



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 03:09 am GMT

PDB ID : 1OS2  
Title : Ternary enzyme-product-inhibitor complexes of human MMP12  
Authors : Bertini, I.; Calderone, V.; Fragai, M.; Luchinat, C.; Mangani, S.; Terni, B.  
Deposited on : 2003-03-18  
Resolution : 2.15 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

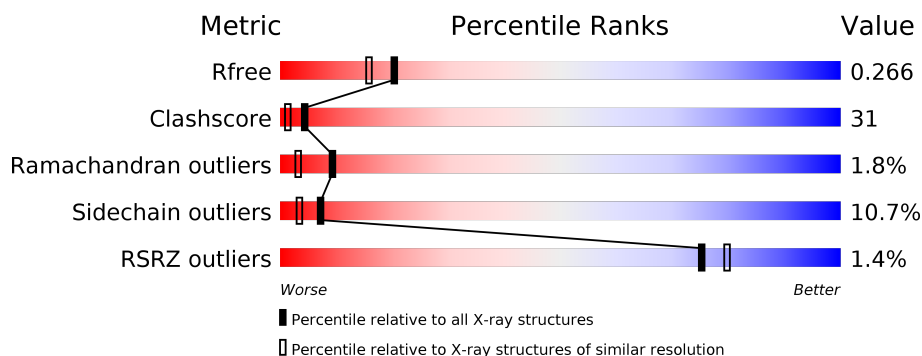
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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))
$R_{free}$	111664	1287 (2.16-2.16)
Clashscore	122126	1390 (2.16-2.16)
Ramachandran outliers	120053	1368 (2.16-2.16)
Sidechain outliers	120020	1367 (2.16-2.16)
RSRZ outliers	108989	1262 (2.16-2.16)

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	165	<div> <div>%</div> <div> <div></div> <div>62%</div> <div>31%</div> <div>6%</div> <div>.</div> </div> </div>
1	B	165	<div> <div>%</div> <div> <div></div> <div>48%</div> <div>37%</div> <div>13%</div> <div>.</div> </div> </div>
1	C	165	<div> <div>2%</div> <div> <div></div> <div>52%</div> <div>34%</div> <div>12%</div> <div>.</div> </div> </div>
1	D	165	<div> <div>%</div> <div> <div></div> <div>62%</div> <div>28%</div> <div>7%</div> <div>.</div> </div> </div>
1	E	165	<div> <div>%</div> <div> <div></div> <div>51%</div> <div>38%</div> <div>8%</div> <div>.</div> </div> </div>
1	F	165	<div> <div>3%</div> <div> <div></div> <div>55%</div> <div>34%</div> <div>8%</div> <div>.</div> </div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8132 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 Macrophage metalloelastase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	0	7	0
			1295	823	225	242	5			
1	B	165	Total	C	N	O	S	0	7	0
			1295	823	225	242	5			
1	C	165	Total	C	N	O	S	0	6	0
			1295	823	225	242	5			
1	D	165	Total	C	N	O	S	0	7	0
			1295	823	225	242	5			
1	E	165	Total	C	N	O	S	0	7	0
			1295	823	225	242	5			
1	F	165	Total	C	N	O	S	0	7	0
			1295	823	225	242	5			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	MET	-	CLONING ARTIFACT	UNP P39900
A	105	MET	-	CLONING ARTIFACT	UNP P39900
A	171	ASP	PHE	ENGINEERED	UNP P39900
B	104	MET	-	CLONING ARTIFACT	UNP P39900
B	105	MET	-	CLONING ARTIFACT	UNP P39900
B	171	ASP	PHE	ENGINEERED	UNP P39900
C	104	MET	-	CLONING ARTIFACT	UNP P39900
C	105	MET	-	CLONING ARTIFACT	UNP P39900
C	171	ASP	PHE	ENGINEERED	UNP P39900
D	104	MET	-	CLONING ARTIFACT	UNP P39900
D	105	MET	-	CLONING ARTIFACT	UNP P39900
D	171	ASP	PHE	ENGINEERED	UNP P39900
E	104	MET	-	CLONING ARTIFACT	UNP P39900
E	105	MET	-	CLONING ARTIFACT	UNP P39900
E	171	ASP	PHE	ENGINEERED	UNP P39900
F	104	MET	-	CLONING ARTIFACT	UNP P39900
F	105	MET	-	CLONING ARTIFACT	UNP P39900

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Chain	Residue	Modelled	Actual	Comment	Reference
F	171	ASP	PHE	ENGINEERED	UNP P39900

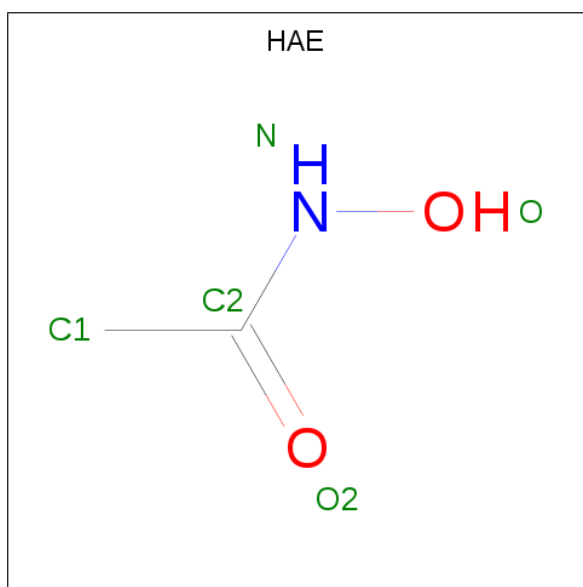
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total 2	Zn 2	0	0
2	E	2	Total 2	Zn 2	0	0
2	B	2	Total 2	Zn 2	0	0
2	C	2	Total 2	Zn 2	0	0
2	A	2	Total 2	Zn 2	0	0
2	F	2	Total 2	Zn 2	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	3	Total 3	Ca 3	0	0
3	E	3	Total 3	Ca 3	0	0
3	B	3	Total 3	Ca 3	0	0
3	C	3	Total 3	Ca 3	0	0
3	A	3	Total 3	Ca 3	0	0
3	F	3	Total 3	Ca 3	0	0

- Molecule 4 is ACETOHYDROXAMIC ACID (three-letter code: HAE) (formula: C<sub>2</sub>H<sub>5</sub>NO<sub>2</sub>).



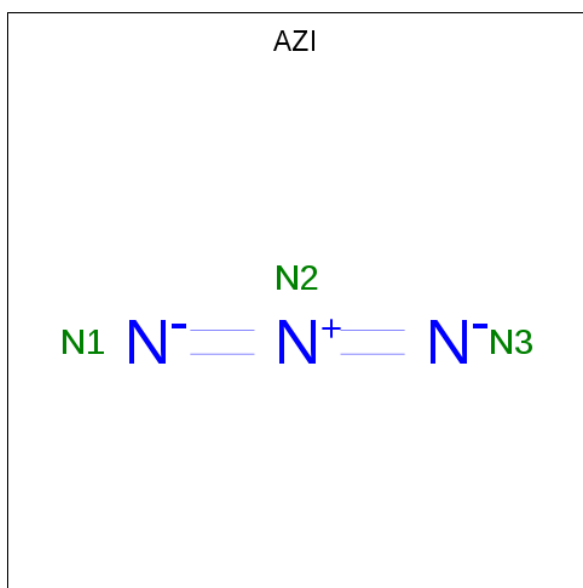
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			5	2	1	2		
4	D	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



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

- Molecule 6 is AZIDE ION (three-letter code: AZI) (formula:  $N_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total N 3 3	0	0
6	F	1	Total N 3 3	0	0

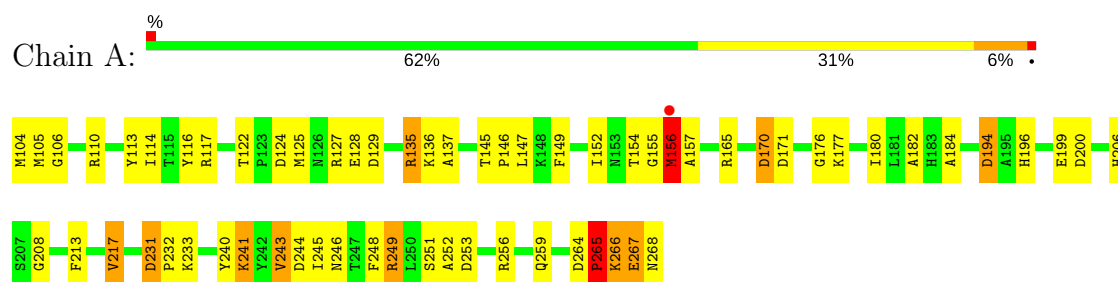
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	46	Total O 46 46	0	0
7	B	67	Total O 67 67	0	0
7	C	51	Total O 51 51	0	0
7	D	44	Total O 44 44	0	0
7	E	59	Total O 59 59	0	0
7	F	41	Total O 41 41	0	0

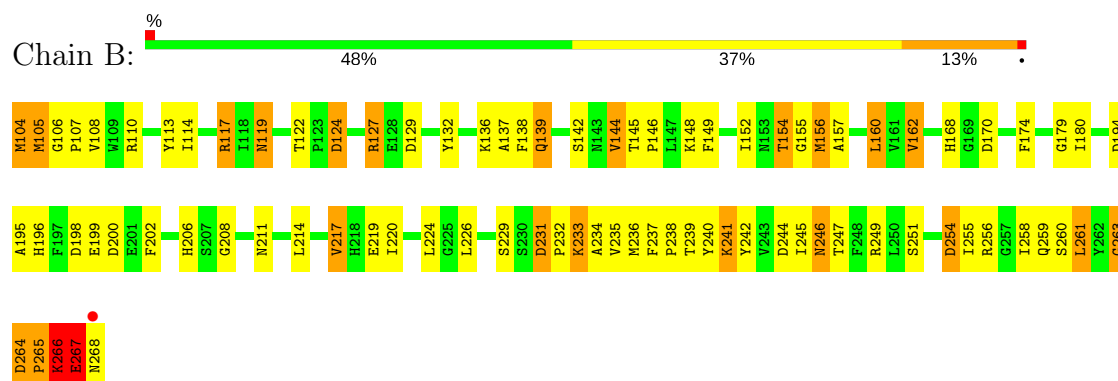
### 3 Residue-property plots [i](#)

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

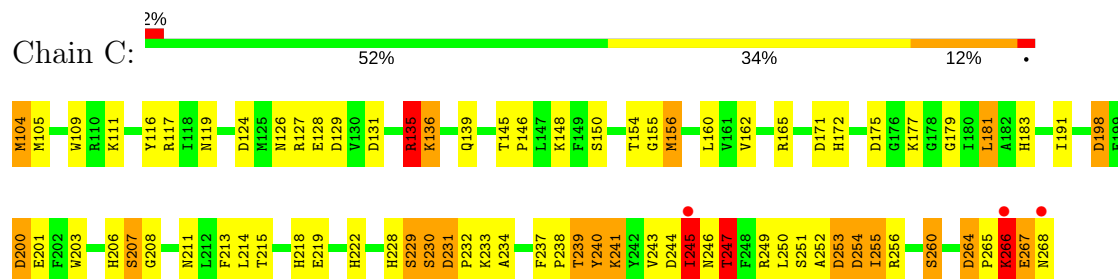
#### • Molecule 1: Macrophage metalloelastase



#### • Molecule 1: Macrophage metalloelastase

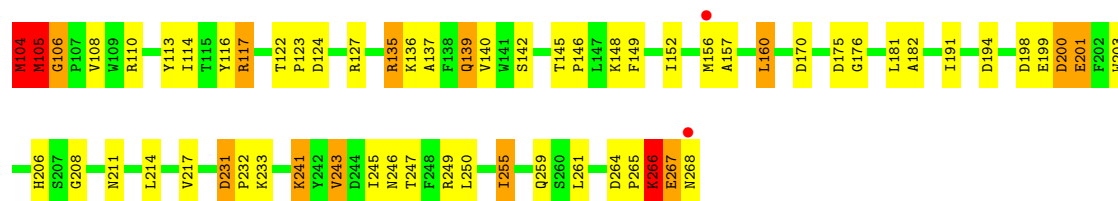


#### • Molecule 1: Macrophage metalloelastase

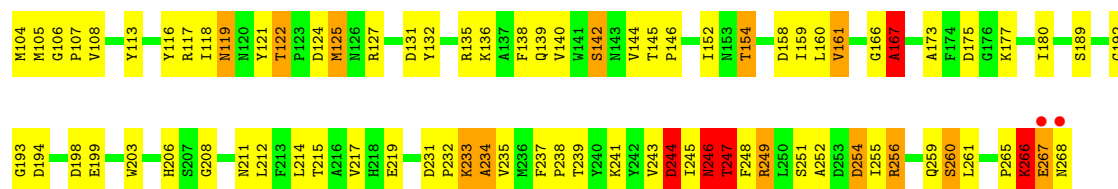


#### • Molecule 1: Macrophage metalloelastase

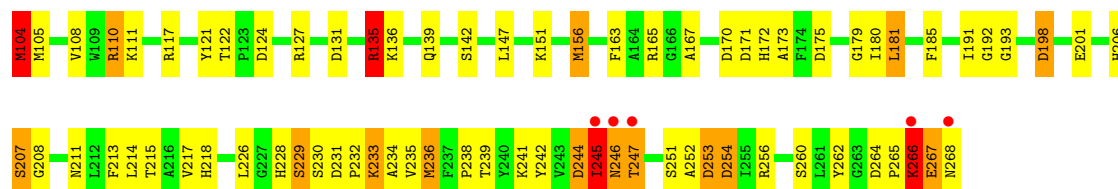




• Molecule 1: Macrophage metalloelastase



• Molecule 1: Macrophage metalloelastase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.84Å 123.84Å 69.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	69.01 – 2.15 69.73 – 2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (69.01-2.15) 100.0 (69.73-2.15)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.1.80	Depositor
R, $R_{free}$	0.212 , 0.271 0.216 , 0.266	Depositor DCC
$R_{free}$ test set	3296 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.2	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 42.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l 0.488 for h,-h-k,-l 0.029 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8132	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AZI, ZN, ACT, CA, HAE

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	1.51	7/1333 (0.5%)	1.40	15/1805 (0.8%)
1	B	1.67	19/1333 (1.4%)	1.49	17/1805 (0.9%)
1	C	1.52	7/1333 (0.5%)	1.53	27/1805 (1.5%)
1	D	1.50	12/1333 (0.9%)	1.35	11/1805 (0.6%)
1	E	1.68	22/1333 (1.7%)	1.57	23/1805 (1.3%)
1	F	1.45	4/1333 (0.3%)	1.47	19/1805 (1.1%)
All	All	1.56	71/7998 (0.9%)	1.47	112/10830 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	2
1	B	0	2
1	C	0	2
1	E	0	4
1	F	1	2
All	All	2	12

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	156	MET	C-O	8.71	1.39	1.23
1	D	139	GLN	CG-CD	7.84	1.69	1.51
1	E	199	GLU	CD-OE1	-7.59	1.17	1.25
1	D	246	ASN	CB-CG	7.44	1.68	1.51
1	A	137	ALA	CA-CB	7.29	1.67	1.52
1	F	252	ALA	CA-CB	7.27	1.67	1.52
1	E	113	TYR	CD1-CE1	6.57	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	135	ARG	CG-CD	6.22	1.67	1.51
1	B	142[A]	SER	CB-OG	-6.20	1.34	1.42
1	B	138	PHE	CE2-CZ	6.18	1.49	1.37
1	D	137	ALA	CA-CB	6.17	1.65	1.52
1	D	117	ARG	CG-CD	6.09	1.67	1.51
1	E	132	TYR	CD2-CE2	6.09	1.48	1.39
1	C	116	TYR	CD1-CE1	6.09	1.48	1.39
1	E	167	ALA	C-O	-5.99	1.11	1.23
1	E	142[A]	SER	CB-OG	-5.99	1.34	1.42
1	D	104	MET	CB-CG	5.95	1.70	1.51
1	C	240	TYR	CD1-CE1	5.92	1.48	1.39
1	F	142[A]	SER	CB-OG	-5.90	1.34	1.42
1	E	144	VAL	CB-CG1	5.87	1.65	1.52
1	E	217	VAL	CB-CG2	5.87	1.65	1.52
1	B	219	GLU	CG-CD	5.87	1.60	1.51
1	D	201	GLU	CD-OE2	-5.84	1.19	1.25
1	C	207	SER	CB-OG	5.80	1.49	1.42
1	E	212	LEU	C-O	5.79	1.34	1.23
1	E	138	PHE	CE2-CZ	5.78	1.48	1.37
1	A	217	VAL	CB-CG2	5.75	1.65	1.52
1	F	135	ARG	NE-CZ	5.67	1.40	1.33
1	B	136	LYS	CE-NZ	5.66	1.63	1.49
1	C	203	TRP	CB-CG	5.62	1.60	1.50
1	D	243	VAL	CB-CG1	5.62	1.64	1.52
1	E	135	ARG	CG-CD	5.59	1.66	1.51
1	E	192	GLY	CA-C	5.56	1.60	1.51
1	C	148	LYS	CB-CG	-5.56	1.37	1.52
1	A	240	TYR	CG-CD1	5.53	1.46	1.39
1	E	219	GLU	CG-CD	5.53	1.60	1.51
1	E	161	VAL	CB-CG2	5.52	1.64	1.52
1	E	234	ALA	CA-CB	5.49	1.64	1.52
1	D	203	TRP	CB-CG	-5.48	1.40	1.50
1	E	161	VAL	CB-CG1	-5.48	1.41	1.52
1	E	136	LYS	CD-CE	5.47	1.65	1.51
1	B	236	MET	CG-SD	5.46	1.95	1.81
1	B	138	PHE	CE1-CZ	5.42	1.47	1.37
1	E	136	LYS	CE-NZ	5.41	1.62	1.49
1	B	113	TYR	CE1-CZ	5.41	1.45	1.38
1	B	132	TYR	CD2-CE2	5.38	1.47	1.39
1	B	136	LYS	CD-CE	5.37	1.64	1.51
1	E	135	ARG	NE-CZ	5.37	1.40	1.33
1	A	252	ALA	CA-CB	5.32	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	116	TYR	CE1-CZ	-5.31	1.31	1.38
1	B	242	TYR	CD1-CE1	-5.29	1.31	1.39
1	B	162	VAL	CB-CG1	5.29	1.64	1.52
1	D	217	VAL	CB-CG2	5.26	1.63	1.52
1	B	240	TYR	CE1-CZ	5.24	1.45	1.38
1	D	142[A]	SER	CB-OG	-5.19	1.35	1.42
1	B	144	VAL	CB-CG1	5.17	1.63	1.52
1	C	117	ARG	CG-CD	5.15	1.64	1.51
1	D	140	VAL	CB-CG2	-5.14	1.42	1.52
1	E	166	GLY	C-N	5.14	1.45	1.34
1	B	139	GLN	CB-CG	5.12	1.66	1.52
1	E	139	GLN	CB-CG	5.11	1.66	1.52
1	B	195	ALA	CA-CB	5.07	1.63	1.52
1	B	117	ARG	NE-CZ	5.07	1.39	1.33
1	E	117	ARG	CG-CD	5.06	1.64	1.51
1	B	217	VAL	CB-CG2	5.06	1.63	1.52
1	B	199	GLU	CD-OE1	-5.06	1.20	1.25
1	C	252	ALA	CA-CB	5.05	1.63	1.52
1	B	246	ASN	CB-CG	5.03	1.62	1.51
1	A	243	VAL	CB-CG1	5.03	1.63	1.52
1	D	116	TYR	CE1-CZ	-5.01	1.32	1.38
1	E	140	VAL	CB-CG1	-5.00	1.42	1.52

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	166	GLY	C-N-CA	-12.70	89.94	121.70
1	E	194	ASP	CB-CG-OD2	12.05	129.15	118.30
1	F	175	ASP	CB-CG-OD2	11.76	128.88	118.30
1	C	175	ASP	CB-CG-OD2	11.17	128.35	118.30
1	B	194	ASP	CB-CG-OD2	10.57	127.82	118.30
1	E	254	ASP	CB-CG-OD2	9.35	126.71	118.30
1	C	231	ASP	CB-CG-OD2	9.32	126.69	118.30
1	E	198	ASP	CB-CG-OD2	9.28	126.65	118.30
1	B	119	ASN	CB-CA-C	9.17	128.73	110.40
1	A	124	ASP	CB-CG-OD2	9.11	126.50	118.30
1	B	261	LEU	CB-CG-CD1	-9.06	95.61	111.00
1	A	231	ASP	CB-CG-OD2	8.88	126.30	118.30
1	D	231	ASP	CB-CG-OD2	8.77	126.19	118.30
1	F	124	ASP	CB-CG-OD1	8.42	125.88	118.30
1	D	170	ASP	CB-CG-OD2	8.34	125.81	118.30
1	E	167	ALA	CA-C-N	-8.29	98.97	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	124	ASP	CB-CG-OD1	8.27	125.74	118.30
1	A	194	ASP	CB-CG-OD2	8.09	125.58	118.30
1	F	198	ASP	CB-CG-OD2	7.92	125.43	118.30
1	B	254	ASP	CB-CG-OD2	7.76	125.29	118.30
1	F	181	LEU	CB-CG-CD1	-7.72	97.87	111.00
1	C	198	ASP	CB-CG-OD2	7.64	125.18	118.30
1	C	254	ASP	CB-CG-OD2	7.62	125.16	118.30
1	C	264	ASP	CB-CG-OD2	7.47	125.03	118.30
1	F	254	ASP	CB-CG-OD2	7.39	124.95	118.30
1	E	244	ASP	CB-CG-OD2	7.36	124.92	118.30
1	E	119	ASN	CB-CA-C	7.35	125.10	110.40
1	D	194	ASP	CB-CG-OD2	7.19	124.77	118.30
1	A	266	LYS	CB-CA-C	7.09	124.58	110.40
1	F	131	ASP	CB-CG-OD2	7.09	124.68	118.30
1	F	253	ASP	CB-CG-OD2	6.87	124.48	118.30
1	C	171	ASP	CB-CG-OD2	6.74	124.36	118.30
1	C	181	LEU	CB-CG-CD1	-6.68	99.64	111.00
1	A	170	ASP	CB-CG-OD2	6.66	124.30	118.30
1	C	131	ASP	CB-CG-OD2	6.62	124.26	118.30
1	C	200	ASP	CB-CG-OD2	6.60	124.24	118.30
1	E	160	LEU	CB-CG-CD2	-6.58	99.81	111.00
1	B	160	LEU	CB-CG-CD1	-6.58	99.82	111.00
1	D	105	MET	CG-SD-CE	-6.45	89.87	100.20
1	C	253	ASP	CB-CG-OD2	6.45	124.10	118.30
1	A	253	ASP	CB-CG-OD1	6.40	124.06	118.30
1	F	117	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	E	158	ASP	CB-CG-OD1	6.32	123.98	118.30
1	E	243	VAL	CG1-CB-CG2	-6.29	100.83	110.90
1	F	246	ASN	N-CA-C	6.23	127.82	111.00
1	E	246	ASN	N-CA-CB	6.20	121.75	110.60
1	B	160	LEU	CB-CG-CD2	-6.19	100.48	111.00
1	B	129	ASP	CB-CG-OD2	6.17	123.86	118.30
1	A	155	GLY	C-N-CA	-6.15	106.31	121.70
1	C	135	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	D	198	ASP	CB-CG-OD2	6.15	123.83	118.30
1	D	124	ASP	CB-CG-OD2	6.14	123.83	118.30
1	E	175	ASP	CB-CG-OD1	6.10	123.79	118.30
1	D	160	LEU	CB-CG-CD1	-6.06	100.70	111.00
1	A	267	GLU	N-CA-C	-5.99	94.82	111.00
1	C	135	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	F	245	ILE	C-N-CA	-5.94	106.84	121.70
1	C	154	THR	CA-CB-CG2	-5.88	104.17	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	236	MET	CG-SD-CE	5.84	109.55	100.20
1	D	267	GLU	N-CA-C	-5.83	95.25	111.00
1	E	117	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	F	111	LYS	CB-CA-C	-5.77	98.86	110.40
1	C	117	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	C	155	GLY	C-N-CA	-5.75	107.32	121.70
1	F	170	ASP	CB-CG-OD1	5.75	123.47	118.30
1	C	239	THR	CA-CB-CG2	-5.64	104.50	112.40
1	B	200	ASP	CB-CG-OD1	5.63	123.36	118.30
1	C	222	HIS	CB-CA-C	-5.63	99.15	110.40
1	C	250	LEU	CB-CG-CD1	-5.59	101.49	111.00
1	C	200	ASP	OD1-CG-OD2	-5.57	112.72	123.30
1	B	124	ASP	CB-CG-OD2	5.56	123.31	118.30
1	A	180	ILE	CG1-CB-CG2	-5.52	99.26	111.40
1	B	231	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	129	ASP	CB-CG-OD2	5.47	123.22	118.30
1	E	122	THR	OG1-CB-CG2	-5.45	97.46	110.00
1	B	263	GLY	N-CA-C	5.45	126.72	113.10
1	F	117	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	D	200	ASP	CB-CG-OD2	5.43	123.19	118.30
1	C	127	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	B	245	ILE	C-N-CA	-5.35	108.33	121.70
1	E	124	ASP	CB-CG-OD2	5.35	123.11	118.30
1	B	127	ARG	CB-CA-C	5.33	121.06	110.40
1	B	170	ASP	C-N-CA	-5.33	108.37	121.70
1	A	156	MET	CB-CA-C	5.32	121.05	110.40
1	E	160	LEU	CB-CG-CD1	-5.32	101.95	111.00
1	F	156	MET	CB-CA-C	5.32	121.05	110.40
1	C	162	VAL	CB-CA-C	-5.31	101.30	111.40
1	C	156	MET	CB-CA-C	5.31	121.02	110.40
1	D	246	ASN	N-CA-CB	5.28	120.11	110.60
1	E	142[A]	SER	CA-CB-OG	-5.28	96.93	111.20
1	A	265	PRO	N-CA-C	-5.27	98.40	112.10
1	C	239	THR	OG1-CB-CG2	-5.27	97.88	110.00
1	F	135	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	C	200	ASP	CB-CG-OD1	5.25	123.03	118.30
1	E	245	ILE	CG1-CB-CG2	-5.23	99.89	111.40
1	D	175	ASP	CB-CG-OD1	5.22	123.00	118.30
1	E	167	ALA	CA-C-O	5.22	131.05	120.10
1	E	177	LYS	CD-CE-NZ	-5.20	99.75	111.70
1	E	233	LYS	CB-CA-C	-5.17	100.07	110.40
1	B	247	THR	OG1-CB-CG2	-5.15	98.15	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	245	ILE	C-N-CA	-5.14	108.85	121.70
1	A	125	MET	CG-SD-CE	5.13	108.41	100.20
1	A	249	ARG	CG-CD-NE	-5.12	101.06	111.80
1	A	194	ASP	CB-CG-OD1	-5.12	113.70	118.30
1	E	131	ASP	CB-CG-OD2	5.12	122.90	118.30
1	B	226	LEU	CB-CG-CD1	5.09	119.65	111.00
1	C	127	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	C	201	GLU	N-CA-C	-5.06	97.33	111.00
1	B	198	ASP	CB-CG-OD2	5.04	122.84	118.30
1	F	256	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	F	110[A]	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	F	104	MET	N-CA-C	-5.02	97.44	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	266	LYS	CA
1	F	246	ASN	CA

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	156	MET	Mainchain
1	A	265	PRO	Peptide
1	B	265	PRO	Peptide
1	B	266	LYS	Peptide
1	C	245	ILE	Peptide
1	C	266	LYS	Peptide
1	E	125	MET	Mainchain
1	E	167	ALA	Mainchain,Peptide
1	E	266	LYS	Peptide
1	F	104	MET	Peptide
1	F	245	ILE	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	1295	0	1210	57	0
1	B	1295	0	1210	118	1
1	C	1295	0	1212	102	0
1	D	1295	0	1210	48	0
1	E	1295	0	1210	75	1
1	F	1295	0	1210	108	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
3	F	3	0	0	0	0
4	A	5	0	4	0	0
4	D	5	0	4	0	0
5	B	4	0	3	1	0
5	E	4	0	3	1	0
6	C	3	0	0	1	0
6	F	3	0	0	1	0
7	A	46	0	0	11	0
7	B	67	0	0	10	0
7	C	51	0	0	2	0
7	D	44	0	0	4	0
7	E	59	0	0	9	0
7	F	41	0	0	5	0
All	All	8132	0	7276	467	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 31.

All (467) 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:F:136:LYS:CE	1:F:245:ILE:HD11	1.33	1.58
1:C:136:LYS:CE	1:C:245:ILE:HD11	1.32	1.55
1:F:136:LYS:HE2	1:F:245:ILE:CD1	1.42	1.49
1:C:136:LYS:HE2	1:C:245:ILE:CD1	1.58	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:LYS:CE	1:C:245:ILE:CD1	2.08	1.31
1:C:267:GLU:CB	1:C:268:ASN:HB2	1.61	1.29
1:F:267:GLU:HB2	1:F:268:ASN:CA	1.66	1.25
1:C:264:ASP:O	1:C:266:LYS:HG2	1.36	1.25
1:B:266:LYS:NZ	1:B:266:LYS:HA	1.54	1.23
1:F:206:HIS:CD2	1:F:208:GLY:H	1.57	1.21
1:B:105:MET:CE	1:B:105:MET:HA	1.67	1.21
1:E:167:ALA:HB1	7:E:688:HOH:O	1.37	1.20
1:C:265:PRO:HA	1:C:266:LYS:HB2	1.21	1.19
1:C:267:GLU:HB2	1:C:268:ASN:CB	1.73	1.19
1:E:231:ASP:OD2	1:E:232:PRO:CD	1.91	1.19
1:B:231:ASP:OD2	1:B:232:PRO:CD	1.94	1.16
1:A:267:GLU:HB2	1:A:268:ASN:HB2	1.23	1.15
1:E:246:ASN:O	1:E:248:PHE:N	1.78	1.15
1:F:136:LYS:HE3	1:F:245:ILE:HD11	1.24	1.14
1:B:231:ASP:OD2	1:B:232:PRO:HD2	1.46	1.12
1:E:231:ASP:OD2	1:E:232:PRO:HD2	1.45	1.12
1:B:263:GLY:O	1:B:264:ASP:CB	1.97	1.12
1:C:265:PRO:HA	1:C:266:LYS:CB	1.79	1.10
1:B:105:MET:HA	1:B:105:MET:HE3	1.20	1.10
1:B:266:LYS:HZ2	1:B:266:LYS:HA	1.02	1.09
1:F:230:SER:O	1:F:232:PRO:HD3	1.52	1.09
1:F:136:LYS:CE	1:F:245:ILE:CD1	2.14	1.08
1:F:267:GLU:CB	1:F:268:ASN:HA	1.80	1.07
1:A:267:GLU:HB2	1:A:268:ASN:CB	1.84	1.07
1:C:267:GLU:HG3	1:C:268:ASN:HB3	1.33	1.05
1:C:244:ASP:H	1:C:247:THR:HG21	1.21	1.05
1:B:107:PRO:HD2	7:B:431:HOH:O	1.57	1.04
1:D:241[A]:LYS:HE3	7:D:615:HOH:O	1.54	1.04
1:B:263:GLY:O	1:B:264:ASP:HB2	1.52	1.03
1:F:136:LYS:HG2	1:F:213:PHE:CE2	1.94	1.02
1:C:206:HIS:CD2	1:C:208:GLY:H	1.77	1.01
1:B:267:GLU:HG2	1:B:268:ASN:HB2	1.42	1.00
1:A:117:ARG:NH1	1:A:154:THR:HA	1.77	1.00
1:B:206:HIS:HD2	1:B:208:GLY:H	1.08	1.00
1:C:136:LYS:HE2	1:C:245:ILE:HD13	1.40	1.00
1:E:167:ALA:HB2	1:E:173:ALA:CB	1.93	0.99
1:C:266:LYS:HA	1:C:266:LYS:HE2	1.45	0.98
1:F:244:ASP:CG	1:F:247:THR:HG22	1.83	0.98
1:C:136:LYS:HE3	1:C:245:ILE:CD1	1.83	0.98
1:E:127:ARG:NH2	7:E:731:HOH:O	1.97	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:136:LYS:HE2	1:F:245:ILE:HD13	1.40	0.98
1:F:265:PRO:HA	1:F:266:LYS:HE2	1.46	0.97
1:F:267:GLU:HB2	1:F:268:ASN:HA	0.97	0.96
1:F:206:HIS:HD2	1:F:208:GLY:N	1.63	0.95
1:E:206:HIS:HD2	1:E:208:GLY:H	0.97	0.95
1:A:231:ASP:OD2	1:A:233:LYS:HE3	1.65	0.95
1:E:107:PRO:HD2	7:E:705:HOH:O	1.65	0.95
1:B:105:MET:HG3	1:B:261:LEU:CD2	1.98	0.93
1:B:267:GLU:HG2	1:B:268:ASN:CB	1.98	0.93
1:C:206:HIS:HD2	1:C:208:GLY:H	0.93	0.92
1:C:244:ASP:H	1:C:247:THR:CG2	1.81	0.92
1:C:136:LYS:HE3	1:C:245:ILE:HD11	0.94	0.92
1:E:105:MET:HA	1:E:105:MET:CE	2.00	0.92
1:E:106:GLY:HA2	1:F:181:LEU:HD11	1.51	0.92
1:C:267:GLU:CB	1:C:268:ASN:CB	2.42	0.91
1:C:267:GLU:HG3	1:C:268:ASN:CB	2.00	0.91
1:E:105:MET:HA	1:E:105:MET:HE3	1.52	0.91
1:B:105:MET:CE	1:B:105:MET:CA	2.49	0.90
1:F:265:PRO:HA	1:F:266:LYS:HB2	1.53	0.90
1:B:105:MET:HB2	1:C:238:PRO:O	1.71	0.90
1:D:152:ILE:HD11	1:D:157:ALA:HB2	1.51	0.90
1:E:206:HIS:CD2	1:E:208:GLY:H	1.88	0.89
1:E:108:VAL:HG22	1:F:239:THR:HG21	1.54	0.89
1:B:206:HIS:CD2	1:B:208:GLY:H	1.92	0.88
1:D:117:ARG:HD3	7:D:617:HOH:O	1.72	0.88
1:B:104:MET:HE1	1:C:215:THR:HA	1.55	0.87
1:A:246:ASN:ND2	7:A:918:HOH:O	1.93	0.87
1:E:107:PRO:CD	7:E:705:HOH:O	2.19	0.86
1:A:267:GLU:CB	1:A:268:ASN:HB2	2.06	0.86
1:E:127:ARG:CZ	7:E:731:HOH:O	2.21	0.86
1:E:167:ALA:HB2	1:E:173:ALA:HB2	1.57	0.85
1:A:117:ARG:HH12	1:A:154:THR:HA	1.41	0.85
1:F:265:PRO:CA	1:F:266:LYS:HB2	2.06	0.84
1:F:206:HIS:CD2	1:F:208:GLY:N	2.41	0.84
1:B:104:MET:HE3	1:C:240:TYR:HD2	1.42	0.84
1:B:148:LYS:HZ2	1:B:148:LYS:HB3	1.40	0.84
1:F:231:ASP:OD2	1:F:233:LYS:HG3	1.76	0.84
1:D:206:HIS:HD2	1:D:208:GLY:H	1.23	0.84
1:B:104:MET:N	6:C:474:AZI:N3	2.25	0.84
1:B:105:MET:HE3	1:B:105:MET:CA	2.06	0.82
1:C:230:SER:O	1:C:232:PRO:HD3	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:ASP:N	1:C:247:THR:CG2	2.41	0.82
1:F:244:ASP:H	1:F:247:THR:CG2	1.93	0.81
1:C:267:GLU:CG	1:C:268:ASN:CB	2.59	0.81
1:E:231:ASP:OD2	1:E:232:PRO:N	2.14	0.81
1:E:167:ALA:HB2	1:E:173:ALA:CA	2.12	0.80
1:B:106:GLY:HA2	1:C:181:LEU:HD11	1.63	0.80
1:F:211[A]:ASN:HD22	1:F:214:LEU:H	1.30	0.79
1:E:108:VAL:CG2	1:F:239:THR:HG21	2.11	0.79
1:C:206:HIS:HD2	1:C:208:GLY:N	1.78	0.79
1:C:264:ASP:O	1:C:266:LYS:CG	2.26	0.79
1:C:136:LYS:HG2	1:C:213:PHE:CD2	2.17	0.79
1:C:231:ASP:OD2	1:C:233:LYS:N	2.16	0.78
1:B:231:ASP:OD2	1:B:232:PRO:N	2.16	0.78
1:F:167:ALA:HA	1:F:173:ALA:HB2	1.66	0.78
1:B:265:PRO:CB	1:B:266:LYS:HB2	2.14	0.78
1:A:136:LYS:HD2	1:A:245:ILE:HD11	1.65	0.77
1:C:104:MET:HA	1:C:104:MET:HE3	1.66	0.76
1:B:146[A]:PRO:HB3	1:B:266:LYS:HG2	1.67	0.76
1:A:264:ASP:HB2	1:A:265:PRO:CD	2.15	0.76
1:D:265:PRO:HA	1:D:266:LYS:HB2	1.68	0.76
1:F:244:ASP:H	1:F:247:THR:HG21	1.50	0.76
1:E:167:ALA:HB2	1:E:173:ALA:HA	1.66	0.76
1:B:117:ARG:NH1	1:B:155:GLY:O	2.19	0.76
1:D:104:MET:HE2	1:E:215:THR:HG23	1.68	0.74
1:F:230:SER:O	1:F:232:PRO:CD	2.32	0.74
1:B:105:MET:CE	1:C:179:GLY:O	2.35	0.74
1:B:266:LYS:CA	1:B:266:LYS:HZ2	1.92	0.74
1:C:241:LYS:HE3	1:C:243:VAL:HG11	1.70	0.74
1:B:265:PRO:HA	1:B:266:LYS:HD2	1.68	0.74
1:B:107:PRO:CD	7:B:431:HOH:O	2.22	0.74
1:A:104:MET:N	5:B:374:ACT:OXT	2.21	0.74
1:D:145:THR:HB	1:D:146[A]:PRO:HD2	1.67	0.74
1:B:263:GLY:O	1:B:264:ASP:HB3	1.84	0.74
1:B:108:VAL:HG22	1:C:239:THR:HG21	1.68	0.73
1:B:104:MET:CE	1:C:240:TYR:HD2	2.00	0.73
1:E:265:PRO:HA	1:E:266:LYS:HB2	1.71	0.73
1:C:244:ASP:O	1:C:246:ASN:N	2.22	0.73
1:F:267:GLU:HB2	1:F:268:ASN:CB	2.18	0.73
1:C:267:GLU:CG	1:C:268:ASN:HB3	2.17	0.73
1:F:167:ALA:HA	1:F:173:ALA:CB	2.18	0.73
1:F:206:HIS:HD2	1:F:208:GLY:H	0.84	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ARG:HG2	1:A:135:ARG:HH11	1.52	0.73
1:C:265:PRO:CA	1:C:266:LYS:HB2	2.11	0.73
1:B:105:MET:HE2	1:B:106:GLY:H	1.54	0.72
1:B:265:PRO:CA	1:B:266:LYS:HB2	2.20	0.72
1:B:156:MET:CE	1:B:156:MET:HA	2.19	0.72
1:C:241:LYS:HE3	1:C:243:VAL:CG1	2.19	0.72
1:C:244:ASP:CG	1:C:247:THR:HG22	2.11	0.71
1:D:206:HIS:CD2	1:D:208:GLY:H	2.08	0.71
1:A:135:ARG:HD3	7:A:915:HOH:O	1.89	0.71
1:A:268:ASN:OXT	7:A:905:HOH:O	2.07	0.71
1:A:105:MET:HE3	1:B:179:GLY:O	1.91	0.71
1:F:206:HIS:HE1	7:F:810:HOH:O	1.72	0.71
1:F:265:PRO:CA	1:F:266:LYS:HE2	2.19	0.71
1:A:206:HIS:HD2	1:A:208:GLY:H	1.36	0.71
1:A:246:ASN:HB2	7:A:918:HOH:O	1.91	0.70
1:A:241[A]:LYS:HD3	7:A:910:HOH:O	1.92	0.70
1:C:267:GLU:CG	1:C:268:ASN:HB2	2.20	0.70
1:A:145:THR:HB	1:A:146[A]:PRO:HD2	1.72	0.70
1:D:249:ARG:HH21	1:D:249:ARG:HG3	1.56	0.70
1:B:139:GLN:HG3	7:B:399:HOH:O	1.91	0.70
1:C:267:GLU:HB2	1:C:268:ASN:HB2	0.79	0.69
1:F:244:ASP:N	1:F:247:THR:CG2	2.54	0.69
1:E:206:HIS:HD2	1:E:208:GLY:N	1.81	0.69
1:A:267:GLU:HB2	1:A:268:ASN:CG	2.13	0.68
1:E:104:MET:N	6:F:774:AZI:N3	2.40	0.68
1:C:265:PRO:HA	1:C:266:LYS:CG	2.22	0.68
1:F:211[A]:ASN:HD21	1:F:213:PHE:HB3	1.56	0.68
1:B:105:MET:CE	1:B:106:GLY:H	2.06	0.68
1:C:135:ARG:NH2	1:C:139:GLN:OE1	2.26	0.68
1:F:229[A]:SER:HB2	1:F:253:ASP:OD1	1.94	0.68
1:F:267:GLU:CB	1:F:268:ASN:CA	2.52	0.68
1:F:267:GLU:HG3	1:F:268:ASN:HB2	1.75	0.68
1:B:148:LYS:NZ	1:B:148:LYS:HB3	2.07	0.68
1:F:266:LYS:HA	1:F:266:LYS:CE	2.23	0.68
1:A:105:MET:HE1	1:B:179:GLY:HA2	1.76	0.67
1:E:108:VAL:HG22	1:F:239:THR:CG2	2.24	0.67
1:B:156:MET:HA	1:B:156:MET:HE3	1.76	0.67
1:E:265:PRO:CA	1:E:266:LYS:HB2	2.24	0.67
1:B:145:THR:HB	1:B:146[A]:PRO:HD2	1.77	0.67
1:B:105:MET:HE1	1:C:179:GLY:C	2.15	0.66
1:E:145:THR:HB	1:E:146[A]:PRO:HD2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:VAL:CG2	1:C:239:THR:HG21	2.25	0.66
1:B:105:MET:HG3	1:B:261:LEU:HD21	1.77	0.66
1:B:105:MET:HG3	1:B:261:LEU:HD23	1.76	0.66
1:B:266:LYS:NZ	1:B:266:LYS:CA	2.46	0.66
1:F:265:PRO:HA	1:F:266:LYS:CB	2.24	0.65
1:D:264:ASP:HB2	1:D:265:PRO:HD2	1.78	0.65
1:D:250:LEU:HB2	1:D:255:ILE:HD11	1.77	0.65
1:D:152:ILE:HD11	1:D:157:ALA:CB	2.27	0.65
1:E:231:ASP:OD2	1:E:231:ASP:C	2.35	0.65
1:D:152:ILE:CD1	1:D:157:ALA:HB2	2.27	0.65
1:A:264:ASP:HB2	1:A:265:PRO:HD2	1.79	0.65
1:D:264:ASP:HB2	1:D:265:PRO:CD	2.27	0.64
1:C:266:LYS:HA	1:C:266:LYS:CE	2.16	0.64
1:F:104:MET:HA	1:F:104:MET:CE	2.28	0.63
1:E:255:ILE:O	1:E:259:GLN:HB2	1.97	0.63
1:C:244:ASP:O	1:C:247:THR:CG2	2.46	0.63
1:D:104:MET:CE	1:E:215:THR:HG23	2.29	0.63
1:B:241[A]:LYS:HD2	7:B:411:HOH:O	1.99	0.63
1:B:266:LYS:HZ3	1:B:266:LYS:HA	1.62	0.63
1:D:249:ARG:NH2	1:D:249:ARG:HG3	2.13	0.63
1:E:251:SER:O	1:E:254:ASP:N	2.31	0.62
1:F:266:LYS:HE2	1:F:266:LYS:CA	2.29	0.62
1:B:139:GLN:CG	7:B:399:HOH:O	2.47	0.62
1:C:211[A]:ASN:HD22	1:C:214:LEU:H	1.47	0.62
1:F:244:ASP:O	1:F:247:THR:CG2	2.46	0.62
1:F:265:PRO:HA	1:F:266:LYS:CE	2.26	0.62
1:C:245:ILE:O	1:C:245:ILE:HG23	2.01	0.61
1:B:251:SER:O	1:B:254:ASP:N	2.29	0.61
1:D:104:MET:N	5:E:674:ACT:O	2.33	0.61
1:C:206:HIS:CD2	1:C:208:GLY:N	2.61	0.61
1:A:246:ASN:CB	7:A:918:HOH:O	2.47	0.61
1:A:135:ARG:HH11	1:A:135:ARG:CG	2.14	0.61
1:B:106:GLY:HA2	1:C:181:LEU:CD1	2.31	0.61
1:B:105:MET:CB	1:C:238:PRO:O	2.46	0.60
1:B:180:ILE:HD12	7:B:419:HOH:O	2.01	0.60
1:B:105:MET:HB3	1:C:239:THR:HA	1.83	0.60
1:B:104:MET:HE3	1:C:240:TYR:CD2	2.31	0.60
1:B:145:THR:N	1:B:265:PRO:HD3	2.16	0.59
1:D:267:GLU:HB2	1:D:268:ASN:CG	2.22	0.59
1:D:267:GLU:HB2	1:D:268:ASN:HB2	1.84	0.59
1:A:259:GLN:NE2	7:A:886:HOH:O	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:LYS:HG2	1:C:213:PHE:CE2	2.38	0.59
1:A:117:ARG:NH1	1:A:154:THR:CA	2.61	0.59
1:D:250:LEU:HB2	1:D:255:ILE:CD1	2.31	0.59
1:B:231:ASP:OD2	1:B:231:ASP:C	2.41	0.59
1:C:266:LYS:O	1:C:267:GLU:O	2.21	0.59
1:F:265:PRO:CB	1:F:266:LYS:HB2	2.32	0.59
1:B:105:MET:HE1	1:C:179:GLY:O	2.01	0.58
1:B:180:ILE:HD13	7:B:386:HOH:O	2.03	0.58
1:B:267:GLU:CG	1:B:268:ASN:HB2	2.26	0.58
1:B:146[A]:PRO:HB3	1:B:266:LYS:CG	2.33	0.58
1:B:265:PRO:HA	1:B:266:LYS:HB2	1.85	0.58
1:E:106:GLY:HA2	1:F:181:LEU:CD1	2.29	0.58
1:A:206:HIS:CD2	1:A:208:GLY:H	2.19	0.58
1:B:105:MET:HE2	1:B:106:GLY:N	2.18	0.58
1:B:146[A]:PRO:HB3	1:B:266:LYS:HD3	1.85	0.57
1:A:117:ARG:NE	7:A:896:HOH:O	2.38	0.57
1:C:244:ASP:O	1:C:247:THR:HG23	2.04	0.57
1:F:244:ASP:CA	1:F:247:THR:CG2	2.83	0.57
1:E:105:MET:CG	1:E:261:LEU:HD21	2.35	0.57
1:F:244:ASP:O	1:F:247:THR:HG22	2.05	0.57
1:A:145:THR:HB	1:A:146[A]:PRO:CD	2.35	0.57
1:D:145:THR:HB	1:D:146[A]:PRO:CD	2.35	0.57
1:D:267:GLU:HB2	1:D:268:ASN:CB	2.35	0.57
1:B:180:ILE:CD1	7:B:419:HOH:O	2.53	0.56
1:E:237:PHE:CD1	1:E:238:PRO:HD2	2.39	0.56
1:A:114:ILE:O	1:A:149:PHE:HA	2.06	0.56
1:C:241:LYS:HD3	7:C:503:HOH:O	2.05	0.56
1:F:211[A]:ASN:ND2	1:F:213:PHE:HB3	2.20	0.56
1:E:256:ARG:O	1:E:260:SER:HB3	2.04	0.56
1:E:105:MET:HE3	1:F:180:ILE:HA	1.88	0.56
1:F:136:LYS:HG2	1:F:213:PHE:HE2	1.61	0.56
1:B:146[A]:PRO:CB	1:B:266:LYS:HG2	2.35	0.56
1:F:207:SER:HB2	1:F:242:TYR:CE2	2.41	0.56
1:F:136:LYS:HE2	1:F:245:ILE:HD11	0.98	0.56
1:E:246:ASN:C	1:E:246:ASN:OD1	2.43	0.55
1:C:218:HIS:CE1	1:C:228:HIS:CD2	2.93	0.55
1:B:108:VAL:HG22	1:C:239:THR:CG2	2.37	0.55
1:E:105:MET:HG2	1:E:261:LEU:CD2	2.36	0.55
1:C:229[A]:SER:HB2	1:C:253:ASP:OD1	2.06	0.55
1:E:246:ASN:O	1:E:247:THR:C	2.41	0.55
1:F:244:ASP:CB	1:F:247:THR:HG22	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:THR:HB	1:B:146[A]:PRO:CD	2.35	0.55
1:C:244:ASP:OD1	1:C:247:THR:HG22	2.06	0.55
1:E:167:ALA:CB	7:E:710:HOH:O	2.55	0.55
1:A:176:GLY:HA2	1:A:200:ASP:OD1	2.08	0.54
1:F:135:ARG:NH2	1:F:139:GLN:OE1	2.36	0.54
1:C:267:GLU:HA	7:C:487:HOH:O	2.05	0.54
1:E:121:TYR:CE1	1:E:127:ARG:HG2	2.42	0.54
1:E:180:ILE:HD13	7:E:684:HOH:O	2.07	0.54
1:F:167:ALA:CA	1:F:173:ALA:HB2	2.35	0.54
1:F:217:VAL:HG12	1:F:235:VAL:HG21	1.90	0.54
1:A:267:GLU:CB	1:A:268:ASN:CB	2.73	0.54
1:F:104:MET:HA	1:F:104:MET:HE2	1.90	0.54
1:F:136:LYS:HE3	1:F:245:ILE:CD1	2.10	0.54
1:C:266:LYS:HE2	1:C:266:LYS:CA	2.29	0.54
1:E:105:MET:HB2	1:F:238:PRO:O	2.07	0.53
1:F:231:ASP:CG	1:F:233:LYS:HG3	2.27	0.53
1:D:114:ILE:O	1:D:149:PHE:HA	2.09	0.53
1:E:167:ALA:CB	1:E:173:ALA:HA	2.35	0.53
1:E:211[A]:ASN:HD22	1:E:214:LEU:H	1.54	0.53
1:C:244:ASP:O	1:C:247:THR:HG22	2.09	0.53
1:F:185:PHE:N	1:F:185:PHE:CD1	2.76	0.53
1:A:117:ARG:HD3	7:A:896:HOH:O	2.09	0.53
1:F:167:ALA:CA	1:F:173:ALA:CB	2.85	0.53
1:E:265:PRO:C	1:E:266:LYS:HE2	2.29	0.53
1:D:259:GLN:NE2	7:D:593:HOH:O	2.38	0.53
1:E:105:MET:HB3	1:F:239:THR:HA	1.91	0.53
1:B:231:ASP:CG	1:B:232:PRO:CD	2.77	0.52
1:C:104:MET:CE	1:C:104:MET:HA	2.38	0.52
1:E:266:LYS:HE2	1:E:266:LYS:N	2.24	0.52
1:F:218:HIS:CE1	1:F:228:HIS:NE2	2.77	0.52
1:A:114:ILE:CD1	1:A:147:LEU:HD22	2.38	0.52
1:A:213:PHE:O	1:A:217:VAL:HG23	2.10	0.52
1:E:237:PHE:CG	1:E:238:PRO:HD2	2.45	0.52
1:F:110[A]:ARG:HH11	1:F:110[A]:ARG:HG3	1.74	0.52
1:E:105:MET:CE	1:F:179:GLY:O	2.57	0.52
1:D:136:LYS:HD2	1:D:245:ILE:HD11	1.92	0.52
1:E:125:MET:HG3	1:E:203:TRP:O	2.10	0.52
1:B:105:MET:CE	1:B:106:GLY:N	2.73	0.51
1:C:136:LYS:CD	1:C:245:ILE:HD11	2.29	0.51
1:F:244:ASP:O	1:F:247:THR:HG23	2.10	0.51
1:A:113:TYR:C	1:A:114:ILE:HG13	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:VAL:HB	1:B:196:HIS:CD2	2.46	0.51
1:B:237:PHE:CG	1:B:238:PRO:HD2	2.45	0.51
1:F:147:LEU:HD21	1:F:262:TYR:CD2	2.46	0.51
1:A:231:ASP:CG	1:A:233:LYS:HE3	2.29	0.51
1:C:244:ASP:CA	1:C:247:THR:CG2	2.89	0.51
1:D:250:LEU:HB3	1:D:255:ILE:HD13	1.93	0.51
1:E:244:ASP:OD1	1:E:247:THR:HB	2.10	0.51
1:F:244:ASP:CA	1:F:247:THR:HG22	2.41	0.50
1:C:244:ASP:C	1:C:246:ASN:N	2.64	0.50
1:C:265:PRO:HA	1:C:266:LYS:HG2	1.92	0.50
1:D:250:LEU:CB	1:D:255:ILE:HD13	2.41	0.50
1:B:127:ARG:HG2	1:B:127:ARG:HH11	1.76	0.50
1:E:167:ALA:HB1	7:E:710:HOH:O	2.11	0.50
1:B:152:ILE:HD11	1:B:157:ALA:HB2	1.94	0.50
1:C:211[A]:ASN:HD21	1:C:213:PHE:HB3	1.77	0.50
1:A:248:PHE:O	1:A:249:ARG:HG2	2.12	0.50
1:B:144:VAL:C	1:B:265:PRO:HD3	2.32	0.50
1:C:237:PHE:CD1	1:C:238:PRO:HD2	2.46	0.50
1:B:106:GLY:HA3	7:B:431:HOH:O	2.11	0.50
1:B:220:ILE:O	1:B:224:LEU:HG	2.12	0.50
1:F:265:PRO:C	1:F:266:LYS:HE2	2.31	0.50
1:F:244:ASP:CG	1:F:247:THR:CG2	2.71	0.50
1:B:237:PHE:CD1	1:B:238:PRO:HD2	2.47	0.49
1:D:211[A]:ASN:HD22	1:D:214:LEU:H	1.59	0.49
1:B:266:LYS:H	1:B:267:GLU:HB3	1.77	0.49
1:F:207:SER:O	1:F:207:SER:OG	2.29	0.49
1:A:135:ARG:NH1	1:A:135:ARG:HG2	2.22	0.49
1:F:191:ILE:HD12	7:F:804:HOH:O	2.13	0.49
1:B:246:ASN:CG	1:B:246:ASN:O	2.50	0.49
1:C:244:ASP:N	1:C:247:THR:HG23	2.25	0.49
1:E:105:MET:CG	1:E:261:LEU:CD2	2.91	0.49
1:F:136:LYS:HG2	1:F:213:PHE:CD2	2.42	0.49
1:F:217:VAL:CG1	1:F:235:VAL:HG21	2.42	0.49
1:C:266:LYS:C	1:C:267:GLU:O	2.50	0.49
1:E:108:VAL:HG21	1:F:239:THR:HG21	1.95	0.49
1:E:267:GLU:HG2	1:E:267:GLU:O	2.11	0.49
1:B:146[A]:PRO:HB3	1:B:266:LYS:CD	2.43	0.49
1:B:104:MET:CE	1:C:215:THR:HA	2.37	0.49
1:B:229[A]:SER:HB3	1:B:234:ALA:HB3	1.95	0.49
1:B:267:GLU:HG2	1:B:268:ASN:CG	2.33	0.49
1:B:267:GLU:HG2	1:B:268:ASN:OD1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ARG:CD	7:A:896:HOH:O	2.61	0.48
1:A:244:ASP:OD2	1:A:246:ASN:N	2.46	0.48
1:E:104:MET:HG2	1:F:215:THR:HG23	1.94	0.48
1:F:267:GLU:HB2	1:F:268:ASN:HB2	1.94	0.48
1:F:110[A]:ARG:NH1	1:F:110[A]:ARG:HG3	2.28	0.48
1:C:145:THR:HB	1:C:146[A]:PRO:CD	2.44	0.48
1:D:250:LEU:CB	1:D:255:ILE:CD1	2.91	0.48
1:D:201:GLU:HA	1:D:201:GLU:OE1	2.13	0.48
1:C:104:MET:CE	1:C:104:MET:CA	2.92	0.48
1:A:105:MET:CE	1:B:179:GLY:HA2	2.44	0.47
1:E:116:TYR:HA	1:E:159:ILE:O	2.15	0.47
1:F:266:LYS:HA	1:F:266:LYS:HE2	1.88	0.47
1:C:172:HIS:O	1:C:183[A]:HIS:HE1	1.96	0.47
1:F:122:THR:HB	1:F:163:PHE:CD2	2.49	0.47
1:E:105:MET:CB	1:F:238:PRO:O	2.62	0.47
1:F:244:ASP:O	1:F:247:THR:N	2.48	0.47
1:B:110[A]:ARG:HH11	1:C:241:LYS:HB2	1.79	0.47
1:B:137:ALA:HA	1:B:217:VAL:HG22	1.97	0.47
1:B:105:MET:CG	1:B:261:LEU:HD23	2.45	0.47
1:D:148:LYS:HD2	1:D:148:LYS:HA	1.64	0.47
1:D:176:GLY:HA2	1:D:200:ASP:OD1	2.14	0.47
1:B:124:ASP:OD1	1:B:202:PHE:HA	2.15	0.47
1:C:231:ASP:OD2	1:C:233:LYS:CB	2.63	0.47
1:B:110[A]:ARG:NH1	1:C:241:LYS:HB2	2.29	0.47
1:D:231:ASP:OD2	1:D:233:LYS:HD3	2.15	0.47
1:F:136:LYS:CE	1:F:245:ILE:CG1	2.91	0.46
1:F:229[A]:SER:OG	1:F:234:ALA:CB	2.63	0.46
1:E:118:ILE:HA	1:E:161:VAL:HB	1.96	0.46
1:F:206:HIS:CD2	1:F:207:SER:N	2.84	0.46
1:C:136:LYS:CE	1:C:245:ILE:CG1	2.89	0.46
1:F:127:ARG:HG3	7:F:800:HOH:O	2.15	0.46
1:F:244:ASP:N	1:F:247:THR:HG23	2.29	0.46
1:F:171:ASP:HB2	1:F:172:HIS:CD2	2.51	0.46
1:A:105:MET:CE	1:B:179:GLY:C	2.85	0.46
1:F:136:LYS:CD	1:F:245:ILE:HD11	2.31	0.46
1:F:244:ASP:O	1:F:246:ASN:N	2.49	0.46
1:C:265:PRO:CA	1:C:266:LYS:HG2	2.47	0.45
1:E:231:ASP:HA	1:E:232:PRO:HD3	1.73	0.45
1:E:267:GLU:HB2	1:E:268:ASN:HB2	1.98	0.45
1:B:265:PRO:HA	1:B:266:LYS:CB	2.46	0.45
1:B:105:MET:CG	1:B:261:LEU:CD2	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:MET:CE	1:E:215:THR:HA	2.47	0.45
1:A:243:VAL:O	1:A:243:VAL:HG23	2.16	0.45
1:C:145:THR:HA	1:C:265:PRO:HD3	1.98	0.45
1:D:181:LEU:O	1:D:182:ALA:HB2	2.16	0.45
1:E:105:MET:HE2	1:F:179:GLY:O	2.17	0.45
1:A:231:ASP:HA	1:A:232:PRO:HD3	1.82	0.45
1:C:251:SER:O	1:C:254:ASP:N	2.46	0.45
1:B:265:PRO:CA	1:B:266:LYS:CB	2.93	0.45
1:B:231:ASP:HA	1:B:232:PRO:HD3	1.76	0.45
1:B:211[A]:ASN:HD22	1:B:214:LEU:H	1.64	0.44
1:C:256:ARG:O	1:C:260:SER:OG	2.34	0.44
1:D:105:MET:HE3	1:D:106:GLY:N	2.32	0.44
1:D:135:ARG:HH21	1:D:136:LYS:HA	1.82	0.44
1:B:152:ILE:HD12	1:B:154:THR:O	2.16	0.44
1:A:105:MET:HE3	1:B:179:GLY:C	2.36	0.44
1:A:245:ILE:HD13	1:A:245:ILE:HG21	1.68	0.44
1:F:218:HIS:CE1	1:F:228:HIS:CD2	3.05	0.44
1:A:182:ALA:HB1	1:A:196:HIS:O	2.18	0.44
1:F:234:ALA:C	1:F:236:MET:N	2.71	0.44
1:F:267:GLU:CG	1:F:268:ASN:HB2	2.46	0.44
1:A:136:LYS:HE2	1:A:245:ILE:HG12	1.99	0.44
1:C:231:ASP:C	1:C:233:LYS:N	2.70	0.44
1:E:159:ILE:HG23	1:E:193:GLY:O	2.18	0.44
1:B:259:GLN:HG2	1:B:264:ASP:N	2.33	0.43
1:E:105:MET:HG3	1:E:261:LEU:HD21	1.99	0.43
1:F:264:ASP:HA	1:F:265:PRO:HD2	1.74	0.43
1:B:255:ILE:O	1:B:259:GLN:HB2	2.18	0.43
1:C:136:LYS:CG	1:C:213:PHE:CE2	3.01	0.43
1:B:259:GLN:HG2	1:B:264:ASP:HB2	2.00	0.43
1:B:168:HIS:CE1	1:B:174:PHE:CD2	3.07	0.43
1:C:191:ILE:HD13	1:C:191:ILE:HG21	1.64	0.43
1:C:198:ASP:OD2	1:C:200:ASP:HB2	2.19	0.43
1:C:255:ILE:HD12	1:C:255:ILE:HA	1.77	0.43
1:C:206:HIS:CD2	1:C:207:SER:N	2.87	0.43
1:A:251:SER:HB2	7:A:893:HOH:O	2.18	0.43
1:F:121:TYR:CG	1:F:127:ARG:HG2	2.53	0.43
1:B:265:PRO:HA	1:B:266:LYS:CD	2.42	0.43
1:E:265:PRO:CB	1:E:266:LYS:HB2	2.49	0.43
1:A:184:ALA:HA	1:A:194:ASP:O	2.19	0.42
1:F:191:ILE:CD1	7:F:804:HOH:O	2.67	0.42
1:C:126:ASN:O	1:C:129:ASP:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:ILE:HD11	1:D:157:ALA:CA	2.49	0.42
1:F:264:ASP:O	1:F:266:LYS:CE	2.67	0.42
1:B:160:LEU:HD12	1:B:160:LEU:HA	1.67	0.42
1:C:231:ASP:O	1:C:234:ALA:N	2.39	0.42
1:F:235:VAL:HG12	1:F:254:ASP:OD1	2.20	0.42
1:D:231:ASP:HA	1:D:232:PRO:HD3	1.88	0.42
1:F:251:SER:O	1:F:254:ASP:N	2.51	0.42
1:C:251:SER:O	1:C:254:ASP:HB2	2.19	0.42
1:C:255:ILE:HD13	1:C:255:ILE:N	2.34	0.42
1:F:151:LYS:HD2	7:F:794:HOH:O	2.18	0.42
1:A:177:LYS:N	1:A:200:ASP:HB3	2.35	0.42
1:C:109:TRP:HB3	1:C:111:LYS:HB2	2.01	0.42
1:E:180:ILE:CD1	7:E:706:HOH:O	2.68	0.42
1:F:231:ASP:CG	1:F:233:LYS:H	2.24	0.42
1:A:114:ILE:HD12	1:A:147:LEU:HD22	2.01	0.41
1:B:229[A]:SER:HB3	1:B:234:ALA:CB	2.50	0.41
1:D:214:LEU:HD11	1:D:243:VAL:H	1.85	0.41
1:E:267:GLU:CB	1:E:268:ASN:HB2	2.50	0.41
1:A:199:GLU:O	1:A:199:GLU:HG3	2.19	0.41
1:D:108:VAL:HG12	1:D:261:LEU:HD13	2.02	0.41
1:B:229[A]:SER:CB	1:B:234:ALA:CB	2.99	0.41
1:D:160:LEU:HA	1:D:160:LEU:HD12	1.60	0.41
1:A:136:LYS:HD3	1:A:213:PHE:CE2	2.55	0.41
1:D:105:MET:HE2	1:D:105:MET:HB3	1.16	0.41
1:F:198:ASP:HB3	1:F:201:GLU:HG2	2.02	0.41
1:E:167:ALA:CB	1:E:173:ALA:HB2	2.38	0.41
1:E:231:ASP:O	1:E:234:ALA:N	2.41	0.41
1:E:105:MET:CE	1:F:179:GLY:C	2.89	0.41
1:D:123:PRO:HD2	1:D:199:GLU:CD	2.41	0.41
1:F:191:ILE:O	1:F:192:GLY:C	2.58	0.41
1:B:258:ILE:HG23	1:B:259:GLN:N	2.35	0.41
1:C:128:GLU:H	1:C:128:GLU:HG2	1.66	0.41
1:A:152:ILE:HD11	1:A:157:ALA:HB2	2.03	0.41
1:D:148:LYS:HD3	7:D:602:HOH:O	2.21	0.41
1:D:123:PRO:HD2	1:D:199:GLU:OE2	2.20	0.41
1:E:248:PHE:O	1:E:249:ARG:HD3	2.21	0.41
1:F:226:LEU:HD23	1:F:226:LEU:HA	1.82	0.41
1:A:105:MET:HE1	1:B:179:GLY:CA	2.47	0.40
1:B:258:ILE:CG2	1:B:259:GLN:N	2.84	0.40
1:C:119:ASN:HB2	1:C:160:LEU:HD11	2.03	0.40
1:D:113:TYR:C	1:D:114:ILE:HG13	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:ILE:HB	1:B:149:PHE:CD1	2.56	0.40
1:C:245:ILE:O	1:C:245:ILE:CG2	2.68	0.40
1:E:251:SER:O	1:E:252:ALA:C	2.59	0.40
1:A:154:THR:HG23	1:A:154:THR:O	2.20	0.40
1:B:231:ASP:O	1:B:234:ALA:HB3	2.22	0.40
1:D:199:GLU:O	1:D:199:GLU:HG3	2.22	0.40
1:B:241[A]:LYS:NZ	7:B:411:HOH:O	2.27	0.40
1:B:259:GLN:HG2	1:B:263:GLY:C	2.42	0.40
1:B:265:PRO:CA	1:B:266:LYS:HD2	2.44	0.40
1:E:152:ILE:HD12	1:E:154:THR:O	2.21	0.40
1:F:108:VAL:HG23	1:F:262:TYR:CZ	2.56	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:233:LYS:NZ	1:E:249:ARG:NH1[1_554]	2.07	0.13

## 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	163/165 (99%)	155 (95%)	6 (4%)	2 (1%)	14	7
1	B	163/165 (99%)	153 (94%)	7 (4%)	3 (2%)	9	3
1	C	163/165 (99%)	152 (93%)	7 (4%)	4 (2%)	6	1
1	D	163/165 (99%)	158 (97%)	3 (2%)	2 (1%)	14	7
1	E	163/165 (99%)	153 (94%)	7 (4%)	3 (2%)	9	3
1	F	163/165 (99%)	151 (93%)	8 (5%)	4 (2%)	6	1
All	All	978/990 (99%)	922 (94%)	38 (4%)	18 (2%)	9	3

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	266	LYS
1	B	266	LYS
1	C	245	ILE
1	C	266	LYS
1	C	267	GLU
1	D	266	LYS
1	E	247	THR
1	E	266	LYS
1	F	267	GLU
1	B	264	ASP
1	B	267	GLU
1	C	247	THR
1	E	246	ASN
1	F	245	ILE
1	F	266	LYS
1	A	106	GLY
1	D	106	GLY
1	F	193	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	134/134 (100%)	123 (92%)	11 (8%)	12	7
1	B	134/134 (100%)	118 (88%)	16 (12%)	6	2
1	C	134/134 (100%)	117 (87%)	17 (13%)	5	1
1	D	134/134 (100%)	121 (90%)	13 (10%)	9	5
1	E	134/134 (100%)	118 (88%)	16 (12%)	6	2
1	F	134/134 (100%)	121 (90%)	13 (10%)	9	5
All	All	804/804 (100%)	718 (89%)	86 (11%)	7	3

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110[A]	ARG
1	A	122	THR
1	A	127	ARG
1	A	128	GLU
1	A	135	ARG
1	A	156	MET
1	A	165	ARG
1	A	170	ASP
1	A	171	ASP
1	A	241[A]	LYS
1	A	256	ARG
1	B	104	MET
1	B	105	MET
1	B	119	ASN
1	B	122	THR
1	B	154	THR
1	B	156	MET
1	B	233	LYS
1	B	235	VAL
1	B	239	THR
1	B	241[A]	LYS
1	B	244	ASP
1	B	249	ARG
1	B	256	ARG
1	B	260	SER
1	B	266	LYS
1	B	267	GLU
1	C	104	MET
1	C	105	MET
1	C	135	ARG
1	C	136	LYS
1	C	150	SER
1	C	156	MET
1	C	165	ARG
1	C	177	LYS
1	C	219	GLU
1	C	229[A]	SER
1	C	230	SER
1	C	241	LYS
1	C	245	ILE
1	C	247	THR
1	C	249	ARG
1	C	255	ILE

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Mol	Chain	Res	Type
1	C	260	SER
1	D	104	MET
1	D	105	MET
1	D	110[A]	ARG
1	D	122	THR
1	D	127	ARG
1	D	135	ARG
1	D	139	GLN
1	D	156	MET
1	D	191	ILE
1	D	241[A]	LYS
1	D	247	THR
1	D	255	ILE
1	D	266	LYS
1	E	119	ASN
1	E	122	THR
1	E	142[A]	SER
1	E	154	THR
1	E	189	SER
1	E	233	LYS
1	E	235	VAL
1	E	239	THR
1	E	241[A]	LYS
1	E	244	ASP
1	E	247	THR
1	E	249	ARG
1	E	256	ARG
1	E	260	SER
1	E	266	LYS
1	E	267	GLU
1	F	104	MET
1	F	105	MET
1	F	135	ARG
1	F	156	MET
1	F	165	ARG
1	F	207	SER
1	F	229[A]	SER
1	F	233	LYS
1	F	241[A]	LYS
1	F	244	ASP
1	F	247	THR
1	F	260	SER

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Mol	Chain	Res	Type
1	F	266	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	ASN
1	A	172	HIS
1	A	206	HIS
1	A	211[A]	ASN
1	A	259	GLN
1	B	172	HIS
1	B	206	HIS
1	B	211[A]	ASN
1	C	119	ASN
1	C	172	HIS
1	C	206	HIS
1	C	211[A]	ASN
1	C	259	GLN
1	D	126	ASN
1	D	172	HIS
1	D	206	HIS
1	D	211[A]	ASN
1	D	259	GLN
1	E	172	HIS
1	E	206	HIS
1	E	211[A]	ASN
1	E	259	GLN
1	F	172	HIS
1	F	206	HIS
1	F	211[A]	ASN
1	F	259	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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



## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 30 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	HAE	A	874	2	4,4,4	1.19	0	2,4,4	4.26	2 (100%)
5	ACT	B	374	2	1,3,3	4.40	1 (100%)	0,3,3	0.00	-
6	AZI	C	474	2	0,2,2	0.00	-	0,1,1	0.00	-
4	HAE	D	574	2	4,4,4	1.31	1 (25%)	2,4,4	5.69	2 (100%)
5	ACT	E	674	2	1,3,3	4.36	1 (100%)	0,3,3	0.00	-
6	AZI	F	774	2	0,2,2	0.00	-	0,1,1	0.00	-

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
4	HAE	A	874	2	-	0/1/2/2	0/0/0/0
5	ACT	B	374	2	-	0/0/0/0	0/0/0/0
6	AZI	C	474	2	-	0/0/0/0	0/0/0/0
4	HAE	D	574	2	-	0/1/2/2	0/0/0/0
5	ACT	E	674	2	-	0/0/0/0	0/0/0/0
6	AZI	F	774	2	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	574	HAE	C2-N	2.05	1.36	1.33
5	E	674	ACT	CH3-C	4.36	1.54	1.48
5	B	374	ACT	CH3-C	4.40	1.54	1.48

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	574	HAE	O2-C2-C1	-5.76	111.66	122.07
4	A	874	HAE	O2-C2-C1	-3.73	115.34	122.07
4	A	874	HAE	C1-C2-N	4.73	124.39	116.08
4	D	574	HAE	C1-C2-N	5.63	125.96	116.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	374	ACT	1	0
6	C	474	AZI	1	0
5	E	674	ACT	1	0
6	F	774	AZI	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	165/165 (100%)	-0.36	1 (0%)	89 91	19, 36, 52, 62	9 (5%)
1	B	165/165 (100%)	-0.31	1 (0%)	89 91	16, 31, 51, 82	9 (5%)
1	C	165/165 (100%)	-0.22	3 (1%)	68 74	18, 34, 56, 86	8 (4%)
1	D	165/165 (100%)	-0.33	2 (1%)	79 83	18, 36, 52, 66	9 (5%)
1	E	165/165 (100%)	-0.30	2 (1%)	79 83	16, 30, 52, 89	9 (5%)
1	F	165/165 (100%)	-0.17	5 (3%)	50 58	18, 35, 56, 82	9 (5%)
All	All	990/990 (100%)	-0.28	14 (1%)	75 80	16, 34, 54, 89	53 (5%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	245	ILE	5.4
1	E	268	ASN	4.7
1	F	245	ILE	4.4
1	C	268	ASN	3.7
1	E	267	GLU	3.6
1	F	268	ASN	3.4
1	D	156	MET	3.2
1	D	268	ASN	3.1
1	F	266	LYS	2.8
1	B	268	ASN	2.5
1	F	246	ASN	2.3
1	F	247	THR	2.3
1	C	266	LYS	2.1
1	A	156	MET	2.0

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

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

## 6.3 Carbohydrates

There are no carbohydrates in this entry.

## 6.4 Ligands

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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CA	B	372	1/1	0.90	0.14	35,35,35,35	0
5	ACT	B	374	4/4	0.93	0.16	33,35,37,40	0
3	CA	D	573	1/1	0.94	0.13	51,51,51,51	0
3	CA	A	872	1/1	0.94	0.13	39,39,39,39	0
5	ACT	E	674	4/4	0.95	0.16	28,33,36,36	0
3	CA	F	773	1/1	0.96	0.11	37,37,37,37	0
3	CA	E	672	1/1	0.97	0.14	32,32,32,32	0
3	CA	C	473	1/1	0.97	0.10	38,38,38,38	0
3	CA	A	871	1/1	0.97	0.07	44,44,44,44	0
6	AZI	F	774	3/3	0.98	0.09	29,29,44,48	0
2	ZN	E	669	1/1	0.98	0.12	33,33,33,33	0
3	CA	D	572	1/1	0.98	0.08	40,40,40,40	0
3	CA	A	873	1/1	0.98	0.13	47,47,47,47	0
2	ZN	F	770	1/1	0.98	0.14	33,33,33,33	0
6	AZI	C	474	3/3	0.98	0.12	29,29,47,47	0
2	ZN	A	870	1/1	0.98	0.09	43,43,43,43	0
2	ZN	E	670	1/1	0.99	0.12	30,30,30,30	0
2	ZN	C	470	1/1	0.99	0.12	33,33,33,33	0
3	CA	E	671	1/1	0.99	0.09	27,27,27,27	0
3	CA	B	373	1/1	0.99	0.08	28,28,28,28	0
3	CA	E	673	1/1	0.99	0.07	30,30,30,30	0
3	CA	C	471	1/1	0.99	0.10	28,28,28,28	0
3	CA	F	772	1/1	0.99	0.07	30,30,30,30	0
3	CA	D	571	1/1	0.99	0.10	43,43,43,43	0
4	HAE	A	874	5/5	0.99	0.13	27,34,38,43	0
2	ZN	B	369	1/1	0.99	0.12	34,34,34,34	0
3	CA	F	771	1/1	0.99	0.10	29,29,29,29	0
2	ZN	F	769	1/1	0.99	0.09	33,33,33,33	0
3	CA	C	472	1/1	0.99	0.09	31,31,31,31	0
2	ZN	C	469	1/1	0.99	0.09	32,32,32,32	0
4	HAE	D	574	5/5	0.99	0.13	28,34,42,43	0
2	ZN	D	570	1/1	0.99	0.10	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CA	B	371	1/1	0.99	0.10	26,26,26,26	0
2	ZN	A	869	1/1	1.00	0.12	29,29,29,29	0
2	ZN	B	370	1/1	1.00	0.10	29,29,29,29	0
2	ZN	D	569	1/1	1.00	0.12	28,28,28,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.