



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:44 am GMT

PDB ID : 3OFU  
Title : Crystal Structure of Cytochrome P450 CYP101C1  
Authors : Zhou, W.; Ma, M.; Bell, S.G.; Yang, W.; Hao, Y.; Rees, N.H.; Bartlam, M.;  
Wong, L.-L.; Rao, Z.  
Deposited on : 2010-08-16  
Resolution : 2.80 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

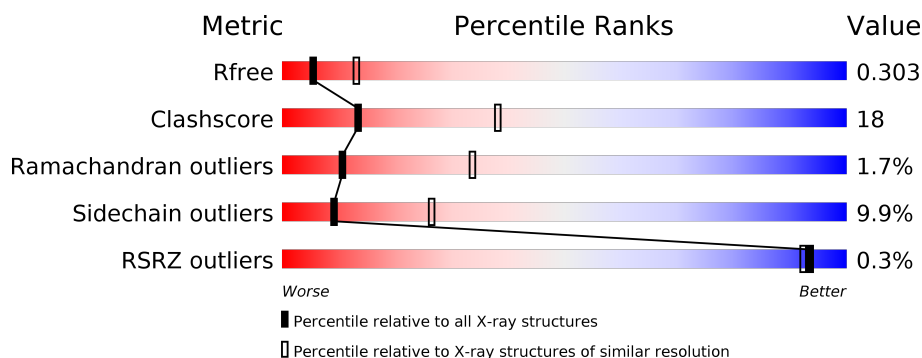
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	396	<div> <div style="width: 61%; background-color: green;"></div> <div style="width: 28%; background-color: yellow;"></div> <div style="width: 10%; background-color: orange;"></div> <div style="width: 1%; background-color: red;"></div> <div style="width: 0%; background-color: grey;"></div> </div> <div>61% 28% 10% .</div>
1	B	396	<div> <div style="width: 57%; background-color: green;"></div> <div style="width: 34%; background-color: yellow;"></div> <div style="width: 7%; background-color: orange;"></div> <div style="width: 1%; background-color: red;"></div> <div style="width: 0%; background-color: grey;"></div> </div> <div>57% 34% 7% .</div>
1	C	396	<div> <div style="width: 58%; background-color: green;"></div> <div style="width: 35%; background-color: yellow;"></div> <div style="width: 6%; background-color: orange;"></div> <div style="width: 1%; background-color: red;"></div> <div style="width: 0%; background-color: grey;"></div> </div> <div>58% 35% 6% .</div>
1	D	396	<div> <div style="width: 61%; background-color: green;"></div> <div style="width: 34%; background-color: yellow;"></div> <div style="width: 3%; background-color: orange;"></div> <div style="width: 1%; background-color: red;"></div> <div style="width: 1%; background-color: grey;"></div> </div> <div>61% 34% . .</div>
1	E	396	<div> <div style="width: 50%; background-color: green;"></div> <div style="width: 38%; background-color: yellow;"></div> <div style="width: 9%; background-color: orange;"></div> <div style="width: 1%; background-color: red;"></div> <div style="width: 2%; background-color: grey;"></div> </div> <div>% 50% 38% 9% . .</div>
1	F	396	<div> <div style="width: 50%; background-color: green;"></div> <div style="width: 38%; background-color: yellow;"></div> <div style="width: 9%; background-color: orange;"></div> <div style="width: 1%; background-color: red;"></div> <div style="width: 2%; background-color: grey;"></div> </div> <div>% 50% 38% 9% . .</div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ID3	A	397	-	-	-	X
3	ID3	B	397	-	-	-	X
3	ID3	C	397	-	-	-	X

## 2 Entry composition [i](#)

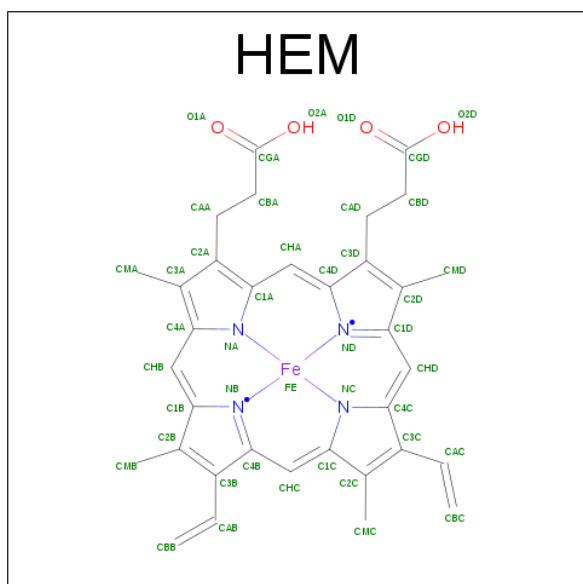
There are 4 unique types of molecules in this entry. The entry contains 18917 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cytochrome P450.

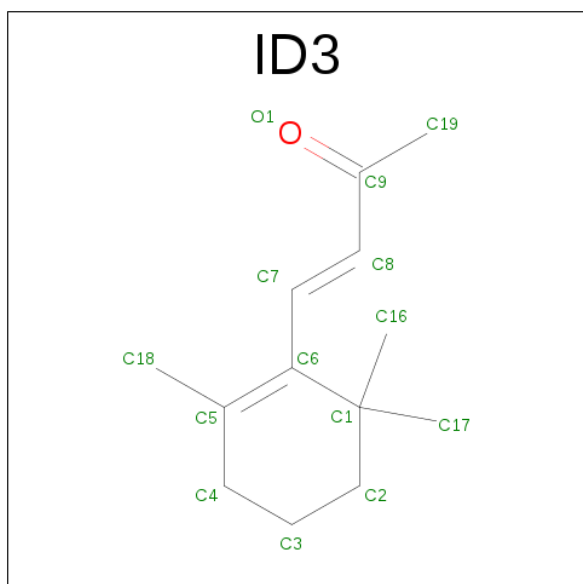
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			3068	1950	552	547	19			
1	B	396	Total	C	N	O	S	0	0	0
			3068	1950	552	547	19			
1	C	396	Total	C	N	O	S	0	0	0
			3068	1950	552	547	19			
1	D	394	Total	C	N	O	S	0	0	0
			3053	1941	550	543	19			
1	E	390	Total	C	N	O	S	0	0	0
			3025	1926	543	537	19			
1	F	390	Total	C	N	O	S	0	0	0
			3025	1926	543	537	19			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	E	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	F	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 3 is (3E)-4-(2,6,6-TRIMETHYLCYCLOHEX-1-EN-1-YL)BUT-3-EN-2-ONE (three-letter code: ID3) (formula: C<sub>13</sub>H<sub>20</sub>O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O		
			14	13	1	0	0
3	B	1	Total	C	O		
			14	13	1	0	0
3	C	1	Total	C	O		
			14	13	1	0	0

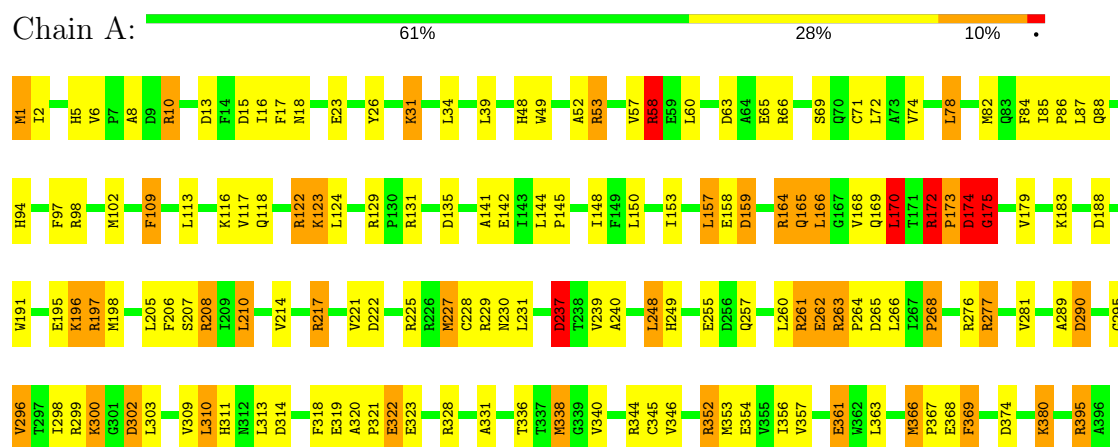
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	51	Total 51	O 51	0	0
4	B	62	Total 62	O 62	0	0
4	C	64	Total 64	O 64	0	0
4	D	52	Total 52	O 52	0	0
4	E	41	Total 41	O 41	0	0
4	F	40	Total 40	O 40	0	0

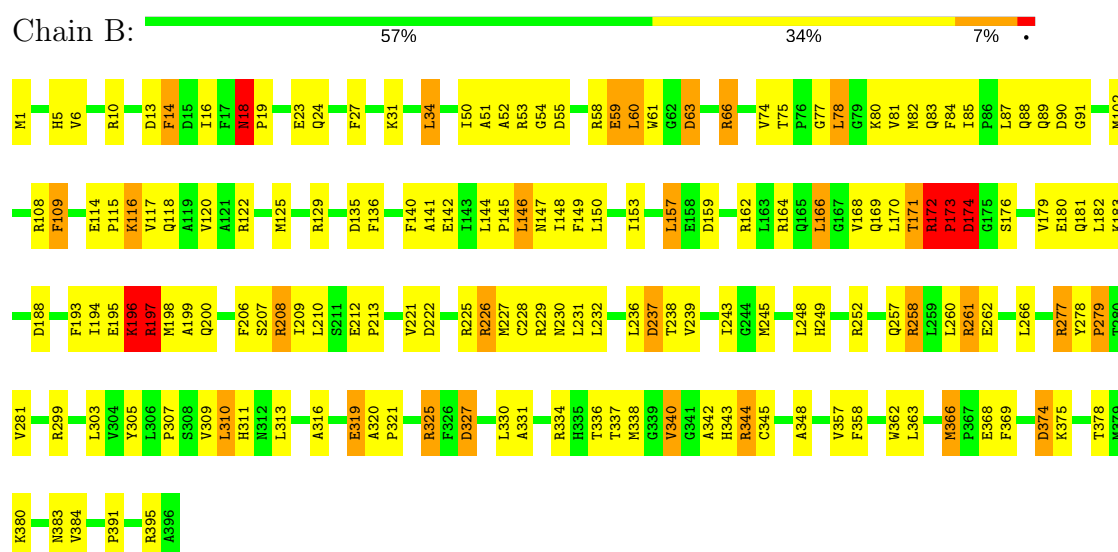
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Cytochrome P450

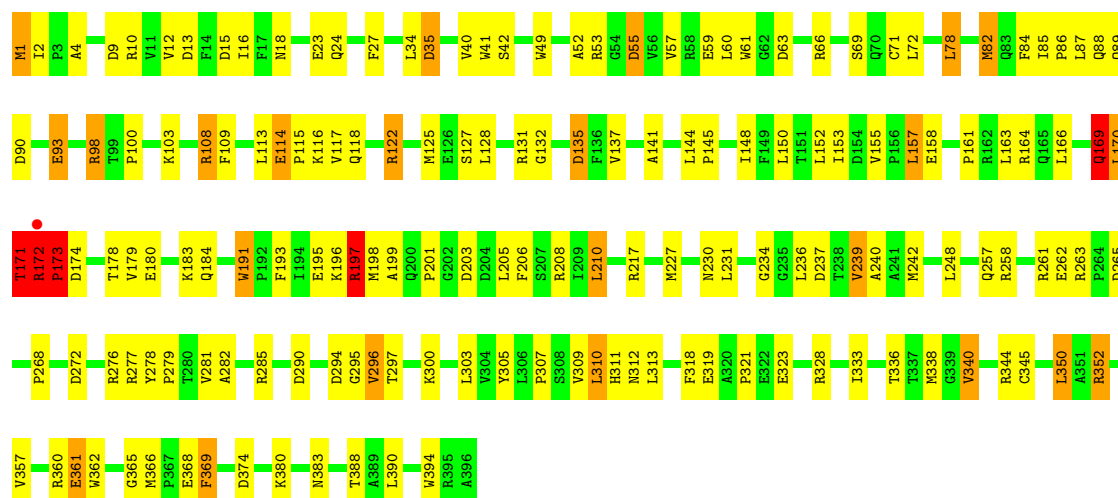


#### • Molecule 1: Cytochrome P450



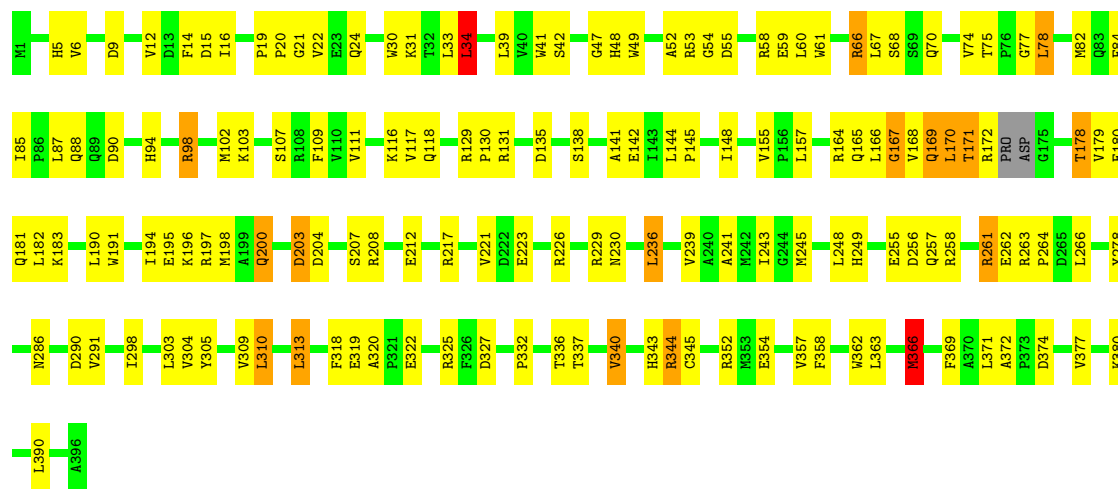
#### • Molecule 1: Cytochrome P450





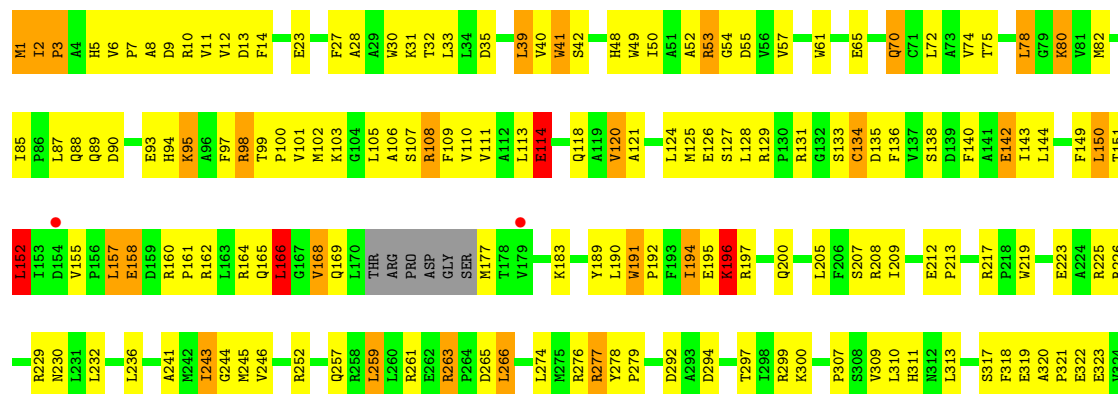
• Molecule 1: Cytochrome P450

Chain D: 61% 34%



• Molecule 1: Cytochrome P450

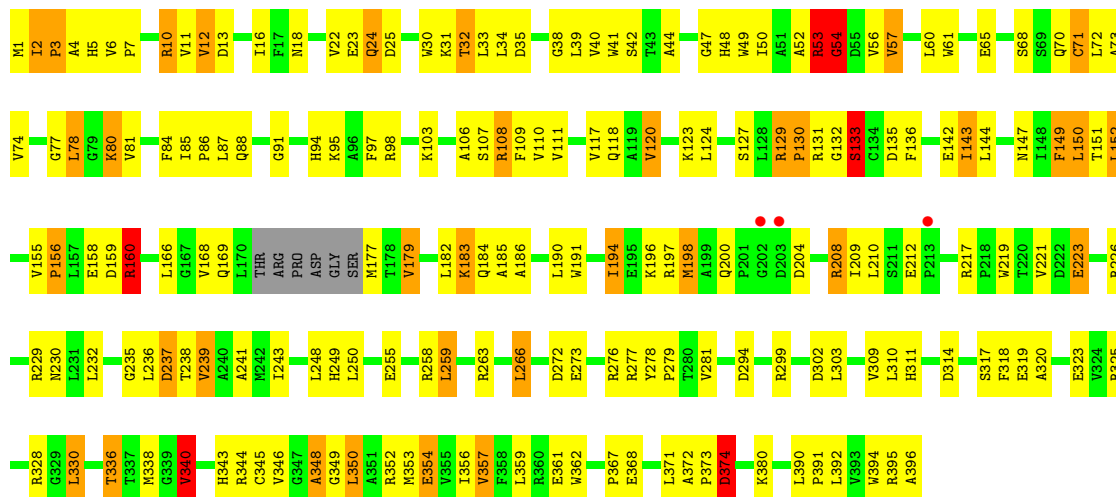
Chain E: 50% 38% 9%







● Molecule 1: Cytochrome P450



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.36Å 113.42Å 150.23Å 90.00° 89.90° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 46.21 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.0 (50.00-2.80) 98.5 (46.21-2.80)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.80 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.193 , 0.303 0.195 , 0.303	Depositor DCC
$R_{free}$ test set	2827 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.6	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 3.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.458 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	18917	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.44 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.7644e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, ID3

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	1.74	39/3140 (1.2%)	1.38	32/4269 (0.7%)
1	B	1.70	37/3140 (1.2%)	1.30	25/4269 (0.6%)
1	C	1.73	45/3140 (1.4%)	1.37	35/4269 (0.8%)
1	D	1.66	24/3123 (0.8%)	1.28	23/4243 (0.5%)
1	E	1.61	26/3095 (0.8%)	1.31	26/4206 (0.6%)
1	F	1.64	33/3095 (1.1%)	1.30	29/4206 (0.7%)
All	All	1.68	204/18733 (1.1%)	1.32	170/25462 (0.7%)

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	B	0	1
1	C	0	2
1	F	0	1
All	All	0	4

All (204) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	262	GLU	CG-CD	12.96	1.71	1.51
1	C	114	GLU	CG-CD	-10.01	1.36	1.51
1	A	17	PHE	CE1-CZ	9.69	1.55	1.37
1	C	319	GLU	CG-CD	9.58	1.66	1.51
1	C	203	ASP	CB-CG	9.41	1.71	1.51
1	B	281	VAL	CB-CG2	9.40	1.72	1.52
1	A	109	PHE	CE2-CZ	8.76	1.53	1.37
1	D	196	LYS	CD-CE	8.46	1.72	1.51
1	A	135	ASP	CB-CG	8.41	1.69	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	395	ARG	CG-CD	8.39	1.73	1.51
1	C	23	GLU	CD-OE1	8.25	1.34	1.25
1	A	195	GLU	CG-CD	8.09	1.64	1.51
1	A	361	GLU	CD-OE1	7.94	1.34	1.25
1	F	111	VAL	CB-CG1	7.92	1.69	1.52
1	F	191	TRP	CB-CG	7.86	1.64	1.50
1	A	109	PHE	CG-CD1	7.84	1.50	1.38
1	C	109	PHE	CD2-CE2	7.82	1.54	1.39
1	F	23	GLU	CG-CD	7.78	1.63	1.51
1	C	135	ASP	CB-CG	7.71	1.68	1.51
1	F	65	GLU	CD-OE2	7.67	1.34	1.25
1	E	318	PHE	CE2-CZ	7.67	1.51	1.37
1	C	103	LYS	CD-CE	7.60	1.70	1.51
1	A	296	VAL	CB-CG1	7.56	1.68	1.52
1	E	65	GLU	CG-CD	7.52	1.63	1.51
1	F	111	VAL	CB-CG2	7.46	1.68	1.52
1	A	319	GLU	CD-OE1	7.44	1.33	1.25
1	A	142	GLU	CG-CD	7.43	1.63	1.51
1	A	319	GLU	CD-OE2	7.36	1.33	1.25
1	B	196	LYS	CD-CE	7.35	1.69	1.51
1	E	278	TYR	CB-CG	-7.31	1.40	1.51
1	B	142	GLU	CG-CD	7.30	1.62	1.51
1	B	195	GLU	CG-CD	7.27	1.62	1.51
1	C	93	GLU	CB-CG	7.14	1.65	1.52
1	B	262	GLU	CB-CG	7.11	1.65	1.52
1	F	142	GLU	CB-CG	7.11	1.65	1.52
1	D	180	GLU	CD-OE1	7.04	1.33	1.25
1	F	354	GLU	CB-CG	6.99	1.65	1.52
1	C	196	LYS	CD-CE	6.96	1.68	1.51
1	D	200	GLN	CG-CD	6.92	1.67	1.51
1	C	361	GLU	CD-OE2	6.91	1.33	1.25
1	D	30	TRP	CZ3-CH2	6.89	1.51	1.40
1	E	319	GLU	CG-CD	6.83	1.62	1.51
1	C	374	ASP	CB-CG	6.80	1.66	1.51
1	B	59	GLU	CD-OE2	6.80	1.33	1.25
1	A	323	GLU	CG-CD	6.79	1.62	1.51
1	C	352	ARG	CZ-NH2	6.78	1.41	1.33
1	E	142	GLU	CB-CG	6.76	1.65	1.52
1	D	195	GLU	CG-CD	6.74	1.62	1.51
1	C	360	ARG	CZ-NH2	6.73	1.41	1.33
1	E	41	TRP	CZ3-CH2	6.70	1.50	1.40
1	C	239	VAL	CB-CG2	6.70	1.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	54	GLY	C-O	-6.67	1.12	1.23
1	B	180	GLU	CD-OE2	6.65	1.32	1.25
1	D	109	PHE	CE1-CZ	6.57	1.49	1.37
1	B	23	GLU	CD-OE1	6.57	1.32	1.25
1	E	336	THR	CA-CB	6.53	1.70	1.53
1	D	322	GLU	CD-OE2	6.50	1.32	1.25
1	B	193	PHE	CE2-CZ	6.50	1.49	1.37
1	A	255	GLU	C-O	6.50	1.35	1.23
1	A	71	CYS	CB-SG	6.48	1.93	1.82
1	B	180	GLU	CG-CD	6.45	1.61	1.51
1	A	221	VAL	CB-CG1	-6.44	1.39	1.52
1	E	354	GLU	CG-CD	6.43	1.61	1.51
1	E	27	PHE	CG-CD2	6.41	1.48	1.38
1	D	322	GLU	CD-OE1	6.40	1.32	1.25
1	C	169	GLN	CG-CD	6.38	1.65	1.51
1	C	23	GLU	CG-CD	6.34	1.61	1.51
1	A	109	PHE	CD2-CE2	6.32	1.51	1.39
1	A	296	VAL	CA-CB	6.29	1.68	1.54
1	E	318	PHE	CD1-CE1	6.29	1.51	1.39
1	D	142	GLU	CD-OE2	6.29	1.32	1.25
1	B	109	PHE	CG-CD1	6.27	1.48	1.38
1	E	354	GLU	CB-CG	6.26	1.64	1.52
1	C	352	ARG	CZ-NH1	6.25	1.41	1.33
1	E	196	LYS	CD-CE	6.21	1.66	1.51
1	B	362	TRP	CZ3-CH2	6.20	1.50	1.40
1	F	318	PHE	CE2-CZ	6.18	1.49	1.37
1	D	318	PHE	CD1-CE1	6.18	1.51	1.39
1	F	241	ALA	CA-CB	-6.17	1.39	1.52
1	D	109	PHE	CG-CD1	6.15	1.48	1.38
1	B	358	PHE	CE1-CZ	6.15	1.49	1.37
1	E	109	PHE	CG-CD1	6.14	1.48	1.38
1	D	374	ASP	CG-OD2	6.14	1.39	1.25
1	C	59	GLU	CD-OE2	6.12	1.32	1.25
1	D	304	VAL	CB-CG2	6.12	1.65	1.52
1	B	109	PHE	CE1-CZ	6.12	1.49	1.37
1	F	18	ASN	CB-CG	6.10	1.65	1.51
1	A	368	GLU	CD-OE1	6.10	1.32	1.25
1	A	281	VAL	CB-CG1	6.10	1.65	1.52
1	B	116	LYS	CB-CG	6.08	1.69	1.52
1	C	262	GLU	CD-OE2	6.07	1.32	1.25
1	F	278	TYR	CE1-CZ	6.06	1.46	1.38
1	C	296	VAL	CB-CG1	6.03	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	223	GLU	CB-CG	-6.02	1.40	1.52
1	E	319	GLU	CD-OE2	5.99	1.32	1.25
1	F	278	TYR	CG-CD1	5.95	1.46	1.39
1	F	340	VAL	CB-CG2	5.95	1.65	1.52
1	F	391	PRO	N-CA	5.91	1.57	1.47
1	C	23	GLU	CB-CG	5.89	1.63	1.52
1	C	174	ASP	CB-CG	5.89	1.64	1.51
1	A	109	PHE	CE1-CZ	5.89	1.48	1.37
1	E	322	GLU	CG-CD	5.88	1.60	1.51
1	C	323	GLU	CD-OE1	5.88	1.32	1.25
1	C	361	GLU	CD-OE1	5.86	1.32	1.25
1	A	8	ALA	CA-CB	-5.85	1.40	1.52
1	E	191	TRP	CB-CG	5.85	1.60	1.50
1	C	59	GLU	CD-OE1	5.84	1.32	1.25
1	C	323	GLU	CG-CD	5.82	1.60	1.51
1	C	13	ASP	C-O	-5.81	1.12	1.23
1	C	282	ALA	CA-CB	-5.81	1.40	1.52
1	F	71	CYS	CB-SG	5.81	1.92	1.82
1	A	262	GLU	CD-OE2	5.80	1.32	1.25
1	C	323	GLU	CD-OE2	5.80	1.32	1.25
1	F	65	GLU	CD-OE1	5.76	1.31	1.25
1	C	114	GLU	CB-CG	-5.74	1.41	1.52
1	B	23	GLU	CG-CD	5.74	1.60	1.51
1	B	228	CYS	CB-SG	5.74	1.92	1.82
1	D	358	PHE	CE1-CZ	5.73	1.48	1.37
1	D	41	TRP	CB-CG	5.71	1.60	1.50
1	E	349	GLY	C-O	5.71	1.32	1.23
1	B	23	GLU	CB-CG	5.69	1.62	1.52
1	F	149	PHE	CE1-CZ	5.66	1.48	1.37
1	D	374	ASP	CB-CG	5.65	1.63	1.51
1	D	195	GLU	CB-CG	5.65	1.62	1.52
1	B	109	PHE	CE2-CZ	5.64	1.48	1.37
1	D	322	GLU	CG-CD	5.62	1.60	1.51
1	B	180	GLU	CD-OE1	5.61	1.31	1.25
1	F	320	ALA	CA-CB	5.60	1.64	1.52
1	A	69	SER	N-CA	-5.59	1.35	1.46
1	A	158	GLU	CG-CD	5.59	1.60	1.51
1	C	109	PHE	CE1-CZ	5.58	1.48	1.37
1	A	322	GLU	CB-CG	-5.57	1.41	1.52
1	B	319	GLU	CD-OE1	5.57	1.31	1.25
1	C	203	ASP	CG-OD1	5.56	1.38	1.25
1	E	114	GLU	CG-CD	-5.53	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	281	VAL	CB-CG1	5.53	1.64	1.52
1	A	380	LYS	CE-NZ	5.53	1.62	1.49
1	E	340	VAL	CB-CG2	5.53	1.64	1.52
1	E	326	PHE	CE1-CZ	5.52	1.47	1.37
1	B	199	ALA	CA-CB	5.51	1.64	1.52
1	C	116	LYS	CD-CE	5.50	1.65	1.51
1	F	143	ILE	CA-CB	5.50	1.67	1.54
1	C	4	ALA	CA-CB	-5.50	1.41	1.52
1	B	325	ARG	CG-CD	5.48	1.65	1.51
1	B	342	ALA	CA-CB	5.48	1.64	1.52
1	A	196	LYS	CD-CE	5.48	1.65	1.51
1	B	6	VAL	CB-CG1	-5.47	1.41	1.52
1	E	65	GLU	CB-CG	5.46	1.62	1.52
1	F	336	THR	CA-CB	5.44	1.67	1.53
1	B	231	LEU	C-O	-5.43	1.13	1.23
1	A	237	ASP	CB-CG	5.42	1.63	1.51
1	B	52	ALA	CA-CB	5.36	1.63	1.52
1	D	180	GLU	CD-OE2	5.36	1.31	1.25
1	D	352	ARG	CG-CD	-5.35	1.38	1.51
1	D	14	PHE	CD2-CE2	-5.34	1.28	1.39
1	A	175	GLY	N-CA	5.34	1.54	1.46
1	F	374	ASP	CB-CG	5.33	1.62	1.51
1	A	369	PHE	CG-CD1	5.32	1.46	1.38
1	B	331	ALA	CA-CB	-5.32	1.41	1.52
1	F	368	GLU	CD-OE1	5.31	1.31	1.25
1	B	200	GLN	CG-CD	5.29	1.63	1.51
1	C	100	PRO	N-CA	-5.28	1.38	1.47
1	B	258	ARG	CZ-NH2	5.26	1.39	1.33
1	B	279	PRO	CB-CG	5.26	1.76	1.50
1	A	240	ALA	CA-CB	5.25	1.63	1.52
1	F	272	ASP	CB-CG	5.25	1.62	1.51
1	C	41	TRP	CZ3-CH2	5.23	1.48	1.40
1	A	319	GLU	CG-CD	5.22	1.59	1.51
1	F	80	LYS	CB-CG	5.22	1.66	1.52
1	B	91	GLY	N-CA	-5.22	1.38	1.46
1	C	297	THR	CA-CB	5.22	1.67	1.53
1	A	361	GLU	CG-CD	5.20	1.59	1.51
1	D	196	LYS	CG-CD	5.20	1.70	1.52
1	C	173	PRO	N-CA	5.19	1.56	1.47
1	F	109	PHE	CG-CD1	5.17	1.46	1.38
1	F	319	GLU	CD-OE1	5.16	1.31	1.25
1	A	352	ARG	CZ-NH1	5.14	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	65	GLU	CD-OE2	5.14	1.31	1.25
1	A	331	ALA	CA-CB	-5.13	1.41	1.52
1	C	180	GLU	CD-OE2	5.13	1.31	1.25
1	A	262	GLU	CD-OE1	5.13	1.31	1.25
1	E	80	LYS	CB-CG	5.13	1.66	1.52
1	F	223	GLU	CG-CD	5.13	1.59	1.51
1	C	127	SER	CA-CB	5.13	1.60	1.52
1	F	131	ARG	CB-CG	5.10	1.66	1.52
1	A	123	LYS	CG-CD	5.09	1.69	1.52
1	A	26	TYR	CD2-CE2	5.09	1.47	1.39
1	C	258	ARG	CZ-NH2	5.08	1.39	1.33
1	B	316	ALA	N-CA	5.08	1.56	1.46
1	C	258	ARG	CZ-NH1	5.08	1.39	1.33
1	A	116	LYS	CD-CE	5.08	1.64	1.51
1	B	74	VAL	C-O	5.08	1.32	1.23
1	F	348	ALA	N-CA	5.07	1.56	1.46
1	F	391	PRO	C-O	5.07	1.33	1.23
1	E	361	GLU	CB-CG	5.06	1.61	1.52
1	E	114	GLU	CB-CG	-5.05	1.42	1.52
1	B	334	ARG	CG-CD	-5.05	1.39	1.51
1	C	360	ARG	CZ-NH1	5.03	1.39	1.33
1	F	354	GLU	CG-CD	5.03	1.59	1.51
1	A	368	GLU	CD-OE2	5.02	1.31	1.25
1	F	239	VAL	CB-CG2	-5.01	1.42	1.52
1	E	219	TRP	CE3-CZ3	5.01	1.47	1.38
1	D	286	ASN	C-O	5.01	1.32	1.23
1	C	369	PHE	CG-CD1	5.00	1.46	1.38

All (170) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	ARG	NE-CZ-NH1	-13.45	113.58	120.30
1	A	66	ARG	NE-CZ-NH1	-11.52	114.54	120.30
1	A	157	LEU	CA-CB-CG	10.49	139.44	115.30
1	A	66	ARG	NE-CZ-NH2	10.36	125.48	120.30
1	C	10	ARG	NE-CZ-NH1	-10.07	115.27	120.30
1	C	66	ARG	NE-CZ-NH1	-9.68	115.46	120.30
1	B	63	ASP	CB-CG-OD1	9.49	126.84	118.30
1	C	66	ARG	NE-CZ-NH2	9.35	124.97	120.30
1	A	208	ARG	NE-CZ-NH1	8.79	124.70	120.30
1	C	276	ARG	NE-CZ-NH1	8.77	124.68	120.30
1	A	328	ARG	NE-CZ-NH1	-8.70	115.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	78	LEU	CA-CB-CG	8.68	135.26	115.30
1	B	262	GLU	OE1-CD-OE2	-8.62	112.96	123.30
1	D	261	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	C	197	ARG	NE-CZ-NH1	-8.36	116.12	120.30
1	F	208	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	F	53	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	B	344	ARG	NE-CZ-NH1	-8.30	116.15	120.30
1	C	122	ARG	NE-CZ-NH1	-8.15	116.22	120.30
1	C	203	ASP	CB-CG-OD1	8.06	125.55	118.30
1	C	164	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	D	217	ARG	NE-CZ-NH2	-7.97	116.31	120.30
1	E	299	ARG	NE-CZ-NH2	-7.97	116.32	120.30
1	C	208	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	C	277	ARG	NE-CZ-NH2	7.91	124.26	120.30
1	B	66	ARG	NE-CZ-NH1	-7.87	116.36	120.30
1	B	208	ARG	NE-CZ-NH2	7.86	124.23	120.30
1	F	217	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	D	258	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	E	129	ARG	NE-CZ-NH2	7.59	124.09	120.30
1	E	299	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	C	157	LEU	CA-CB-CG	7.56	132.68	115.30
1	A	277	ARG	NE-CZ-NH2	7.51	124.06	120.30
1	A	374	ASP	CB-CG-OD1	-7.51	111.54	118.30
1	F	53	ARG	NE-CZ-NH2	-7.41	116.59	120.30
1	C	285	ARG	NE-CZ-NH1	-7.41	116.59	120.30
1	C	1	MET	CG-SD-CE	7.38	112.01	100.20
1	B	10	ARG	NE-CZ-NH1	-7.33	116.63	120.30
1	B	90	ASP	CB-CG-OD1	7.19	124.77	118.30
1	A	395	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	E	252	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	C	63	ASP	CB-CG-OD1	7.06	124.65	118.30
1	A	129	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	C	98	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	F	299	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	C	328	ARG	NE-CZ-NH1	-6.94	116.83	120.30
1	A	261	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	A	63	ASP	CB-CG-OD1	6.85	124.47	118.30
1	E	277	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	B	303	LEU	CA-CB-CG	6.82	130.98	115.30
1	E	330	LEU	CA-CB-CG	6.82	130.98	115.30
1	A	170	LEU	CA-CB-CG	6.81	130.96	115.30
1	C	374	ASP	CB-CG-OD2	6.77	124.39	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	53	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	A	276	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	F	272	ASP	CB-CG-OD1	6.70	124.33	118.30
1	F	226	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	F	266	LEU	CB-CG-CD1	6.65	122.31	111.00
1	A	191	TRP	CA-CB-CG	-6.62	101.12	113.70
1	B	157	LEU	CA-CB-CG	6.61	130.50	115.30
1	B	327	ASP	CB-CG-OD2	6.59	124.23	118.30
1	A	290	ASP	CB-CG-OD1	6.58	124.22	118.30
1	A	15	ASP	CB-CG-OD1	-6.53	112.43	118.30
1	D	344	ARG	NE-CZ-NH1	-6.53	117.04	120.30
1	C	258	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	B	122	ARG	NE-CZ-NH2	6.44	123.52	120.30
1	F	78	LEU	CB-CG-CD2	6.44	121.94	111.00
1	F	25	ASP	CB-CG-OD1	-6.40	112.54	118.30
1	B	60	LEU	CB-CG-CD1	6.40	121.88	111.00
1	C	172	ARG	N-CA-C	6.33	128.09	111.00
1	B	277	ARG	NE-CZ-NH1	-6.31	117.14	120.30
1	E	259	LEU	CB-CG-CD1	6.31	121.73	111.00
1	C	374	ASP	CB-CG-OD1	-6.28	112.64	118.30
1	D	344	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	B	197	ARG	NE-CZ-NH1	-6.23	117.18	120.30
1	D	197	ARG	NE-CZ-NH1	-6.21	117.20	120.30
1	C	55	ASP	CB-CG-OD2	6.20	123.88	118.30
1	E	98	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	A	210	LEU	CB-CG-CD2	6.19	121.52	111.00
1	D	352	ARG	NE-CZ-NH1	-6.14	117.23	120.30
1	F	78	LEU	CA-CB-CG	6.14	129.41	115.30
1	A	302	ASP	CB-CG-OD2	6.13	123.82	118.30
1	A	302	ASP	CB-CG-OD1	-6.02	112.88	118.30
1	F	266	LEU	CB-CG-CD2	-6.01	100.78	111.00
1	C	164	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	124	LEU	CB-CG-CD2	-5.99	100.82	111.00
1	B	226	ARG	NE-CZ-NH2	5.98	123.29	120.30
1	A	395	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	F	129	ARG	NE-CZ-NH2	5.87	123.23	120.30
1	B	299	ARG	NE-CZ-NH1	-5.86	117.37	120.30
1	C	338	MET	CG-SD-CE	-5.84	90.85	100.20
1	F	152	LEU	CA-CB-CG	5.84	128.73	115.30
1	D	15	ASP	CB-CG-OD2	5.82	123.54	118.30
1	B	188	ASP	CB-CG-OD1	5.81	123.53	118.30
1	C	15	ASP	CB-CG-OD1	-5.80	113.08	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	LEU	CB-CG-CD1	5.79	120.84	111.00
1	E	152	LEU	CA-CB-CG	5.78	128.60	115.30
1	F	39	LEU	CB-CG-CD2	-5.74	101.24	111.00
1	D	131	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	E	208	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	E	276	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	F	259	LEU	CB-CG-CD2	-5.70	101.31	111.00
1	F	160	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	E	265	ASP	CB-CG-OD1	5.66	123.40	118.30
1	B	129	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	E	39	LEU	CB-CG-CD2	-5.60	101.48	111.00
1	F	266	LEU	CA-CB-CG	5.59	128.15	115.30
1	E	78	LEU	CB-CG-CD2	5.58	120.49	111.00
1	B	226	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	C	191	TRP	CA-CB-CG	-5.56	103.14	113.70
1	C	108	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	A	98	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	E	128	LEU	CA-CB-CG	5.53	128.01	115.30
1	B	319	GLU	OE1-CD-OE2	5.52	129.92	123.30
1	D	34	LEU	CA-CB-CG	5.51	127.97	115.30
1	B	225	ARG	NE-CZ-NH2	5.48	123.04	120.30
1	B	261	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	B	222	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	164	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	F	1	MET	CG-SD-CE	5.45	108.92	100.20
1	C	290	ASP	CB-CG-OD1	5.45	123.20	118.30
1	E	252	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	F	350	LEU	CB-CG-CD1	5.43	120.23	111.00
1	D	98	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	A	338	MET	CG-SD-CE	-5.42	91.52	100.20
1	E	105	LEU	CB-CG-CD2	-5.42	101.78	111.00
1	F	277	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	F	359	LEU	CB-CG-CD1	-5.39	101.83	111.00
1	C	90	ASP	CB-CG-OD1	5.38	123.14	118.30
1	D	390	LEU	CA-CB-CG	5.36	127.63	115.30
1	D	167	GLY	N-CA-C	-5.36	99.70	113.10
1	E	261	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	F	328	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	D	66	ARG	NE-CZ-NH1	-5.29	117.66	120.30
1	E	166	LEU	CB-CG-CD1	5.25	119.93	111.00
1	A	263	ARG	NE-CZ-NH1	-5.25	117.67	120.30
1	D	164	ARG	NE-CZ-NH1	5.25	122.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	217	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	C	35	ASP	CB-CG-OD1	-5.24	113.58	118.30
1	D	263	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	B	166	LEU	CA-CB-CG	5.24	127.36	115.30
1	D	204	ASP	CB-CG-OD2	-5.23	113.60	118.30
1	E	344	ARG	NE-CZ-NH2	5.21	122.90	120.30
1	F	371	LEU	CB-CG-CD1	-5.20	102.16	111.00
1	E	266	LEU	CB-CG-CD1	5.20	119.84	111.00
1	E	334	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	188	ASP	CB-CG-OD1	5.18	122.97	118.30
1	E	208	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	C	290	ASP	CB-CG-OD2	-5.16	113.65	118.30
1	D	313	LEU	CB-CG-CD2	-5.16	102.23	111.00
1	A	53	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	A	58	ARG	NE-CZ-NH1	-5.15	117.72	120.30
1	F	237	ASP	CB-CA-C	5.15	120.69	110.40
1	F	10	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	C	350	LEU	CB-CG-CD1	-5.13	102.27	111.00
1	D	303	LEU	CA-CB-CG	5.13	127.11	115.30
1	A	13	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	F	359	LEU	CA-CB-CG	-5.13	103.51	115.30
1	C	294	ASP	CB-CG-OD2	5.12	122.90	118.30
1	D	39	LEU	CA-CB-CG	5.12	127.06	115.30
1	F	217	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	D	366	MET	CG-SD-CE	-5.08	92.07	100.20
1	E	226	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	D	77	GLY	N-CA-C	5.07	125.77	113.10
1	A	122	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	B	18	ASN	N-CA-CB	5.04	119.67	110.60
1	C	210	LEU	CB-CG-CD2	5.03	119.56	111.00
1	C	350	LEU	CB-CG-CD2	-5.03	102.45	111.00
1	D	203	ASP	CB-CG-OD1	-5.02	113.78	118.30
1	F	354	GLU	OE1-CD-OE2	-5.01	117.28	123.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	172	ARG	Peptide
1	C	171	THR	Peptide
1	C	172	ARG	Peptide
1	F	197	ARG	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	3068	0	3088	100	0
1	B	3068	0	3088	119	1
1	C	3068	0	3088	101	0
1	D	3053	0	3076	97	1
1	E	3025	0	3048	133	0
1	F	3025	0	3048	123	0
2	A	43	0	30	4	0
2	B	43	0	30	1	0
2	C	43	0	30	2	0
2	D	43	0	30	5	0
2	E	43	0	30	3	0
2	F	43	0	30	5	0
3	A	14	0	20	2	0
3	B	14	0	20	5	0
3	C	14	0	20	2	0
4	A	51	0	0	0	0
4	B	62	0	0	6	0
4	C	64	0	0	5	0
4	D	52	0	0	6	0
4	E	41	0	0	4	0
4	F	40	0	0	3	0
All	All	18917	0	18676	672	1

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 18.

All (672) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:PRO:CG	1:B:279:PRO:CB	1.76	1.32
1:C:172:ARG:HH22	1:C:237:ASP:HB3	1.03	1.12
1:C:257:GLN:HE21	1:C:261:ARG:NH2	1.46	1.11
1:A:172:ARG:NH1	1:A:237:ASP:HB3	1.66	1.09
1:B:172:ARG:NH2	1:B:237:ASP:HB3	1.65	1.09
1:C:172:ARG:NH2	1:C:237:ASP:HB3	1.70	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:ARG:HD2	1:B:55:ASP:OD1	1.55	1.05
1:B:172:ARG:C	1:B:174:ASP:H	1.57	1.03
1:A:172:ARG:H	1:A:173:PRO:CD	1.71	1.03
1:A:257:GLN:HE21	1:A:261:ARG:HH22	1.04	1.02
1:A:153:ILE:O	1:A:197:ARG:NH1	1.97	0.97
1:B:245:MET:HE3	1:B:245:MET:HA	1.43	0.97
1:C:84:PHE:H	1:C:88:GLN:NE2	1.64	0.95
1:E:232:LEU:O	1:E:236:LEU:HG	1.68	0.94
1:E:124:LEU:O	1:E:127:SER:HB3	1.68	0.92
1:B:172:ARG:HH22	1:B:237:ASP:HB3	1.22	0.92
1:F:204:ASP:O	1:F:208:ARG:HG3	1.70	0.92
1:A:257:GLN:HE21	1:A:261:ARG:NH2	1.68	0.91
1:C:153:ILE:O	1:C:197:ARG:NH1	2.02	0.91
1:D:53:ARG:HD2	1:D:55:ASP:OD1	1.73	0.89
1:A:197:ARG:HG2	1:A:207:SER:OG	1.72	0.89
1:C:257:GLN:HE21	1:C:261:ARG:HH22	1.19	0.89
1:C:199:ALA:O	1:C:201:PRO:HD3	1.72	0.89
1:E:162:ARG:HG2	1:E:166:LEU:HD22	1.54	0.86
1:C:318:PHE:O	1:C:321:PRO:HD3	1.75	0.86
1:B:82:MET:O	1:B:229:ARG:NH1	2.09	0.85
1:B:245:MET:CE	1:B:245:MET:HA	2.05	0.85
1:F:196:LYS:O	1:F:200:GLN:N	2.09	0.85
1:B:153:ILE:O	1:B:197:ARG:NH1	2.09	0.85
1:E:196:LYS:O	1:E:200:GLN:N	2.11	0.84
1:A:169:GLN:O	1:A:170:LEU:HB3	1.78	0.83
1:B:84:PHE:H	1:B:88:GLN:NE2	1.77	0.83
1:C:118:GLN:HG3	1:C:357:VAL:HG13	1.59	0.82
1:D:84:PHE:H	1:D:88:GLN:NE2	1.78	0.82
1:F:3:PRO:O	1:F:5:HIS:N	2.13	0.81
1:B:172:ARG:C	1:B:174:ASP:N	2.34	0.81
1:B:309:VAL:CG2	1:B:313:LEU:HD12	2.10	0.81
1:E:279:PRO:HG2	1:E:309:VAL:HA	1.62	0.80
1:E:99:THR:HB	1:E:100:PRO:HD3	1.64	0.80
1:B:257:GLN:HE21	1:B:261:ARG:NH2	1.80	0.80
1:D:84:PHE:H	1:D:88:GLN:HE21	1.25	0.80
1:D:245:MET:HE3	1:D:245:MET:HA	1.64	0.79
1:E:362:TRP:O	1:E:366:MET:HB2	1.83	0.78
1:F:12:VAL:O	1:F:42:SER:HA	1.83	0.78
1:A:172:ARG:NH1	1:A:237:ASP:CB	2.45	0.77
1:F:323:GLU:OE1	1:F:325:ARG:HD3	1.84	0.77
1:D:290:ASP:O	1:E:395:ARG:NH1	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:417:HEM:HBB2	2:D:417:HEM:CMB	2.16	0.76
1:C:191:TRP:NE1	1:C:195:GLU:OE2	2.18	0.76
1:E:157:LEU:HA	1:E:160:ARG:HD2	1.68	0.76
1:B:194:ILE:O	1:B:198:MET:HG3	1.85	0.76
1:E:40:VAL:HG22	1:E:50:ILE:HB	1.67	0.75
1:D:309:VAL:HG13	1:D:310:LEU:HD13	1.69	0.75
1:E:311:HIS:CD2	1:E:336:THR:OG1	2.40	0.75
1:C:257:GLN:HE21	1:C:261:ARG:HH21	1.35	0.74
1:F:232:LEU:O	1:F:236:LEU:HG	1.87	0.74
1:B:84:PHE:H	1:B:88:GLN:HE21	1.33	0.74
1:B:61:TRP:HB3	1:B:340:VAL:HG13	1.68	0.74
1:F:135:ASP:HB3	4:F:397:HOH:O	1.85	0.73
1:E:196:LYS:HE2	1:E:200:GLN:HB2	1.70	0.73
1:A:172:ARG:H	1:A:173:PRO:HD2	1.51	0.73
1:D:118:GLN:HG3	1:D:357:VAL:HG13	1.68	0.73
1:E:165:GLN:O	1:E:168:VAL:HG23	1.88	0.73
1:F:132:GLY:CA	1:F:396:ALA:HB2	2.18	0.73
1:E:6:VAL:HG11	1:E:41:TRP:HB3	1.70	0.73
1:C:171:THR:CG2	1:C:171:THR:O	2.36	0.73
1:A:172:ARG:HH12	1:A:237:ASP:CB	2.02	0.73
1:F:54:GLY:HA2	1:F:311:HIS:HA	1.70	0.73
1:E:98:ARG:NH1	1:E:346:VAL:CG1	2.52	0.72
1:A:172:ARG:HH22	1:A:237:ASP:HA	1.54	0.72
1:B:118:GLN:HG3	1:B:357:VAL:HG13	1.72	0.72
1:B:245:MET:CE	1:B:245:MET:CA	2.67	0.71
1:C:122:ARG:HG3	1:C:361:GLU:OE2	1.90	0.71
1:A:366:MET:HG3	1:A:367:PRO:HD2	1.72	0.71
1:F:132:GLY:HA3	1:F:396:ALA:HB2	1.71	0.70
1:E:1:MET:CE	1:E:1:MET:H1	2.05	0.70
1:D:6:VAL:HG12	1:D:6:VAL:O	1.89	0.70
1:A:262:GLU:O	1:A:264:PRO:HD3	1.92	0.70
1:A:311:HIS:HD2	1:A:336:THR:OG1	1.75	0.69
1:E:367:PRO:HG2	1:E:394:TRP:HB2	1.74	0.69
1:F:311:HIS:CD2	1:F:336:THR:OG1	2.45	0.69
1:A:172:ARG:H	1:A:173:PRO:HD3	1.54	0.69
1:D:102:MET:CG	4:D:414:HOH:O	2.40	0.69
1:F:156:PRO:HG2	1:F:159:ASP:OD2	1.92	0.69
1:D:78:LEU:HG	1:D:179:VAL:HG21	1.75	0.69
1:E:89:GLN:NE2	1:E:93:GLU:HG2	2.08	0.68
1:A:78:LEU:HG	1:A:179:VAL:HG21	1.74	0.68
1:A:290:ASP:OD1	1:A:300:LYS:HG2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:GLN:O	1:A:170:LEU:CB	2.41	0.68
1:D:257:GLN:HE21	1:D:261:ARG:NH2	1.92	0.68
1:F:235:GLY:O	1:F:239:VAL:HG23	1.94	0.68
1:A:172:ARG:HH12	1:A:237:ASP:HB3	1.54	0.68
1:F:276:ARG:HD3	1:F:330:LEU:HD12	1.76	0.67
1:B:108:ARG:NH2	1:F:31:LYS:HE2	2.09	0.67
1:E:155:VAL:CG2	1:E:160:ARG:HG2	2.24	0.67
1:A:172:ARG:N	1:A:173:PRO:CD	2.49	0.67
1:E:12:VAL:O	1:E:42:SER:HA	1.94	0.67
1:C:171:THR:HG22	1:C:171:THR:O	1.95	0.67
1:F:53:ARG:HH22	1:F:294:ASP:CG	1.97	0.66
1:E:196:LYS:HE2	1:E:200:GLN:CB	2.25	0.66
1:F:98:ARG:NH1	1:F:346:VAL:HG12	2.11	0.66
1:B:87:LEU:H	1:B:230:ASN:ND2	1.92	0.66
1:E:263:ARG:HB3	1:E:266:LEU:HD23	1.78	0.66
1:F:124:LEU:HD21	1:F:143:ILE:HG22	1.77	0.66
1:B:63:ASP:OD2	1:B:66:ARG:HB2	1.95	0.66
1:A:122:ARG:HG3	1:A:361:GLU:OE2	1.95	0.65
1:D:257:GLN:HE21	1:D:261:ARG:HH21	1.43	0.65
1:F:71:CYS:O	1:F:73:ALA:N	2.29	0.65
1:D:24:GLN:OE1	4:D:434:HOH:O	2.13	0.65
1:E:311:HIS:HD2	1:E:336:THR:OG1	1.79	0.65
1:F:151:THR:HA	1:F:160:ARG:HH22	1.62	0.65
1:E:162:ARG:CG	1:E:166:LEU:HD22	2.26	0.65
1:F:106:ALA:HB1	1:F:108:ARG:HH21	1.60	0.65
1:F:374:ASP:N	1:F:374:ASP:OD2	2.29	0.65
1:A:227:MET:HE1	1:A:228:CYS:SG	2.37	0.65
1:C:114:GLU:HB3	1:C:115:PRO:HD3	1.78	0.65
1:D:178:THR:HG22	1:D:181:GLN:OE1	1.96	0.65
1:E:95:LYS:HB2	1:E:95:LYS:HZ2	1.61	0.65
1:A:356:ILE:HG22	1:A:357:VAL:N	2.11	0.65
1:B:85:ILE:C	1:B:230:ASN:HD22	2.00	0.65
1:D:16:ILE:HD12	1:D:305:TYR:CZ	2.31	0.65
1:F:33:LEU:C	1:F:35:ASP:H	2.00	0.65
1:D:102:MET:HG2	4:D:414:HOH:O	1.95	0.64
1:D:61:TRP:HB3	1:D:340:VAL:HG13	1.79	0.64
1:A:1:MET:C	1:A:2:ILE:HD13	2.18	0.64
1:D:98:ARG:NH2	1:D:344:ARG:O	2.27	0.64
1:F:87:LEU:H	1:F:230:ASN:HD21	1.46	0.64
1:B:78:LEU:HG	1:B:179:VAL:HG21	1.80	0.64
1:D:85:ILE:C	1:D:230:ASN:HD22	2.01	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:HIS:CD2	1:A:336:THR:OG1	2.51	0.64
1:F:183:LYS:C	1:F:183:LYS:HD3	2.18	0.64
1:F:338:MET:HE2	1:F:348:ALA:HA	1.80	0.64
1:C:257:GLN:NE2	1:C:261:ARG:HH22	1.91	0.63
1:D:166:LEU:N	1:D:167:GLY:HA3	2.13	0.63
1:C:257:GLN:NE2	1:C:261:ARG:NH2	2.32	0.63
1:B:309:VAL:HG23	1:B:313:LEU:HD12	1.79	0.63
1:D:169:GLN:CD	1:D:169:GLN:H	2.02	0.63
1:A:172:ARG:NH2	1:A:237:ASP:HA	2.13	0.63
1:C:117:VAL:HG13	1:C:148:ILE:HG12	1.79	0.63
1:D:165:GLN:O	1:D:169:GLN:NE2	2.32	0.63
2:D:417:HEM:HBB2	2:D:417:HEM:HMB1	1.80	0.63
1:E:98:ARG:NH1	1:E:346:VAL:HG13	2.13	0.63
1:B:338:MET:HE2	1:B:348:ALA:HA	1.80	0.63
1:E:135:ASP:HB3	4:E:401:HOH:O	1.97	0.63
1:F:52:ALA:HA	1:F:310:LEU:HD23	1.79	0.63
1:C:84:PHE:HB2	1:C:88:GLN:HE21	1.63	0.63
1:E:98:ARG:HH12	1:E:346:VAL:CG1	2.12	0.63
1:E:194:ILE:O	1:E:196:LYS:N	2.32	0.63
1:F:32:THR:O	1:F:35:ASP:HB2	1.98	0.63
1:F:350:LEU:HD12	1:F:354:GLU:HG3	1.79	0.62
1:C:89:GLN:NE2	1:C:93:GLU:OE1	2.29	0.62
1:A:205:LEU:HD21	1:A:231:LEU:HD13	1.82	0.62
1:E:320:ALA:O	1:E:323:GLU:HB2	2.00	0.62
1:A:172:ARG:N	1:A:173:PRO:HD2	2.13	0.62
1:B:146:LEU:HD12	1:B:236:LEU:HD21	1.82	0.62
1:E:98:ARG:NH1	1:E:346:VAL:HG12	2.15	0.61
1:F:3:PRO:HB2	1:F:5:HIS:CD2	2.34	0.61
1:C:118:GLN:HA	1:C:357:VAL:CG1	2.30	0.61
1:B:108:ARG:N	1:F:35:ASP:OD1	2.32	0.61
1:E:40:VAL:CG2	1:E:50:ILE:HB	2.31	0.61
1:A:84:PHE:H	1:A:88:GLN:NE2	1.98	0.61
1:E:108:ARG:HB3	1:E:108:ARG:CZ	2.30	0.61
1:E:89:GLN:HE22	1:E:93:GLU:HG2	1.65	0.61
1:F:117:VAL:HG12	1:F:357:VAL:HG11	1.81	0.61
1:B:257:GLN:HE21	1:B:261:ARG:HH21	1.47	0.61
1:C:1:MET:HA	1:C:1:MET:CE	2.30	0.61
1:E:377:VAL:HG13	1:E:390:LEU:HD13	1.83	0.61
1:A:85:ILE:C	1:A:230:ASN:HD22	2.04	0.61
1:E:263:ARG:HD3	1:E:266:LEU:CD2	2.30	0.60
1:F:6:VAL:HG11	1:F:41:TRP:CB	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ARG:O	1:A:168:VAL:HG23	2.01	0.60
1:B:277:ARG:NH1	1:B:277:ARG:O	2.35	0.60
1:C:362:TRP:O	1:C:366:MET:HB2	2.02	0.60
1:B:141:ALA:O	1:B:145:PRO:CD	2.49	0.60
3:B:397:ID3:H17	3:B:397:ID3:H8	1.82	0.60
1:A:102:MET:HG3	1:A:346:VAL:HG12	1.83	0.60
1:E:53:ARG:NH2	1:E:294:ASP:OD1	2.28	0.60
1:F:84:PHE:HE1	1:F:229:ARG:HG2	1.67	0.60
1:F:3:PRO:C	1:F:5:HIS:H	2.05	0.60
1:B:196:LYS:NZ	1:B:197:ARG:HH21	2.00	0.60
1:B:108:ARG:HH22	1:F:31:LYS:HE2	1.66	0.60
1:E:14:PHE:CD1	1:E:33:LEU:HD21	2.36	0.60
1:D:344:ARG:O	1:D:345:CYS:C	2.41	0.59
1:A:16:ILE:HD11	1:A:74:VAL:HG21	1.83	0.59
1:A:227:MET:CE	1:A:228:CYS:SG	2.90	0.59
1:E:118:GLN:HG3	1:E:361:GLU:HG2	1.83	0.59
1:F:6:VAL:HG11	1:F:41:TRP:HB3	1.82	0.59
1:F:124:LEU:O	1:F:127:SER:HB3	2.02	0.59
1:B:171:THR:O	1:B:173:PRO:CD	2.50	0.59
1:F:367:PRO:HG2	1:F:394:TRP:HB2	1.84	0.59
1:B:135:ASP:HB3	4:B:445:HOH:O	2.03	0.59
1:D:117:VAL:HG13	1:D:148:ILE:HG12	1.84	0.59
1:B:172:ARG:O	1:B:174:ASP:N	2.34	0.59
1:B:383:ASN:HB2	3:B:397:ID3:H17B	1.84	0.58
1:C:312:ASN:C	1:C:313:LEU:HD23	2.23	0.58
1:F:24:GLN:H	1:F:24:GLN:CD	2.06	0.58
1:D:245:MET:HA	1:D:245:MET:CE	2.33	0.58
1:D:102:MET:HG3	4:D:414:HOH:O	2.03	0.58
1:B:82:MET:HE1	1:B:182:LEU:HD23	1.85	0.58
1:C:311:HIS:CD2	1:C:336:THR:OG1	2.57	0.58
1:F:56:VAL:HG12	1:F:60:LEU:HD22	1.86	0.58
1:F:13:ASP:O	1:F:44:ALA:HB2	2.04	0.58
1:F:392:LEU:HB2	1:F:394:TRP:HZ3	1.69	0.58
1:A:227:MET:HE3	1:A:228:CYS:N	2.20	0.57
1:B:109:PHE:HB2	1:B:208:ARG:NH2	2.19	0.57
1:C:12:VAL:O	1:C:42:SER:HA	2.04	0.57
1:E:196:LYS:HG3	1:E:200:GLN:HB2	1.86	0.57
1:D:129:ARG:HB3	1:D:130:PRO:HD3	1.87	0.57
1:B:61:TRP:HB3	1:B:340:VAL:CG1	2.34	0.57
1:E:97:PHE:CZ	1:E:223:GLU:HG2	2.40	0.57
1:E:95:LYS:NZ	1:E:95:LYS:HB2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:259:LEU:O	1:F:263:ARG:HB2	2.05	0.57
1:C:198:MET:HG3	1:C:210:LEU:HD13	1.87	0.57
1:E:99:THR:HB	1:E:100:PRO:CD	2.33	0.57
1:F:30:TRP:HB3	1:F:310:LEU:CD1	2.35	0.57
1:A:78:LEU:HG	1:A:179:VAL:CG2	2.35	0.57
1:F:68:SER:OG	1:F:70:GLN:HB2	2.05	0.57
1:B:311:HIS:CD2	1:B:336:THR:OG1	2.58	0.56
1:D:48:HIS:HD2	1:D:49:TRP:O	1.87	0.56
1:E:98:ARG:HG2	1:E:98:ARG:HH11	1.69	0.56
1:F:56:VAL:O	1:F:60:LEU:HB2	2.05	0.56
1:A:257:GLN:NE2	1:A:261:ARG:NH2	2.46	0.56
1:B:245:MET:HE3	1:B:245:MET:CA	2.24	0.56
1:F:48:HIS:HD2	1:F:49:TRP:O	1.88	0.56
1:F:311:HIS:HD2	1:F:336:THR:OG1	1.87	0.56
1:B:206:PHE:O	1:B:210:LEU:HD12	2.06	0.56
1:B:102:MET:CG	4:B:425:HOH:O	2.54	0.56
1:F:343:HIS:O	2:F:417:HEM:HAA2	2.06	0.56
1:A:353:MET:O	1:A:354:GLU:C	2.44	0.56
1:C:84:PHE:H	1:C:88:GLN:HE21	1.52	0.55
1:E:85:ILE:C	1:E:230:ASN:HD22	2.08	0.55
1:E:190:LEU:O	1:E:194:ILE:HG13	2.06	0.55
1:C:172:ARG:HD2	1:C:173:PRO:N	2.21	0.55
1:A:49:TRP:NE1	1:A:298:ILE:HG23	2.20	0.55
1:A:94:HIS:HE1	2:A:417:HEM:O2D	1.89	0.55
1:D:66:ARG:O	1:D:67:LEU:HD23	2.05	0.55
1:E:72:LEU:HD22	1:E:88:GLN:NE2	2.21	0.55
1:A:118:GLN:HA	1:A:357:VAL:CG1	2.37	0.55
1:B:311:HIS:HD2	1:B:336:THR:OG1	1.90	0.55
1:E:10:ARG:HD2	1:E:39:LEU:O	2.07	0.55
1:C:87:LEU:HG	1:C:87:LEU:O	2.07	0.55
1:E:113:LEU:HD13	1:E:152:LEU:CD2	2.37	0.55
1:E:133:SER:O	1:E:134:CYS:HB3	2.07	0.55
1:F:136:PHE:CD1	1:F:392:LEU:HD11	2.42	0.55
1:F:106:ALA:HB1	1:F:108:ARG:NH2	2.21	0.55
1:C:163:LEU:HD22	1:C:193:PHE:HZ	1.72	0.55
4:B:439:HOH:O	1:D:5:HIS:HD2	1.90	0.54
1:C:295:GLY:O	1:C:296:VAL:CG1	2.55	0.54
1:E:1:MET:H1	1:E:1:MET:HE1	1.71	0.54
1:E:28:ALA:O	1:E:32:THR:HG23	2.06	0.54
1:D:66:ARG:HH11	1:E:395:ARG:HD2	1.72	0.54
1:A:117:VAL:HG13	1:A:148:ILE:HG12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:319:GLU:O	1:D:320:ALA:C	2.45	0.54
1:F:108:ARG:HH11	1:F:108:ARG:HB3	1.72	0.54
1:B:248:LEU:HD11	1:B:252:ARG:NH1	2.23	0.54
1:D:169:GLN:CD	1:D:169:GLN:N	2.60	0.54
1:E:87:LEU:H	1:E:230:ASN:HD21	1.53	0.54
1:F:209:ILE:O	1:F:212:GLU:HB2	2.08	0.54
1:A:344:ARG:O	1:A:345:CYS:C	2.45	0.54
1:C:118:GLN:HA	1:C:357:VAL:HG13	1.88	0.54
1:F:72:LEU:HD22	1:F:88:GLN:NE2	2.23	0.54
1:F:124:LEU:HD21	1:F:143:ILE:CG2	2.37	0.54
1:F:198:MET:HE1	1:F:221:VAL:HG22	1.89	0.54
1:C:263:ARG:HD3	1:C:265:ASP:OD1	2.08	0.54
1:E:263:ARG:HD3	1:E:266:LEU:HD23	1.89	0.54
1:E:113:LEU:HD13	1:E:152:LEU:HD22	1.90	0.54
1:A:2:ILE:N	1:A:2:ILE:HD13	2.23	0.53
1:D:362:TRP:O	1:D:366:MET:HB2	2.08	0.53
1:F:85:ILE:C	1:F:230:ASN:HD22	2.11	0.53
1:D:85:ILE:HD11	1:D:226:ARG:CZ	2.38	0.53
1:E:161:PRO:O	1:E:165:GLN:HG3	2.08	0.53
1:F:124:LEU:HA	1:F:127:SER:HB3	1.89	0.53
2:D:417:HEM:CBB	2:D:417:HEM:HMB1	2.38	0.53
1:C:163:LEU:HD22	1:C:193:PHE:CZ	2.44	0.53
1:B:144:LEU:HB3	1:B:145:PRO:HD3	1.90	0.53
1:F:255:GLU:OE1	1:F:255:GLU:N	2.28	0.53
1:B:27:PHE:O	1:B:31:LYS:HG3	2.08	0.53
1:E:94:HIS:HE1	2:E:417:HEM:O2D	1.91	0.53
1:A:172:ARG:CZ	1:A:237:ASP:HB3	2.35	0.53
1:B:319:GLU:O	1:B:320:ALA:C	2.44	0.53
1:D:239:VAL:O	1:D:243:ILE:HG12	2.09	0.52
1:B:82:MET:CE	1:B:182:LEU:HD23	2.39	0.52
1:C:172:ARG:HH22	1:C:237:ASP:CB	1.97	0.52
1:C:242:MET:HB2	4:C:431:HOH:O	2.10	0.52
1:D:12:VAL:O	1:D:42:SER:HA	2.08	0.52
1:A:277:ARG:NH2	1:A:322:GLU:HG2	2.25	0.52
1:E:53:ARG:HD2	1:E:55:ASP:OD1	2.08	0.52
1:E:149:PHE:HZ	1:E:190:LEU:HD21	1.75	0.52
1:E:52:ALA:HA	1:E:310:LEU:HD23	1.90	0.52
1:C:344:ARG:O	1:C:345:CYS:C	2.48	0.52
1:E:120:VAL:O	1:E:121:ALA:C	2.46	0.52
1:E:243:ILE:HG22	1:E:244:GLY:N	2.25	0.52
1:E:277:ARG:O	1:E:313:LEU:HD21	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:LEU:O	1:A:87:LEU:HG	2.10	0.52
1:B:13:ASP:N	1:B:13:ASP:OD2	2.43	0.52
1:C:272:ASP:OD1	1:C:352:ARG:NE	2.39	0.52
1:C:61:TRP:CG	1:C:340:VAL:HG13	2.45	0.52
1:E:133:SER:HB2	1:E:393:VAL:HG12	1.92	0.52
1:B:197:ARG:HG2	1:B:207:SER:OG	2.10	0.52
1:B:61:TRP:CG	1:B:340:VAL:HG13	2.45	0.52
1:F:190:LEU:HB3	1:F:194:ILE:HD11	1.92	0.52
1:B:309:VAL:HG23	1:B:313:LEU:CD1	2.39	0.51
1:E:151:THR:HA	1:E:160:ARG:HH22	1.75	0.51
1:B:61:TRP:CB	1:B:340:VAL:HG13	2.39	0.51
1:E:98:ARG:HH12	1:E:346:VAL:HG12	1.70	0.51
1:B:164:ARG:O	1:B:168:VAL:HG23	2.10	0.51
1:B:58:ARG:HD2	1:B:340:VAL:HG21	1.93	0.51
1:E:197:ARG:HG2	1:E:207:SER:OG	2.10	0.51
1:E:1:MET:CE	1:E:1:MET:N	2.72	0.51
1:E:257:GLN:HE22	1:E:369:PHE:H	1.57	0.51
1:D:78:LEU:HA	1:D:179:VAL:HG21	1.93	0.51
1:E:323:GLU:OE1	1:E:325:ARG:HD3	2.10	0.51
1:F:33:LEU:C	1:F:35:ASP:N	2.64	0.51
1:A:85:ILE:O	1:A:227:MET:HA	2.10	0.51
1:D:248:LEU:HD13	1:D:377:VAL:HG11	1.92	0.51
1:D:87:LEU:H	1:D:230:ASN:ND2	2.08	0.51
1:E:338:MET:HE2	1:E:348:ALA:HA	1.92	0.51
1:B:309:VAL:HG13	1:B:310:LEU:HD13	1.93	0.51
1:D:144:LEU:HG	1:D:148:ILE:HD12	1.93	0.51
1:F:344:ARG:O	1:F:345:CYS:C	2.48	0.51
1:F:3:PRO:C	1:F:5:HIS:N	2.63	0.51
1:A:289:ALA:HB2	1:F:95:LYS:HE2	1.93	0.51
1:E:98:ARG:NH2	1:E:344:ARG:O	2.42	0.51
1:F:186:ALA:O	1:F:190:LEU:HG	2.10	0.51
1:A:82:MET:O	1:A:229:ARG:NH1	2.44	0.51
1:D:58:ARG:HD2	1:D:340:VAL:HG11	1.93	0.51
1:B:320:ALA:N	1:B:321:PRO:HD3	2.25	0.51
1:C:153:ILE:HG13	1:C:155:VAL:HG13	1.93	0.51
1:C:248:LEU:HD13	1:C:390:LEU:CD1	2.41	0.51
1:D:53:ARG:HH11	1:D:55:ASP:CG	2.13	0.51
1:E:140:PHE:CE2	1:E:144:LEU:HD22	2.45	0.51
1:B:277:ARG:HG3	1:B:278:TYR:CE2	2.46	0.50
1:D:53:ARG:NH1	1:D:55:ASP:OD2	2.44	0.50
1:F:120:VAL:HG11	1:F:147:ASN:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:PRO:HA	1:A:356:ILE:HD11	1.92	0.50
1:E:374:ASP:OD2	1:E:374:ASP:N	2.42	0.50
1:F:210:LEU:HA	1:F:219:TRP:CD1	2.47	0.50
1:B:257:GLN:O	1:B:261:ARG:HG3	2.12	0.50
1:B:102:MET:HG2	4:B:425:HOH:O	2.10	0.50
1:F:94:HIS:HE1	2:F:417:HEM:O2D	1.95	0.50
1:B:279:PRO:HB3	1:B:337:THR:OG1	2.12	0.50
1:B:374:ASP:CG	1:B:374:ASP:O	2.49	0.50
1:E:136:PHE:HE2	1:E:243:ILE:HG22	1.77	0.50
1:F:16:ILE:HD12	1:F:16:ILE:C	2.32	0.50
1:B:102:MET:HG3	4:B:425:HOH:O	2.12	0.50
1:A:295:GLY:O	1:A:296:VAL:HG13	2.12	0.50
1:A:52:ALA:HA	1:A:310:LEU:HD23	1.93	0.50
1:C:71:CYS:HB2	4:C:450:HOH:O	2.10	0.49
1:A:239:VAL:HA	2:A:417:HEM:HBB1	1.94	0.49
1:E:111:VAL:O	1:E:114:GLU:HB3	2.12	0.49
1:E:375:LYS:HB2	1:E:391:PRO:HG3	1.94	0.49
1:A:109:PHE:CZ	1:A:113:LEU:HD21	2.48	0.49
1:A:6:VAL:HG12	1:A:6:VAL:O	2.13	0.49
1:C:16:ILE:HD12	1:C:305:TYR:CZ	2.47	0.49
1:B:196:LYS:HZ3	1:B:197:ARG:HH21	1.60	0.49
1:B:239:VAL:O	1:B:243:ILE:HG12	2.13	0.49
1:D:207:SER:O	1:D:208:ARG:C	2.49	0.49
1:E:30:TRP:O	1:E:310:LEU:HD11	2.13	0.49
1:F:97:PHE:CZ	1:F:223:GLU:HG2	2.48	0.49
1:C:135:ASP:HB3	4:C:399:HOH:O	2.12	0.49
1:D:343:HIS:O	2:D:417:HEM:HAA2	2.12	0.49
1:E:292:ASP:OD1	1:E:297:THR:HG23	2.13	0.49
1:F:273:GLU:CD	1:F:276:ARG:HH21	2.15	0.49
1:E:246:VAL:HG13	1:E:274:LEU:HD13	1.94	0.49
1:A:309:VAL:HG13	1:A:310:LEU:HD13	1.95	0.49
1:E:241:ALA:O	1:E:245:MET:HG2	2.12	0.49
1:B:53:ARG:O	1:B:54:GLY:C	2.51	0.48
1:C:234:GLY:HA2	3:C:397:ID3:H18B	1.94	0.48
1:A:257:GLN:HE22	1:A:369:PHE:H	1.60	0.48
1:A:257:GLN:HG2	1:A:261:ARG:NH2	2.28	0.48
1:F:106:ALA:O	1:F:110:VAL:HG23	2.13	0.48
1:D:52:ALA:O	4:D:433:HOH:O	2.20	0.48
1:C:132:GLY:HA2	1:C:394:TRP:NE1	2.29	0.48
1:C:137:VAL:HA	1:C:141:ALA:HB3	1.95	0.48
1:C:257:GLN:HE22	1:C:369:PHE:H	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:ARG:HD3	1:D:363:LEU:O	2.14	0.48
1:D:255:GLU:HG2	1:D:256:ASP:N	2.29	0.48
1:E:362:TRP:NE1	1:E:369:PHE:CZ	2.80	0.48
1:E:1:MET:N	1:E:1:MET:SD	2.87	0.48
1:A:144:LEU:HG	1:A:148:ILE:CD1	2.44	0.48
1:A:118:GLN:HA	1:A:357:VAL:HG11	1.96	0.48
1:B:309:VAL:HG22	1:B:313:LEU:HD12	1.94	0.48
1:B:87:LEU:H	1:B:230:ASN:HD21	1.61	0.48
1:D:82:MET:CE	1:D:182:LEU:HD23	2.43	0.48
1:C:183:LYS:HG3	1:C:184:GLN:N	2.27	0.48
1:C:84:PHE:CB	1:C:88:GLN:HE21	2.26	0.48
1:E:150:LEU:HD12	1:E:155:VAL:HG11	1.95	0.48
1:F:136:PHE:HE2	1:F:243:ILE:HG22	1.79	0.48
1:F:86:PRO:HG2	2:F:417:HEM:CGD	2.44	0.48
1:B:31:LYS:O	1:B:34:LEU:HB2	2.14	0.47
1:C:239:VAL:HA	2:C:417:HEM:HBB1	1.96	0.47
1:E:343:HIS:O	2:E:417:HEM:HAA2	2.13	0.47
1:F:336:THR:HG23	1:F:340:VAL:HG12	1.95	0.47
1:E:320:ALA:N	1:E:321:PRO:CD	2.76	0.47
1:A:206:PHE:O	1:A:207:SER:C	2.51	0.47
1:C:144:LEU:HB3	1:C:145:PRO:HD3	1.96	0.47
1:D:178:THR:HG22	1:D:181:GLN:CD	2.33	0.47
1:F:190:LEU:HB3	1:F:194:ILE:CD1	2.43	0.47
1:C:2:ILE:N	1:C:2:ILE:HD13	2.29	0.47
1:F:118:GLN:HG2	1:F:361:GLU:OE1	2.14	0.47
1:F:87:LEU:HD13	2:F:417:HEM:HAD2	1.97	0.47
1:A:318:PHE:O	1:A:321:PRO:HG3	2.15	0.47
1:C:82:MET:HG3	1:C:84:PHE:CZ	2.49	0.47
1:E:259:LEU:O	1:E:263:ARG:HB2	2.14	0.47
1:F:309:VAL:HG13	1:F:310:LEU:N	2.29	0.47
1:F:52:ALA:O	1:F:53:ARG:HB2	2.13	0.47
1:B:248:LEU:O	1:B:249:HIS:C	2.52	0.47
1:B:383:ASN:CB	3:B:397:ID3:H17B	2.44	0.47
1:D:241:ALA:O	1:D:245:MET:HG2	2.15	0.47
1:E:3:PRO:O	1:E:5:HIS:N	2.47	0.47
1:C:239:VAL:HA	2:C:417:HEM:CBB	2.45	0.47
1:B:159:ASP:OD1	1:B:162:ARG:NH2	2.42	0.47
1:C:248:LEU:HB3	4:C:410:HOH:O	2.15	0.47
1:F:179:VAL:O	1:F:182:LEU:HB3	2.14	0.47
1:A:170:LEU:C	1:A:172:ARG:HA	2.35	0.47
1:A:338:MET:HE2	1:A:345:CYS:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:VAL:H	1:D:169:GLN:NE2	2.13	0.47
1:D:178:THR:HG23	1:D:181:GLN:HB2	1.97	0.47
1:A:10:ARG:HD2	1:A:39:LEU:O	2.15	0.47
1:B:55:ASP:O	1:B:59:GLU:HG2	2.15	0.47
1:C:205:LEU:HD21	1:C:231:LEU:HD13	1.97	0.47
1:F:84:PHE:CE1	1:F:229:ARG:HG2	2.49	0.47
1:A:118:GLN:HG3	1:A:357:VAL:HG13	1.97	0.46
1:A:257:GLN:HE22	1:A:369:PHE:N	2.13	0.46
1:D:236:LEU:HD23	1:D:236:LEU:HA	1.72	0.46
1:E:12:VAL:HG12	1:E:13:ASP:H	1.80	0.46
1:F:24:GLN:N	1:F:24:GLN:CD	2.68	0.46
1:C:144:LEU:HG	1:C:148:ILE:HD12	1.97	0.46
1:C:53:ARG:NH1	1:C:55:ASP:OD2	2.49	0.46
1:D:141:ALA:O	1:D:145:PRO:HD3	2.15	0.46
1:E:30:TRP:HB3	1:E:310:LEU:CD1	2.45	0.46
1:F:61:TRP:CG	1:F:340:VAL:HG13	2.51	0.46
1:A:262:GLU:C	1:A:264:PRO:HD3	2.36	0.46
1:C:85:ILE:C	1:C:230:ASN:HD22	2.18	0.46
1:F:40:VAL:HG22	1:F:50:ILE:HB	1.97	0.46
1:C:85:ILE:O	1:C:227:MET:HA	2.15	0.46
1:A:144:LEU:HG	1:A:148:ILE:HD12	1.97	0.46
1:D:325:ARG:NH2	1:D:327:ASP:OD1	2.47	0.46
1:E:2:ILE:HG22	1:E:3:PRO:HD2	1.97	0.46
1:F:263:ARG:HB3	1:F:266:LEU:HD22	1.97	0.46
1:F:279:PRO:HG2	1:F:309:VAL:HA	1.97	0.46
1:E:149:PHE:CZ	1:E:190:LEU:HD21	2.51	0.46
1:F:38:GLY:HA3	1:F:53:ARG:NH2	2.31	0.46
1:E:217:ARG:NH1	1:E:223:GLU:OE1	2.43	0.46
1:A:31:LYS:HE2	1:A:313:LEU:HB3	1.98	0.45
1:D:148:ILE:HD13	1:D:354:GLU:HG2	1.97	0.45
1:B:172:ARG:HB2	1:B:174:ASP:OD1	2.16	0.45
1:B:245:MET:HE2	1:B:245:MET:HB3	1.53	0.45
1:E:106:ALA:O	1:E:110:VAL:HG23	2.16	0.45
1:E:11:VAL:HA	1:E:41:TRP:O	2.16	0.45
1:C:313:LEU:HD23	1:C:313:LEU:N	2.31	0.45
1:D:155:VAL:O	1:D:155:VAL:HG23	2.15	0.45
1:D:16:ILE:HD11	1:D:74:VAL:HG21	1.97	0.45
1:A:198:MET:HG3	1:A:210:LEU:HD13	1.98	0.45
1:A:5:HIS:HE1	1:A:302:ASP:OD1	1.99	0.45
1:A:310:LEU:O	1:A:314:ASP:HB2	2.17	0.45
1:C:383:ASN:HB3	3:C:397:ID3:H17B	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ALA:O	1:A:145:PRO:CD	2.64	0.45
1:D:103:LYS:HE2	1:D:212:GLU:OE1	2.16	0.45
1:D:135:ASP:HB3	4:D:405:HOH:O	2.16	0.45
1:F:56:VAL:CG1	1:F:60:LEU:HD22	2.46	0.45
1:B:258:ARG:NH1	1:B:368:GLU:OE2	2.49	0.45
1:B:77:GLY:O	1:B:81:VAL:HG23	2.17	0.45
1:D:68:SER:OG	1:D:90:ASP:OD2	2.31	0.45
1:F:198:MET:HB2	1:F:198:MET:HE2	1.80	0.45
1:D:166:LEU:O	1:D:169:GLN:HG2	2.17	0.45
1:D:309:VAL:CG2	1:D:313:LEU:HD12	2.47	0.45
1:E:131:ARG:NH2	1:E:134:CYS:HA	2.31	0.45
1:E:225:ARG:O	1:E:229:ARG:HB2	2.17	0.45
1:F:336:THR:O	1:F:336:THR:HG22	2.17	0.45
1:F:53:ARG:O	1:F:54:GLY:C	2.55	0.45
1:B:125:MET:HG2	1:B:366:MET:SD	2.57	0.45
1:B:85:ILE:O	1:B:227:MET:HA	2.16	0.45
1:C:191:TRP:HA	1:C:191:TRP:CE3	2.52	0.45
1:D:42:SER:O	1:D:47:GLY:HA2	2.17	0.45
1:E:124:LEU:HD21	1:E:143:ILE:HB	1.99	0.45
1:E:189:TYR:O	1:E:192:PRO:HD2	2.17	0.45
1:B:140:PHE:CE2	1:B:144:LEU:HD22	2.52	0.45
1:B:18:ASN:HA	1:B:19:PRO:HD3	1.73	0.45
1:D:194:ILE:O	1:D:198:MET:HG3	2.16	0.45
1:C:53:ARG:O	1:C:57:VAL:HG23	2.18	0.44
1:B:118:GLN:HA	1:B:357:VAL:HG11	1.99	0.44
1:B:83:GLN:HB3	1:B:226:ARG:HE	1.82	0.44
1:D:67:LEU:HD21	1:D:291:VAL:HG21	1.98	0.44
1:B:114:GLU:N	1:B:115:PRO:CD	2.79	0.44
1:B:257:GLN:NE2	1:B:261:ARG:NH2	2.58	0.44
1:E:98:ARG:CG	1:E:98:ARG:HH11	2.30	0.44
1:F:344:ARG:HD2	4:F:421:HOH:O	2.16	0.44
1:B:257:GLN:HE22	1:B:369:PHE:H	1.66	0.44
1:D:257:GLN:HE22	1:D:369:PHE:H	1.65	0.44
1:E:155:VAL:HG21	1:E:160:ARG:HG2	1.99	0.44
1:A:72:LEU:HD22	1:A:88:GLN:NE2	2.33	0.44
1:D:21:GLY:O	1:D:22:VAL:C	2.54	0.44
1:D:34:LEU:HD13	1:D:310:LEU:HG	2.00	0.44
1:F:392:LEU:CB	1:F:394:TRP:HZ3	2.30	0.44
1:E:54:GLY:HA2	1:E:311:HIS:HA	2.00	0.44
1:F:184:GLN:O	1:F:185:ALA:C	2.55	0.44
1:A:166:LEU:HD12	1:A:166:LEU:HA	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:397:ID3:H17A	3:A:397:ID3:H4A	2.00	0.44
1:C:113:LEU:HD13	1:C:152:LEU:HD22	1.98	0.44
1:A:214:VAL:O	1:A:217:ARG:HG3	2.18	0.44
1:C:380:LYS:HD3	1:C:388:THR:CG2	2.47	0.44
1:D:94:HIS:HE1	2:D:417:HEM:O2D	2.00	0.44
1:D:82:MET:O	1:D:229:ARG:NH1	2.46	0.44
1:F:2:ILE:HG22	1:F:3:PRO:HD2	2.00	0.44
1:F:77:GLY:O	1:F:81:VAL:HG23	2.18	0.44
1:A:263:ARG:HD3	1:A:265:ASP:OD1	2.18	0.43
1:B:209:ILE:O	1:B:212:GLU:HB2	2.17	0.43
1:B:261:ARG:HD3	1:B:363:LEU:O	2.18	0.43
1:F:136:PHE:HD1	1:F:392:LEU:CD1	2.31	0.43
1:A:165:GLN:HE21	1:A:165:GLN:HA	1.83	0.43
1:A:53:ARG:O	1:A:57:VAL:HG23	2.18	0.43
1:D:203:ASP:N	1:D:203:ASP:OD1	2.51	0.43
1:E:57:VAL:O	1:E:61:TRP:HB2	2.18	0.43
1:C:55:ASP:OD1	1:C:55:ASP:N	2.51	0.43
1:F:352:ARG:O	1:F:356:ILE:HG13	2.18	0.43
1:A:159:ASP:N	1:A:159:ASP:OD1	2.52	0.43
1:B:120:VAL:HG11	1:B:147:ASN:HB3	2.00	0.43
1:B:260:LEU:HB2	1:B:363:LEU:HD13	2.00	0.43
1:C:145:PRO:HG2	1:C:240:ALA:HB2	2.00	0.43
1:E:142:GLU:OE1	4:E:435:HOH:O	2.21	0.43
1:F:150:LEU:HA	1:F:150:LEU:HD12	1.87	0.43
1:A:174:ASP:HB2	1:A:175:GLY:HA2	2.01	0.43
1:B:236:LEU:HA	1:B:236:LEU:HD23	1.77	0.43
1:C:78:LEU:HG	1:C:179:VAL:HG21	2.01	0.43
1:D:53:ARG:NH1	1:D:55:ASP:OD1	2.51	0.43
1:E:196:LYS:HE2	1:E:200:GLN:HG3	2.01	0.43
1:B:212:GLU:OE2	1:B:213:PRO:HD2	2.18	0.43
1:B:384:VAL:HG23	3:B:397:ID3:H17A	2.00	0.43
1:D:309:VAL:HG23	1:D:313:LEU:CD1	2.48	0.43
1:E:152:LEU:HD13	1:E:205:LEU:HD22	2.00	0.43
3:A:397:ID3:H17A	3:A:397:ID3:C4	2.49	0.43
1:B:136:PHE:HE2	1:B:243:ILE:HG22	1.82	0.43
1:C:125:MET:HE1	1:C:365:GLY:HA3	2.00	0.43
1:C:206:PHE:HE1	1:C:231:LEU:HD12	1.83	0.43
1:C:380:LYS:HD3	1:C:388:THR:HG22	2.01	0.43
1:D:249:HIS:ND1	1:D:278:TYR:OH	2.44	0.43
1:D:336:THR:O	1:D:337:THR:C	2.56	0.43
1:E:336:THR:HG23	1:E:340:VAL:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:343:HIS:ND1	2:E:417:HEM:O1D	2.43	0.43
1:A:48:HIS:HD2	1:A:49:TRP:O	2.01	0.43
1:C:114:GLU:HB3	1:C:115:PRO:CD	2.46	0.43
1:C:98:ARG:NH2	1:C:344:ARG:O	2.41	0.43
1:E:87:LEU:HA	1:E:87:LEU:HD12	1.54	0.43
1:E:95:LYS:CB	1:E:95:LYS:NZ	2.82	0.43
1:F:349:GLY:O	1:F:352:ARG:HB3	2.18	0.43
1:B:245:MET:CE	1:B:248:LEU:HD23	2.49	0.43
1:D:19:PRO:HA	1:D:20:PRO:HD3	1.71	0.43
1:B:343:HIS:O	2:B:417:HEM:HAA2	2.19	0.43
3:B:397:ID3:H7	3:B:397:ID3:H18	1.80	0.43
1:C:350:LEU:HD12	1:C:350:LEU:HA	1.80	0.43
1:C:85:ILE:HG12	1:C:89:GLN:CD	2.40	0.43
1:F:372:ALA:HA	1:F:373:PRO:HD2	1.72	0.43
1:B:325:ARG:NE	1:B:327:ASP:OD2	2.47	0.42
1:B:89:GLN:O	1:B:343:HIS:HE1	2.01	0.42
1:F:40:VAL:HG22	1:F:50:ILE:O	2.18	0.42
1:F:49:TRP:CD1	1:F:302:ASP:HB3	2.54	0.42
1:F:40:VAL:CG2	1:F:50:ILE:HB	2.48	0.42
1:A:86:PRO:HD2	2:A:417:HEM:HMD2	2.01	0.42
1:B:16:ILE:CD1	1:B:305:TYR:CZ	3.03	0.42
1:B:344:ARG:O	1:B:345:CYS:C	2.57	0.42
1:C:263:ARG:O	1:C:265:ASP:N	2.52	0.42
1:D:155:VAL:O	1:D:155:VAL:CG2	2.67	0.42
1:D:31:LYS:O	1:D:34:LEU:HB2	2.19	0.42
1:D:53:ARG:HH11	1:D:53:ARG:HD2	1.65	0.42
1:E:338:MET:CE	1:E:348:ALA:HA	2.49	0.42
1:A:65:GLU:OE2	1:F:91:GLY:HA2	2.18	0.42
1:C:125:MET:CE	1:C:365:GLY:HA3	2.49	0.42
1:D:49:TRP:CD1	1:D:298:ILE:HG23	2.55	0.42
1:E:6:VAL:CG1	1:E:41:TRP:HB3	2.47	0.42
1:B:141:ALA:O	1:B:145:PRO:HD3	2.16	0.42
1:B:5:HIS:H	1:B:5:HIS:CD2	2.37	0.42
1:C:336:THR:O	1:C:336:THR:HG22	2.19	0.42
1:C:128:LEU:O	1:C:131:ARG:HB2	2.19	0.42
1:F:281:VAL:HG21	2:F:417:HEM:HHB	2.01	0.42
1:A:320:ALA:N	1:A:321:PRO:HD3	2.34	0.42
1:A:97:PHE:CZ	1:A:214:VAL:HG11	2.55	0.42
1:B:87:LEU:O	1:B:87:LEU:HD12	2.19	0.42
1:E:160:ARG:O	1:E:164:ARG:HB2	2.20	0.42
1:A:222:ASP:O	1:A:225:ARG:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:THR:HG23	1:C:171:THR:O	2.17	0.42
1:C:295:GLY:O	1:C:296:VAL:HG12	2.19	0.42
1:E:8:ALA:O	1:E:10:ARG:N	2.51	0.42
1:A:205:LEU:CD2	1:A:231:LEU:HD13	2.49	0.42
1:C:113:LEU:HA	1:C:113:LEU:HD23	1.63	0.42
1:B:207:SER:O	1:B:208:ARG:C	2.58	0.42
1:C:231:LEU:HD23	1:C:231:LEU:HA	1.64	0.42
1:C:52:ALA:HA	1:C:310:LEU:HD23	2.00	0.42
1:B:166:LEU:O	1:B:169:GLN:HB2	2.20	0.42
1:B:16:ILE:HD12	1:B:305:TYR:CZ	2.55	0.42
1:B:170:LEU:HD13	1:B:232:LEU:HD21	2.01	0.42
1:C:333:ILE:HG13	1:C:344:ARG:CZ	2.50	0.42
1:D:371:LEU:O	1:D:372:ALA:C	2.57	0.42
1:E:125:MET:C	1:E:125:MET:SD	2.99	0.42
1:E:160:ARG:H	1:E:160:ARG:HG3	1.60	0.42
1:F:129:ARG:HB3	1:F:130:PRO:CD	2.50	0.42
1:D:118:GLN:HA	1:D:357:VAL:CG1	2.50	0.41
1:D:168:VAL:HA	1:D:171:THR:HG23	2.02	0.41
1:F:156:PRO:O	1:F:159:ASP:HB2	2.19	0.41
1:F:133:SER:HA	1:F:392:LEU:O	2.20	0.41
1:B:148:ILE:O	1:B:149:PHE:C	2.58	0.41
1:B:172:ARG:HE	1:B:172:ARG:HB3	1.60	0.41
1:C:307:PRO:HG3	1:C:310:LEU:HD22	2.01	0.41
1:E:380:LYS:HB3	1:E:380:LYS:HE2	1.29	0.41
1:E:87:LEU:H	1:E:230:ASN:ND2	2.17	0.41
1:E:90:ASP:N	4:E:421:HOH:O	2.36	0.41
1:F:155:VAL:HG23	1:F:156:PRO:O	2.20	0.41
1:C:122:ARG:HB2	1:C:361:GLU:OE2	2.21	0.41
1:C:362:TRP:O	1:C:366:MET:CB	2.68	0.41
1:D:170:LEU:HA	1:D:170:LEU:HD12	1.68	0.41
1:B:307:PRO:CG	1:B:310:LEU:HD22	2.49	0.41
1:C:40:VAL:O	1:C:49:TRP:HA	2.20	0.41
1:D:190:LEU:O	1:D:191:TRP:C	2.59	0.41
1:E:149:PHE:C	1:E:149:PHE:CD2	2.93	0.41
1:A:239:VAL:HA	2:A:417:HEM:CBB	2.50	0.41
1:B:375:LYS:HB2	1:B:391:PRO:HG3	2.03	0.41
1:C:158:GLU:O	1:C:161:PRO:HD2	2.21	0.41
1:D:87:LEU:O	1:D:87:LEU:HD12	2.20	0.41
1:E:8:ALA:O	1:E:11:VAL:HG23	2.20	0.41
1:A:248:LEU:O	1:A:249:HIS:C	2.57	0.41
1:E:263:ARG:HD3	1:E:266:LEU:HD21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:249:HIS:HD2	1:F:250:LEU:HD23	1.86	0.41
1:F:57:VAL:HG12	1:F:311:HIS:HB2	2.02	0.41
1:B:89:GLN:O	1:B:343:HIS:CE1	2.73	0.41
1:E:380:LYS:HG2	1:E:381:GLY:N	2.35	0.41
1:D:66:ARG:NH1	1:E:395:ARG:HD2	2.35	0.41
1:E:70:GLN:NE2	4:E:421:HOH:O	2.51	0.41
1:A:299:ARG:O	1:A:300:LYS:C	2.59	0.41
1:A:58:ARG:HH11	1:A:311:HIS:CD2	2.39	0.41
1:D:129:ARG:HE	1:D:129:ARG:HB3	1.60	0.41
1:E:48:HIS:HD2	1:E:49:TRP:O	2.04	0.41
1:F:61:TRP:CD1	1:F:340:VAL:HG13	2.56	0.41
1:A:49:TRP:CD1	1:A:298:ILE:HG23	2.56	0.41
1:B:50:ILE:HG22	1:B:51:ALA:O	2.21	0.41
1:C:153:ILE:C	1:C:197:ARG:HH12	2.14	0.41
1:C:279:PRO:HG2	1:C:309:VAL:HA	2.03	0.41
1:C:257:GLN:NE2	1:C:368:GLU:HG3	2.36	0.41
1:C:61:TRP:HB3	1:C:340:VAL:HG13	2.03	0.41
1:E:136:PHE:CD1	1:E:392:LEU:HD12	2.56	0.41
1:F:136:PHE:HD1	1:F:392:LEU:HD11	1.85	0.41
1:F:258:ARG:HH11	1:F:258:ARG:HG3	1.86	0.41
1:F:54:GLY:N	1:F:314:ASP:OD2	2.50	0.41
1:F:54:GLY:HA3	1:F:317:SER:OG	2.21	0.41
1:F:350:LEU:O	1:F:353:MET:HB3	2.20	0.41
1:B:117:VAL:HG13	1:B:148:ILE:HG12	2.03	0.41
1:C:27:PHE:CZ	1:C:278:TYR:HD1	2.39	0.41
1:D:107:SER:O	1:D:111:VAL:HG23	2.21	0.41
1:E:125:MET:CE	1:E:126:GLU:HG3	2.50	0.41
1:B:109:PHE:HA	1:B:109:PHE:HD1	1.76	0.41
1:E:101:VAL:HA	1:E:209:ILE:HG12	2.03	0.41
1:F:136:PHE:HB3	1:F:390:LEU:HB3	2.02	0.41
1:A:260:LEU:HB3	1:A:363:LEU:HD13	2.02	0.40
1:A:263:ARG:NH1	1:A:265:ASP:OD2	2.54	0.40
1:A:352:ARG:HH21	1:A:352:ARG:HD3	1.77	0.40
1:C:132:GLY:HA3	4:C:447:HOH:O	2.21	0.40
1:D:53:ARG:O	1:D:54:GLY:C	2.59	0.40
4:B:439:HOH:O	1:D:5:HIS:CD2	2.69	0.40
1:E:212:GLU:HA	1:E:213:PRO:HD2	1.86	0.40
1:D:262:GLU:O	1:D:264:PRO:HD2	2.21	0.40
1:E:191:TRP:O	1:E:192:PRO:C	2.57	0.40
1:A:338:MET:CE	1:A:345:CYS:CB	3.00	0.40
1:B:141:ALA:O	1:B:145:PRO:HD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:ASP:O	1:D:59:GLU:HG2	2.21	0.40
1:F:159:ASP:HA	4:F:425:HOH:O	2.20	0.40
1:B:14:PHE:CZ	1:B:19:PRO:HB3	2.56	0.40
1:C:336:THR:HG23	1:C:340:VAL:HG12	2.03	0.40
1:E:32:THR:O	1:E:35:ASP:HB2	2.21	0.40
1:F:149:PHE:CD2	1:F:149:PHE:C	2.94	0.40
1:A:78:LEU:HA	1:A:179:VAL:HG21	2.02	0.40
1:B:53:ARG:HH11	1:B:55:ASP:CG	2.25	0.40
1:C:170:LEU:C	1:C:172:ARG:HG3	2.42	0.40
1:D:168:VAL:N	1:D:169:GLN:NE2	2.70	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:LYS:NZ	1:D:200:GLN:OE1[1_455]	2.19	0.01

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	394/396 (100%)	355 (90%)	34 (9%)	5 (1%)	14	41
1	B	394/396 (100%)	365 (93%)	25 (6%)	4 (1%)	18	50
1	C	394/396 (100%)	360 (91%)	30 (8%)	4 (1%)	18	50
1	D	390/396 (98%)	351 (90%)	38 (10%)	1 (0%)	44	77
1	E	386/396 (98%)	331 (86%)	42 (11%)	13 (3%)	4	15
1	F	386/396 (98%)	321 (83%)	52 (14%)	13 (3%)	4	15
All	All	2344/2376 (99%)	2083 (89%)	221 (9%)	40 (2%)	11	34

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	LEU
1	A	172	ARG
1	B	172	ARG
1	B	173	PRO
1	B	174	ASP
1	C	172	ARG
1	C	173	PRO
1	E	9	ASP
1	F	4	ALA
1	A	173	PRO
1	E	152	LEU
1	E	195	GLU
1	C	72	LEU
1	C	169	GLN
1	E	194	ILE
1	E	307	PRO
1	E	345	CYS
1	F	3	PRO
1	F	53	ARG
1	F	152	LEU
1	F	168	VAL
1	A	175	GLY
1	E	3	PRO
1	E	158	GLU
1	E	169	GLN
1	F	7	PRO
1	F	133	SER
1	F	362	TRP
1	A	174	ASP
1	B	14	PHE
1	D	33	LEU
1	E	157	LEU
1	E	367	PRO
1	F	130	PRO
1	F	194	ILE
1	E	7	PRO
1	E	346	VAL
1	F	47	GLY
1	F	156	PRO
1	F	54	GLY

### 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	321/321 (100%)	287 (89%)	34 (11%)	8	23
1	B	321/321 (100%)	290 (90%)	31 (10%)	9	27
1	C	321/321 (100%)	295 (92%)	26 (8%)	14	37
1	D	319/321 (99%)	296 (93%)	23 (7%)	17	43
1	E	316/321 (98%)	279 (88%)	37 (12%)	6	19
1	F	316/321 (98%)	278 (88%)	38 (12%)	6	18
All	All	1914/1926 (99%)	1725 (90%)	189 (10%)	9	26

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	18	ASN
1	A	23	GLU
1	A	31	LYS
1	A	34	LEU
1	A	58	ARG
1	A	60	LEU
1	A	78	LEU
1	A	123	LYS
1	A	131	ARG
1	A	150	LEU
1	A	157	LEU
1	A	159	ASP
1	A	165	GLN
1	A	166	LEU
1	A	170	LEU
1	A	172	ARG
1	A	174	ASP
1	A	183	LYS
1	A	196	LYS
1	A	197	ARG
1	A	208	ARG

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Mol	Chain	Res	Type
1	A	217	ARG
1	A	227	MET
1	A	237	ASP
1	A	266	LEU
1	A	268	PRO
1	A	300	LYS
1	A	303	LEU
1	A	310	LEU
1	A	340	VAL
1	A	366	MET
1	A	380	LYS
1	A	395	ARG
1	B	1	MET
1	B	18	ASN
1	B	24	GLN
1	B	34	LEU
1	B	60	LEU
1	B	75	THR
1	B	78	LEU
1	B	116	LYS
1	B	146	LEU
1	B	150	LEU
1	B	157	LEU
1	B	171	THR
1	B	172	ARG
1	B	173	PRO
1	B	174	ASP
1	B	176	SER
1	B	181	GLN
1	B	183	LYS
1	B	196	LYS
1	B	197	ARG
1	B	221	VAL
1	B	237	ASP
1	B	238	THR
1	B	266	LEU
1	B	310	LEU
1	B	330	LEU
1	B	340	VAL
1	B	366	MET
1	B	374	ASP
1	B	378	THR

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Mol	Chain	Res	Type
1	B	380	LYS
1	C	9	ASP
1	C	18	ASN
1	C	24	GLN
1	C	34	LEU
1	C	35	ASP
1	C	60	LEU
1	C	69	SER
1	C	78	LEU
1	C	82	MET
1	C	86	PRO
1	C	108	ARG
1	C	150	LEU
1	C	157	LEU
1	C	166	LEU
1	C	169	GLN
1	C	170	LEU
1	C	171	THR
1	C	172	ARG
1	C	178	THR
1	C	197	ARG
1	C	236	LEU
1	C	268	PRO
1	C	300	LYS
1	C	303	LEU
1	C	310	LEU
1	C	340	VAL
1	D	9	ASP
1	D	34	LEU
1	D	60	LEU
1	D	70	GLN
1	D	75	THR
1	D	78	LEU
1	D	116	LYS
1	D	138	SER
1	D	157	LEU
1	D	169	GLN
1	D	170	LEU
1	D	171	THR
1	D	172	ARG
1	D	178	THR
1	D	183	LYS

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Mol	Chain	Res	Type
1	D	221	VAL
1	D	236	LEU
1	D	266	LEU
1	D	310	LEU
1	D	332	PRO
1	D	340	VAL
1	D	366	MET
1	D	380	LYS
1	E	1	MET
1	E	2	ILE
1	E	23	GLU
1	E	31	LYS
1	E	70	GLN
1	E	74	VAL
1	E	75	THR
1	E	78	LEU
1	E	80	LYS
1	E	82	MET
1	E	95	LYS
1	E	102	MET
1	E	103	LYS
1	E	107	SER
1	E	108	ARG
1	E	114	GLU
1	E	120	VAL
1	E	134	CYS
1	E	138	SER
1	E	150	LEU
1	E	158	GLU
1	E	166	LEU
1	E	168	VAL
1	E	177	MET
1	E	183	LYS
1	E	196	LYS
1	E	243	ILE
1	E	263	ARG
1	E	300	LYS
1	E	317	SER
1	E	330	LEU
1	E	340	VAL
1	E	357	VAL
1	E	363	LEU

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Mol	Chain	Res	Type
1	E	380	LYS
1	E	390	LEU
1	E	395	ARG
1	F	2	ILE
1	F	10	ARG
1	F	11	VAL
1	F	12	VAL
1	F	22	VAL
1	F	24	GLN
1	F	32	THR
1	F	34	LEU
1	F	57	VAL
1	F	74	VAL
1	F	78	LEU
1	F	80	LYS
1	F	103	LYS
1	F	107	SER
1	F	108	ARG
1	F	120	VAL
1	F	123	LYS
1	F	133	SER
1	F	144	LEU
1	F	150	LEU
1	F	158	GLU
1	F	160	ARG
1	F	166	LEU
1	F	169	GLN
1	F	177	MET
1	F	179	VAL
1	F	183	LYS
1	F	198	MET
1	F	237	ASP
1	F	238	THR
1	F	248	LEU
1	F	303	LEU
1	F	330	LEU
1	F	340	VAL
1	F	357	VAL
1	F	374	ASP
1	F	380	LYS
1	F	395	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	A	88	GLN
1	A	94	HIS
1	A	165	GLN
1	A	230	ASN
1	A	257	GLN
1	A	311	HIS
1	B	5	HIS
1	B	48	HIS
1	B	88	GLN
1	B	230	ASN
1	B	257	GLN
1	B	311	HIS
1	C	5	HIS
1	C	48	HIS
1	C	88	GLN
1	C	230	ASN
1	C	257	GLN
1	C	311	HIS
1	D	5	HIS
1	D	45	ASN
1	D	48	HIS
1	D	88	GLN
1	D	94	HIS
1	D	169	GLN
1	D	200	GLN
1	D	230	ASN
1	D	257	GLN
1	D	311	HIS
1	E	5	HIS
1	E	48	HIS
1	E	83	GLN
1	E	88	GLN
1	E	89	GLN
1	E	94	HIS
1	E	165	GLN
1	E	230	ASN
1	E	257	GLN
1	E	311	HIS
1	F	5	HIS
1	F	48	HIS
1	F	83	GLN

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Mol	Chain	Res	Type
1	F	88	GLN
1	F	94	HIS
1	F	165	GLN
1	F	230	ASN
1	F	257	GLN
1	F	311	HIS

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	ID3	A	397	-	14,14,14	1.85	7 (50%)	20,20,20	2.18	6 (30%)
2	HEM	A	417	1	28,50,50	2.44	10 (35%)	17,82,82	2.57	6 (35%)
3	ID3	B	397	-	14,14,14	1.75	6 (42%)	20,20,20	3.01	7 (35%)
2	HEM	B	417	1	28,50,50	2.56	12 (42%)	17,82,82	1.81	4 (23%)
3	ID3	C	397	-	14,14,14	2.10	7 (50%)	20,20,20	2.69	8 (40%)
2	HEM	C	417	1	28,50,50	2.54	9 (32%)	17,82,82	2.15	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HEM	D	417	1	28,50,50	2.34	9 (32%)	17,82,82	2.28	6 (35%)
2	HEM	E	417	1	28,50,50	2.59	9 (32%)	17,82,82	2.41	7 (41%)
2	HEM	F	417	1	28,50,50	2.64	11 (39%)	17,82,82	2.48	5 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ID3	A	397	-	-	0/5/22/22	0/1/1/1
2	HEM	A	417	1	-	0/6/54/54	0/0/8/8
3	ID3	B	397	-	-	2/5/22/22	0/1/1/1
2	HEM	B	417	1	-	0/6/54/54	0/0/8/8
3	ID3	C	397	-	-	0/5/22/22	0/1/1/1
2	HEM	C	417	1	-	0/6/54/54	0/0/8/8
2	HEM	D	417	1	-	0/6/54/54	0/0/8/8
2	HEM	E	417	1	-	0/6/54/54	0/0/8/8
2	HEM	F	417	1	-	0/6/54/54	0/0/8/8

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	417	HEM	C3B-C2B	-6.62	1.31	1.40
2	B	417	HEM	C3B-C2B	-6.35	1.32	1.40
2	D	417	HEM	C3B-C2B	-5.95	1.32	1.40
2	E	417	HEM	C3C-C2C	-4.99	1.33	1.40
2	E	417	HEM	C3B-C2B	-4.96	1.33	1.40
2	C	417	HEM	C1A-CHA	-4.58	1.28	1.40
2	C	417	HEM	C3B-C2B	-4.38	1.34	1.40
2	A	417	HEM	C3C-C2C	-4.19	1.34	1.40
2	F	417	HEM	C3C-C2C	-3.87	1.35	1.40
2	A	417	HEM	C3B-C2B	-3.17	1.36	1.40
2	D	417	HEM	C3C-C2C	-2.74	1.36	1.40
2	A	417	HEM	C1A-CHA	-2.53	1.33	1.40
2	D	417	HEM	C1A-CHA	-2.37	1.33	1.40
2	B	417	HEM	C1A-CHA	-2.30	1.34	1.40
2	B	417	HEM	C3C-C2C	-2.12	1.37	1.40
3	A	397	ID3	C2-C3	2.00	1.57	1.52
3	B	397	ID3	C4-C5	2.03	1.55	1.51
2	F	417	HEM	CMD-C2D	2.04	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	417	HEM	C4A-NA	2.08	1.40	1.36
3	A	397	ID3	C8-C7	2.08	1.39	1.33
2	B	417	HEM	C4D-ND	2.18	1.39	1.36
3	A	397	ID3	C5-C6	2.21	1.38	1.34
3	C	397	ID3	C2-C1	2.21	1.59	1.54
2	B	417	HEM	C1D-ND	2.23	1.40	1.36
2	F	417	HEM	C1D-ND	2.27	1.41	1.36
3	C	397	ID3	C8-C7	2.30	1.40	1.33
2	F	417	HEM	CAD-C3D	2.32	1.56	1.52
3	B	397	ID3	C7-C6	2.41	1.54	1.45
2	E	417	HEM	CMC-C2C	2.41	1.56	1.51
3	B	397	ID3	C8-C7	2.44	1.40	1.33
3	B	397	ID3	C2-C3	2.44	1.58	1.52
2	A	417	HEM	CMA-C3A	2.50	1.56	1.51
2	D	417	HEM	CMB-C2B	2.54	1.57	1.51
2	A	417	HEM	CMD-C2D	2.55	1.56	1.51
2	F	417	HEM	C3B-CAB	2.55	1.53	1.47
2	B	417	HEM	CMC-C2C	2.58	1.57	1.51
3	A	397	ID3	C8-C9	2.60	1.55	1.47
2	B	417	HEM	C3B-CAB	2.63	1.53	1.47
2	E	417	HEM	CMD-C2D	2.64	1.57	1.51
3	A	397	ID3	C1-C6	2.72	1.57	1.53
3	C	397	ID3	C5-C6	2.75	1.39	1.34
2	F	417	HEM	CAA-C2A	2.76	1.56	1.52
2	B	417	HEM	C4C-NC	2.78	1.40	1.36
3	C	397	ID3	C8-C9	2.79	1.55	1.47
2	F	417	HEM	CMA-C3A	2.79	1.57	1.51
3	A	397	ID3	C7-C6	2.81	1.55	1.45
2	A	417	HEM	CMC-C2C	2.82	1.57	1.51
3	B	397	ID3	C1-C6	2.83	1.57	1.53
3	C	397	ID3	C7-C6	2.89	1.56	1.45
2	B	417	HEM	CMB-C2B	2.91	1.57	1.51
2	D	417	HEM	C1C-NC	2.92	1.40	1.36
3	A	397	ID3	C4-C5	2.92	1.57	1.51
3	B	397	ID3	C2-C1	2.96	1.61	1.54
2	B	417	HEM	CMA-C3A	2.97	1.57	1.51
2	C	417	HEM	C3B-CAB	2.98	1.53	1.47
2	C	417	HEM	C1D-ND	3.00	1.42	1.36
2	C	417	HEM	C1B-NB	3.04	1.40	1.36
2	A	417	HEM	C3B-CAB	3.05	1.53	1.47
2	E	417	HEM	C3B-CAB	3.12	1.54	1.47
3	C	397	ID3	C1-C6	3.21	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	417	HEM	CMB-C2B	3.22	1.58	1.51
3	C	397	ID3	C4-C5	3.58	1.58	1.51
2	E	417	HEM	CMA-C3A	3.67	1.59	1.51
2	F	417	HEM	C1C-NC	3.72	1.41	1.36
2	E	417	HEM	CMB-C2B	3.84	1.59	1.51
2	A	417	HEM	C1D-ND	4.28	1.45	1.36
2	D	417	HEM	CMA-C3A	4.40	1.60	1.51
2	D	417	HEM	C3D-C2D	4.63	1.51	1.37
2	C	417	HEM	C3C-CAC	4.68	1.57	1.47
2	C	417	HEM	C3D-C2D	4.75	1.51	1.37
2	B	417	HEM	C3D-C2D	4.81	1.51	1.37
2	D	417	HEM	C3C-CAC	4.92	1.57	1.47
2	A	417	HEM	C3C-CAC	5.37	1.58	1.47
2	E	417	HEM	C3D-C2D	5.49	1.53	1.37
2	F	417	HEM	C3C-CAC	5.62	1.58	1.47
2	E	417	HEM	C3C-CAC	5.67	1.59	1.47
2	C	417	HEM	C4C-NC	5.79	1.43	1.36
2	F	417	HEM	C3D-C2D	5.86	1.55	1.37
2	A	417	HEM	C3D-C2D	6.36	1.56	1.37
2	B	417	HEM	C3C-CAC	6.38	1.60	1.47

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	397	ID3	C18-C5-C6	-7.57	116.03	124.51
3	A	397	ID3	C1-C6-C5	-6.44	113.55	122.59
3	C	397	ID3	C1-C6-C5	-5.69	114.59	122.59
3	C	397	ID3	C18-C5-C6	-5.58	118.27	124.51
2	E	417	HEM	C1D-C2D-C3D	-5.47	103.19	107.00
2	D	417	HEM	CBA-CAA-C2A	-5.18	102.57	112.48
3	B	397	ID3	C1-C6-C5	-5.17	115.32	122.59
2	C	417	HEM	CBA-CAA-C2A	-4.73	103.44	112.48
2	A	417	HEM	CBA-CAA-C2A	-4.63	103.63	112.48
3	B	397	ID3	C17-C1-C6	-4.60	102.85	110.31
2	F	417	HEM	C1D-C2D-C3D	-4.56	103.83	107.00
2	B	417	HEM	CBA-CAA-C2A	-4.34	104.19	112.48
2	D	417	HEM	CMA-C3A-C4A	-4.14	122.10	128.46
3	A	397	ID3	C18-C5-C6	-3.77	120.28	124.51
2	F	417	HEM	C3C-C4C-NC	-3.19	104.92	110.94
3	C	397	ID3	C17-C1-C6	-3.17	105.16	110.31
2	B	417	HEM	CMA-C3A-C4A	-2.81	124.14	128.46
2	E	417	HEM	C3C-C4C-NC	-2.81	105.64	110.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	397	ID3	C16-C1-C6	-2.39	106.43	110.31
2	E	417	HEM	CMA-C3A-C4A	-2.28	124.96	128.46
2	A	417	HEM	C3C-C4C-NC	-2.17	106.84	110.94
2	E	417	HEM	CAD-C3D-C2D	-2.15	122.86	129.00
3	A	397	ID3	C16-C1-C6	-2.10	106.90	110.31
2	D	417	HEM	C3C-C4C-NC	-2.00	107.17	110.94
3	A	397	ID3	C18-C5-C4	2.01	117.27	113.45
3	C	397	ID3	C1-C6-C7	2.05	121.49	115.73
3	C	397	ID3	C18-C5-C4	2.09	117.41	113.45
2	B	417	HEM	CMA-C3A-C2A	2.24	129.16	124.94
3	A	397	ID3	C2-C1-C6	2.35	114.15	110.48
2	C	417	HEM	C4C-C3C-C2C	2.43	108.59	106.90
2	D	417	HEM	CMC-C2C-C3C	2.44	129.42	124.89
3	B	397	ID3	O1-C9-C19	2.55	125.47	119.13
2	C	417	HEM	CAD-CBD-CGD	2.77	117.39	112.66
2	E	417	HEM	CAA-CBA-CGA	2.95	117.69	112.66
3	B	397	ID3	C1-C6-C7	2.95	124.01	115.73
2	F	417	HEM	CAD-CBD-CGD	3.05	117.87	112.66
2	B	417	HEM	CMB-C2B-C3B	3.08	130.62	124.89
2	A	417	HEM	CMB-C2B-C3B	3.12	130.69	124.89
3	A	397	ID3	C7-C8-C9	3.26	129.28	123.90
2	E	417	HEM	CMD-C2D-C1D	3.28	133.50	128.46
2	D	417	HEM	CMA-C3A-C2A	3.52	131.59	124.94
2	C	417	HEM	CMB-C2B-C3B	3.58	131.53	124.89
2	C	417	HEM	CMC-C2C-C3C	3.59	131.56	124.89
2	D	417	HEM	C4C-C3C-C2C	3.69	109.47	106.90
2	F	417	HEM	CAA-CBA-CGA	3.84	119.22	112.66
2	A	417	HEM	CAD-CBD-CGD	3.96	119.43	112.66
2	A	417	HEM	CMC-C2C-C3C	4.01	132.33	124.89
3	B	397	ID3	C2-C1-C6	4.19	117.03	110.48
2	E	417	HEM	C4C-C3C-C2C	4.39	109.97	106.90
3	C	397	ID3	C7-C8-C9	4.79	131.80	123.90
3	C	397	ID3	C2-C1-C6	4.90	118.14	110.48
3	B	397	ID3	C18-C5-C4	5.35	123.61	113.45
2	A	417	HEM	C4C-C3C-C2C	5.48	110.72	106.90
2	F	417	HEM	C4C-C3C-C2C	6.26	111.27	106.90

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	397	ID3	O1-C9-C8-C7

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Mol	Chain	Res	Type	Atoms
3	B	397	ID3	C7-C8-C9-C19

There are no ring outliers.

9 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	397	ID3	2	0
2	A	417	HEM	4	0
3	B	397	ID3	5	0
2	B	417	HEM	1	0
3	C	397	ID3	2	0
2	C	417	HEM	2	0
2	D	417	HEM	5	0
2	E	417	HEM	3	0
2	F	417	HEM	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	396/396 (100%)	-0.73	0	100   100	5, 17, 39, 75	0
1	B	396/396 (100%)	-0.68	0	100   100	6, 19, 44, 71	0
1	C	396/396 (100%)	-0.69	1 (0%)	93   92	5, 18, 37, 80	0
1	D	394/396 (99%)	-0.65	0	100   100	7, 19, 43, 64	0
1	E	390/396 (98%)	-0.12	2 (0%)	90   88	19, 38, 70, 78	0
1	F	390/396 (98%)	-0.15	3 (0%)	86   81	22, 38, 67, 77	0
All	All	2362/2376 (99%)	-0.50	6 (0%)	93   92	5, 23, 60, 80	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	202	GLY	3.4
1	F	203	ASP	2.7
1	E	179	VAL	2.7
1	F	213	PRO	2.3
1	E	154	ASP	2.2
1	C	172	ARG	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	ID3	B	397	14/14	0.85	0.27	6.31	28,44,50,52	0
3	ID3	C	397	14/14	0.76	0.60	6.04	54,59,63,65	14
3	ID3	A	397	14/14	0.91	0.18	2.49	31,41,43,43	0
2	HEM	C	417	43/43	0.97	0.14	0.72	2,10,16,21	0
2	HEM	A	417	43/43	0.98	0.14	0.53	2,7,14,17	0
2	HEM	D	417	43/43	0.98	0.13	0.34	3,12,18,27	0
2	HEM	B	417	43/43	0.98	0.13	0.30	3,10,16,22	0
2	HEM	F	417	43/43	0.97	0.16	0.08	13,22,27,32	0
2	HEM	E	417	43/43	0.97	0.15	-0.34	17,24,29,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.