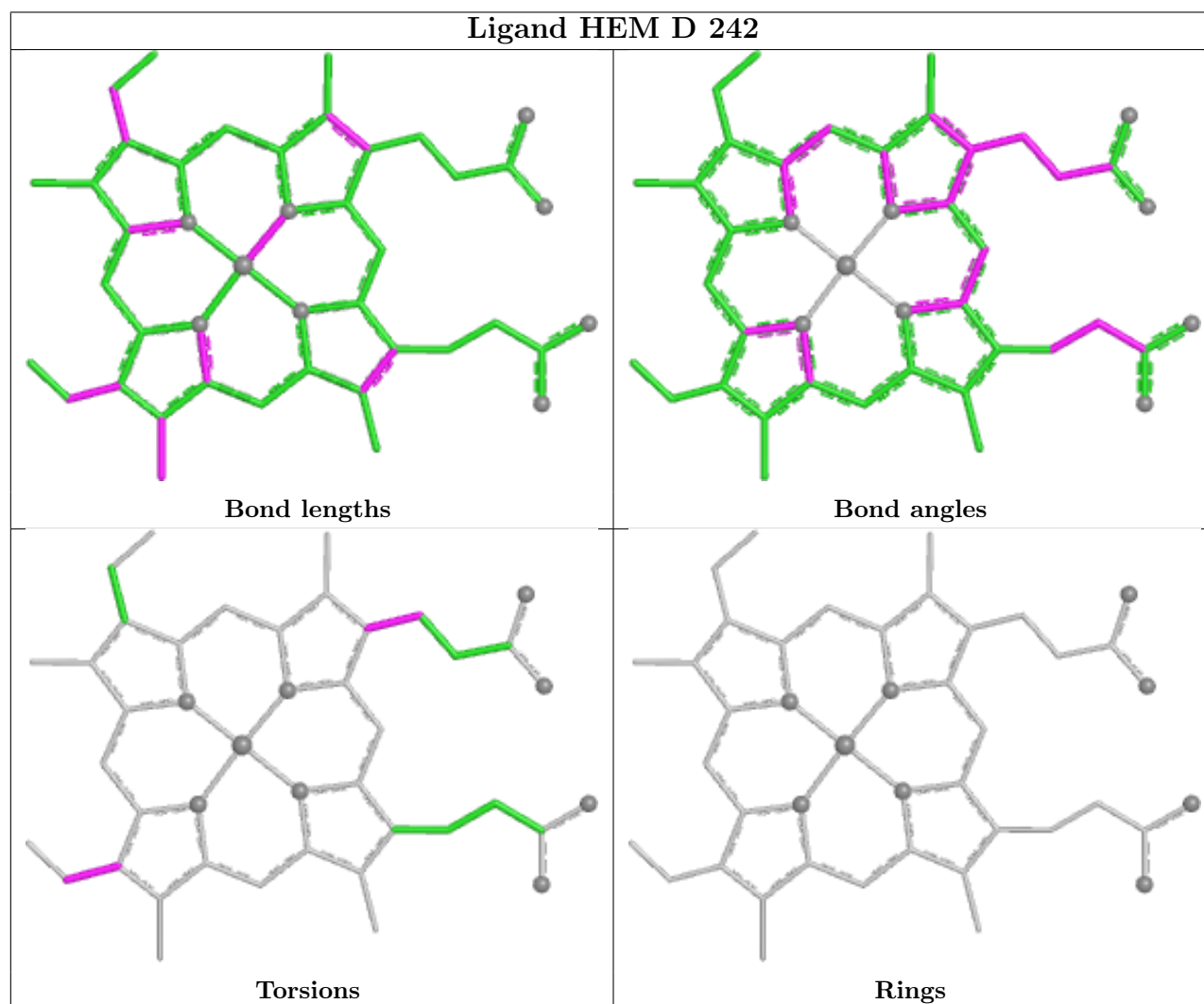
There are no ring outliers.

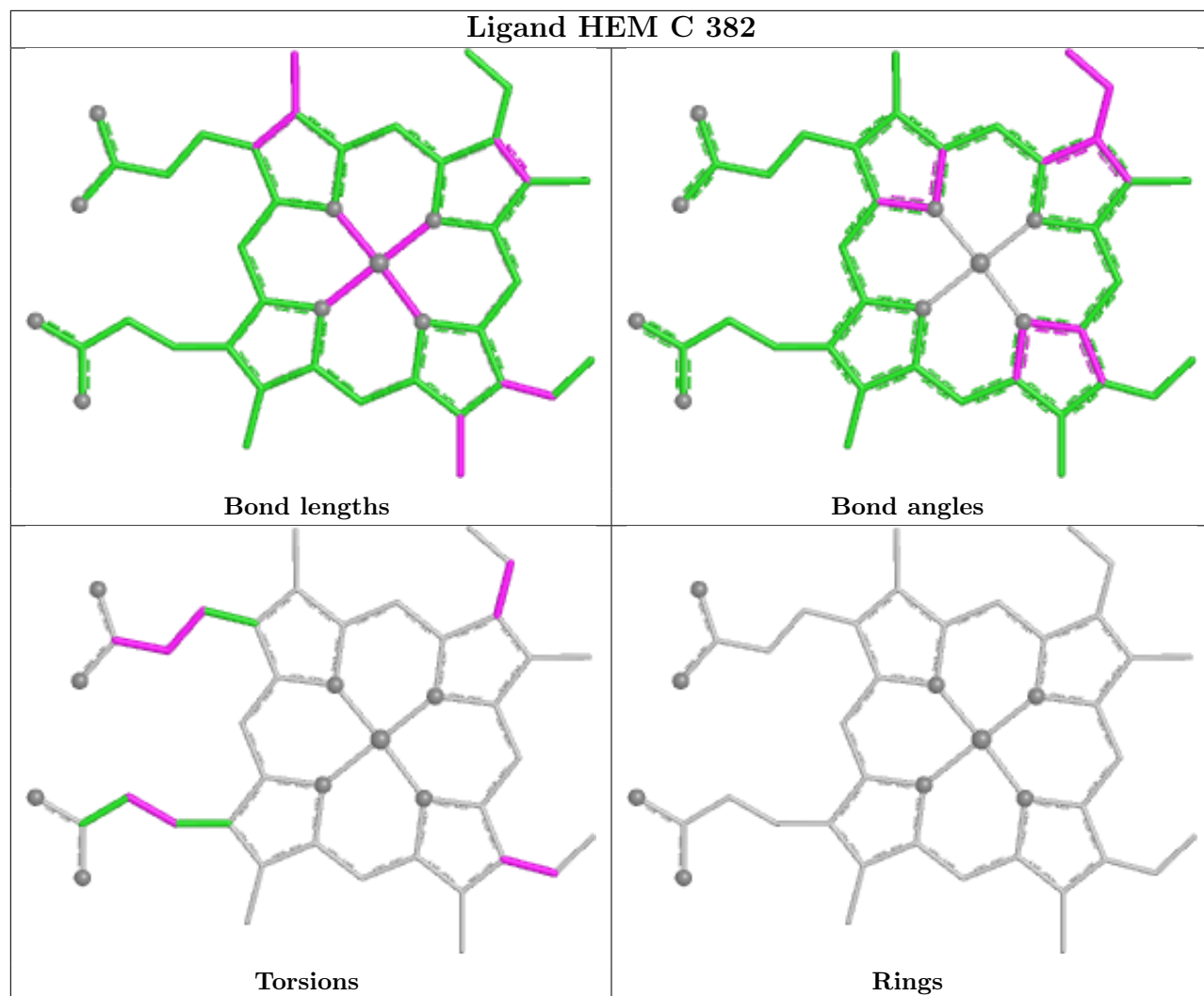
3 monomers are involved in 11 short contacts:

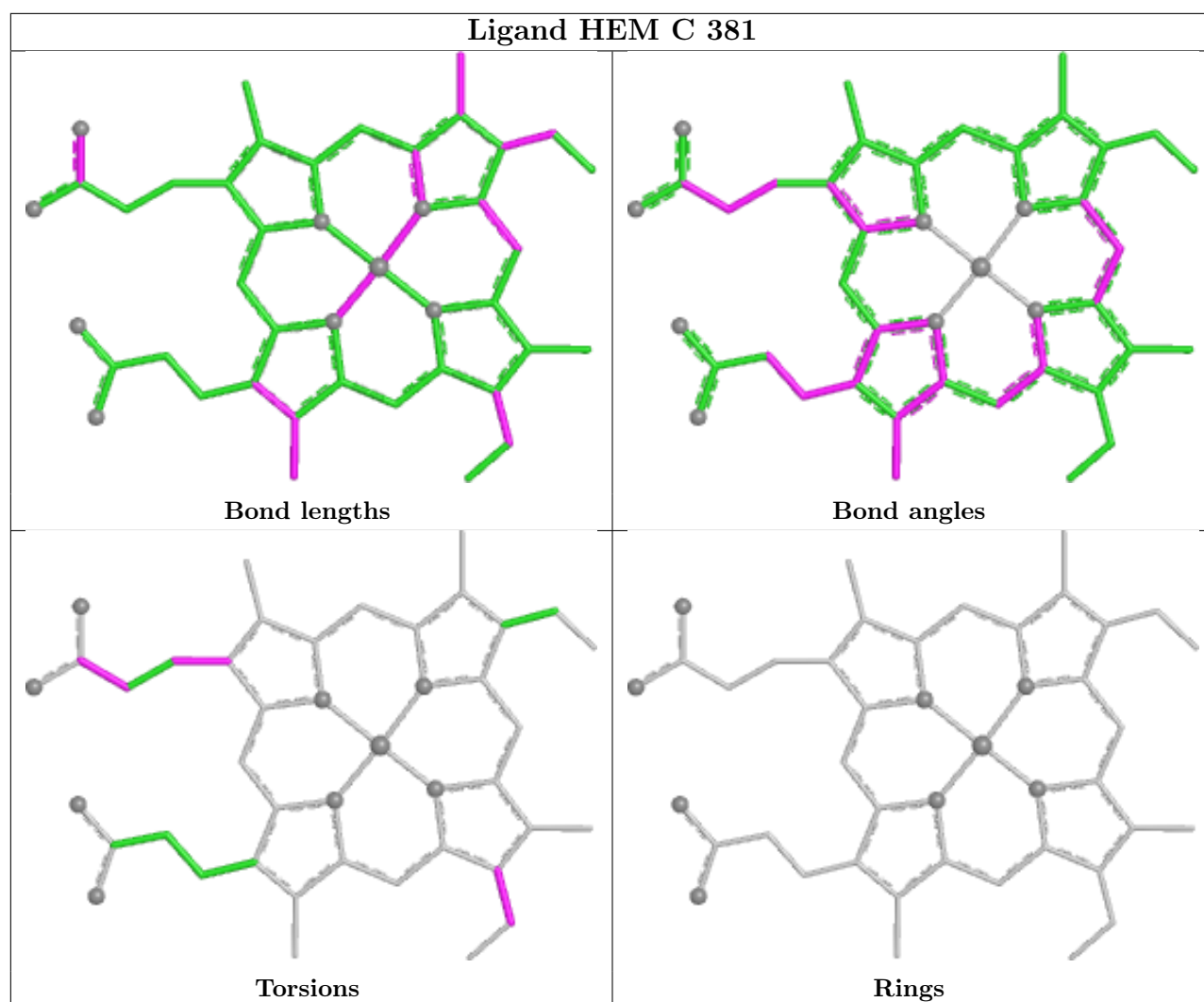
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	D	242	HEM	7	0
13	E	197	FES	1	0
12	C	381	HEM	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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.