



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:33 AM GMT

PDB ID : 3BA0  
Title : Crystal structure of full-length human MMP-12  
Authors : Bertini, I.; Calderone, V.; Fragai, M.; Jaiswal, R.; Luchinat, C.; Melikian, M.; Myonas, E.; Svergun, D.I.  
Deposited on : 2007-11-07  
Resolution : 3.00 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

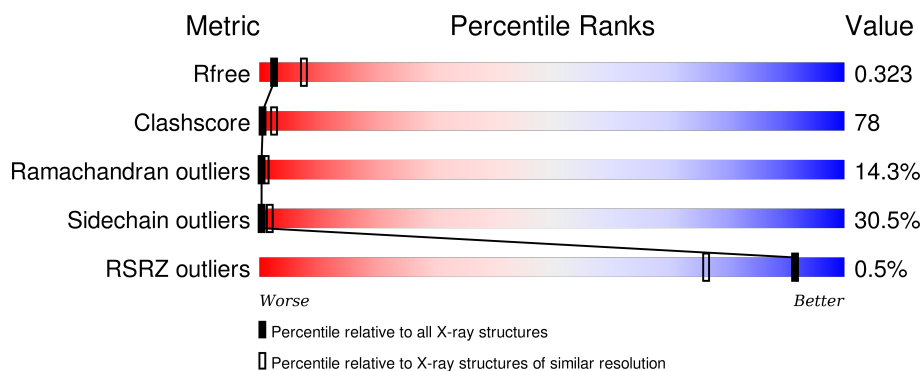
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	365	<div> <div></div> <div>12%</div> <div>34%</div> <div>29%</div> <div>25%</div> </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
4	HAE	A	477	-	X	-	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3063 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	365	Total	C	N	O	S	0	0	0
			2990	1939	504	540	7			

There is a discrepancy between the modelled and reference sequences:

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

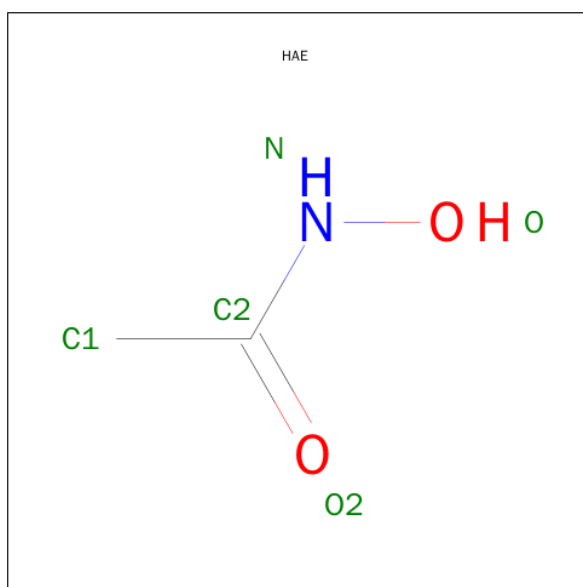
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Ca	0	0
			4	4		

- 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		

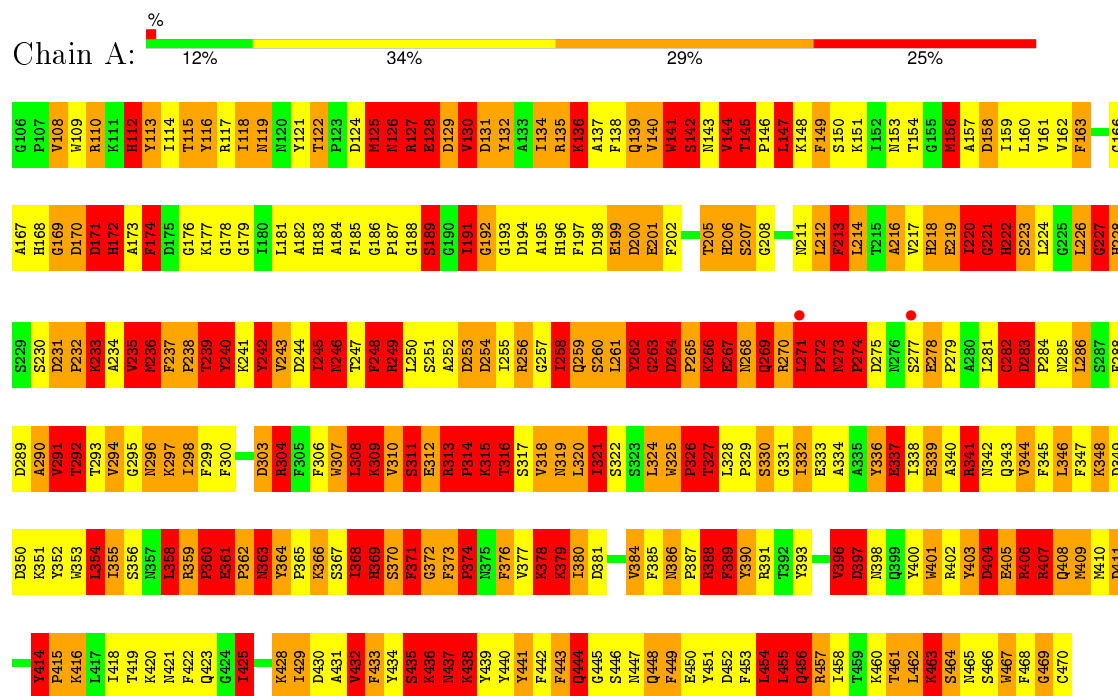
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	62	Total	O	0	0
			62	62		

### 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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.04Å 60.15Å 59.61Å 90.00° 90.74° 90.00°	Depositor
Resolution (Å)	30.70 – 3.00 30.70 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.70-3.00) 95.6 (30.70-3.00)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.63 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.236 , 0.319 0.241 , 0.323	Depositor DCC
$R_{free}$ test set	844 reflections (9.97%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.8	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 10.7	EDS
Estimated twinning fraction	0.055 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 9308 reflections	Xtriage
$F_o, F_c$ correlation	0.82	EDS
Total number of atoms	3063	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	6.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.62% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, 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	2.33	125/3089 (4.0%)	2.36	195/4189 (4.7%)

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	A	1	40

All (125) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	PRO	N-CD	10.59	1.62	1.47
1	A	436	LYS	CD-CE	10.29	1.76	1.51
1	A	108	VAL	CB-CG1	10.20	1.74	1.52
1	A	361	GLU	CD-OE2	9.36	1.35	1.25
1	A	219	GLU	CD-OE2	9.21	1.35	1.25
1	A	439	TYR	CE1-CZ	-9.20	1.26	1.38
1	A	361	GLU	CG-CD	9.02	1.65	1.51
1	A	233	LYS	CE-NZ	8.86	1.71	1.49
1	A	400	TYR	CE1-CZ	-8.51	1.27	1.38
1	A	326	PRO	N-CD	8.36	1.59	1.47
1	A	439	TYR	CE2-CZ	-8.15	1.27	1.38
1	A	393	TYR	CE2-CZ	8.00	1.49	1.38
1	A	449	PHE	CE2-CZ	7.99	1.52	1.37
1	A	192	GLY	C-O	7.97	1.36	1.23
1	A	239	THR	CA-CB	7.96	1.74	1.53
1	A	282	CYS	CB-SG	7.92	1.95	1.82
1	A	364	TYR	CD2-CE2	7.89	1.51	1.39
1	A	379	LYS	CD-CE	7.56	1.70	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	149	PHE	CE2-CZ	7.53	1.51	1.37
1	A	339	GLU	CG-CD	7.49	1.63	1.51
1	A	167	ALA	CA-CB	-7.43	1.36	1.52
1	A	341	ARG	CZ-NH2	7.39	1.42	1.33
1	A	219	GLU	CB-CG	7.36	1.66	1.52
1	A	272	PRO	CA-C	7.32	1.67	1.52
1	A	401	TRP	CB-CG	-7.32	1.37	1.50
1	A	336	TYR	CE2-CZ	-7.29	1.29	1.38
1	A	219	GLU	CG-CD	7.23	1.62	1.51
1	A	242	TYR	CE2-CZ	7.17	1.47	1.38
1	A	339	GLU	CD-OE1	7.09	1.33	1.25
1	A	361	GLU	CD-OE1	7.06	1.33	1.25
1	A	294	VAL	CB-CG2	-7.05	1.38	1.52
1	A	197	PHE	CE2-CZ	-7.04	1.24	1.37
1	A	310	VAL	CA-CB	-7.00	1.40	1.54
1	A	403	TYR	CB-CG	-6.80	1.41	1.51
1	A	376	PHE	CE2-CZ	6.79	1.50	1.37
1	A	108	VAL	CB-CG2	6.73	1.67	1.52
1	A	208	GLY	C-O	6.62	1.34	1.23
1	A	325	TRP	C-N	6.60	1.46	1.34
1	A	376	PHE	CD1-CE1	6.49	1.52	1.39
1	A	343	GLN	CB-CG	-6.46	1.35	1.52
1	A	195	ALA	C-O	-6.46	1.11	1.23
1	A	376	PHE	CG-CD1	6.45	1.48	1.38
1	A	216	ALA	CA-CB	-6.44	1.39	1.52
1	A	351	LYS	CE-NZ	6.43	1.65	1.49
1	A	432	VAL	CB-CG1	6.40	1.66	1.52
1	A	344	VAL	CB-CG1	-6.39	1.39	1.52
1	A	400	TYR	CD2-CE2	-6.36	1.29	1.39
1	A	288	PHE	CE2-CZ	6.34	1.49	1.37
1	A	434	TYR	CD2-CE2	6.34	1.48	1.39
1	A	294	VAL	CB-CG1	-6.34	1.39	1.52
1	A	163	PHE	CD1-CE1	-6.32	1.26	1.39
1	A	274	PRO	CB-CG	6.27	1.81	1.50
1	A	403	TYR	CE2-CZ	-6.25	1.30	1.38
1	A	199	GLU	CB-CG	-6.23	1.40	1.52
1	A	341	ARG	CZ-NH1	6.22	1.41	1.33
1	A	110	ARG	CG-CD	6.16	1.67	1.51
1	A	173	ALA	C-O	-6.11	1.11	1.23
1	A	378	LYS	CD-CE	6.08	1.66	1.51
1	A	132	TYR	CG-CD2	-6.07	1.31	1.39
1	A	127	ARG	CB-CG	-6.06	1.36	1.52

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	414	TYR	CE1-CZ	-6.06	1.30	1.38
1	A	285	ASN	CB-CG	6.01	1.64	1.51
1	A	196	HIS	N-CA	-5.98	1.34	1.46
1	A	219	GLU	CD-OE1	5.97	1.32	1.25
1	A	384	VAL	CB-CG2	-5.93	1.40	1.52
1	A	130	VAL	CB-CG1	-5.91	1.40	1.52
1	A	378	LYS	CE-NZ	5.89	1.63	1.49
1	A	397	ASP	C-N	-5.89	1.20	1.34
1	A	314	PRO	N-CD	-5.88	1.39	1.47
1	A	243	VAL	CB-CG1	5.88	1.65	1.52
1	A	351	LYS	CD-CE	5.86	1.66	1.51
1	A	439	TYR	CD1-CE1	-5.85	1.30	1.39
1	A	227	GLY	C-O	5.83	1.32	1.23
1	A	251	SER	CB-OG	5.82	1.49	1.42
1	A	219	GLU	N-CA	-5.79	1.34	1.46
1	A	444	GLN	CG-CD	5.70	1.64	1.51
1	A	324	LEU	CA-CB	-5.69	1.40	1.53
1	A	463	LYS	CE-NZ	5.67	1.63	1.49
1	A	147	LEU	CG-CD1	5.66	1.72	1.51
1	A	439	TYR	CG-CD2	-5.66	1.31	1.39
1	A	443	PHE	CE2-CZ	-5.66	1.26	1.37
1	A	131	ASP	CB-CG	5.63	1.63	1.51
1	A	116	TYR	CG-CD2	5.62	1.46	1.39
1	A	125	MET	C-N	5.61	1.47	1.34
1	A	240	TYR	CG-CD2	5.59	1.46	1.39
1	A	199	GLU	CA-CB	-5.57	1.41	1.53
1	A	202	PHE	CE2-CZ	5.56	1.48	1.37
1	A	177	LYS	CD-CE	5.51	1.65	1.51
1	A	113	TYR	CE2-CZ	-5.51	1.31	1.38
1	A	312	GLU	N-CA	-5.50	1.35	1.46
1	A	313	ARG	C-N	-5.49	1.23	1.34
1	A	347	PHE	CE1-CZ	-5.48	1.26	1.37
1	A	230	SER	CB-OG	5.48	1.49	1.42
1	A	116	TYR	CB-CG	5.45	1.59	1.51
1	A	254	ASP	C-O	5.39	1.33	1.23
1	A	400	TYR	CD1-CE1	-5.38	1.31	1.39
1	A	278	GLU	C-O	5.38	1.33	1.23
1	A	405	GLU	C-N	-5.36	1.21	1.34
1	A	339	GLU	CD-OE2	5.31	1.31	1.25
1	A	242	TYR	CG-CD2	5.31	1.46	1.39
1	A	310	VAL	C-O	5.30	1.33	1.23
1	A	444	GLN	CD-NE2	5.27	1.46	1.32

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	291	VAL	CB-CG2	-5.26	1.41	1.52
1	A	336	TYR	CD1-CE1	-5.26	1.31	1.39
1	A	246	ASN	CB-CG	5.26	1.63	1.51
1	A	372	GLY	C-N	-5.25	1.22	1.34
1	A	251	SER	CA-CB	5.23	1.60	1.52
1	A	290	ALA	CA-CB	5.22	1.63	1.52
1	A	441	TYR	CB-CG	5.22	1.59	1.51
1	A	439	TYR	CD2-CE2	-5.19	1.31	1.39
1	A	136	LYS	CD-CE	5.17	1.64	1.51
1	A	247	THR	C-O	5.16	1.33	1.23
1	A	174	PHE	CD2-CE2	-5.15	1.28	1.39
1	A	279	PRO	CA-CB	-5.13	1.43	1.53
1	A	406	ARG	C-O	-5.12	1.13	1.23
1	A	403	TYR	CG-CD1	-5.10	1.32	1.39
1	A	124	ASP	CB-CG	5.10	1.62	1.51
1	A	275	ASP	CG-OD1	5.06	1.36	1.25
1	A	353	TRP	CG-CD1	5.06	1.43	1.36
1	A	351	LYS	CG-CD	5.06	1.69	1.52
1	A	147	LEU	C-O	5.05	1.32	1.23
1	A	149	PHE	CG-CD2	5.05	1.46	1.38
1	A	240	TYR	CD2-CE2	5.05	1.47	1.39
1	A	223	SER	C-N	-5.04	1.22	1.34
1	A	128	GLU	CG-CD	5.03	1.59	1.51

All (195) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	414	TYR	C-N-CD	18.14	166.51	128.40
1	A	402	ARG	NE-CZ-NH1	-16.82	111.89	120.30
1	A	263	GLY	C-N-CA	15.82	161.26	121.70
1	A	158	ASP	CB-CG-OD1	14.19	131.07	118.30
1	A	227	GLY	O-C-N	-13.82	100.58	122.70
1	A	359	ARG	NE-CZ-NH1	13.50	127.05	120.30
1	A	368	ILE	O-C-N	-13.44	101.20	122.70
1	A	402	ARG	NE-CZ-NH2	13.42	127.01	120.30
1	A	158	ASP	CB-CG-OD2	-13.08	106.52	118.30
1	A	279	PRO	CA-N-CD	-12.05	94.62	111.50
1	A	142	SER	O-C-N	11.86	141.67	122.70
1	A	341	ARG	NE-CZ-NH1	-11.56	114.52	120.30
1	A	192	GLY	N-CA-C	-11.55	84.23	113.10
1	A	231	ASP	CB-CG-OD1	-11.52	107.93	118.30
1	A	414	TYR	C-N-CA	-10.55	77.67	122.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	397	ASP	CA-C-O	-10.40	98.26	120.10
1	A	249	ARG	NE-CZ-NH1	10.36	125.48	120.30
1	A	315	LYS	C-N-CA	10.30	147.44	121.70
1	A	406	ARG	CA-C-O	10.29	141.70	120.10
1	A	373	PHE	C-N-CD	9.94	149.26	128.40
1	A	396	VAL	CA-CB-CG2	9.93	125.80	110.90
1	A	397	ASP	C-N-CA	9.87	146.38	121.70
1	A	359	ARG	NE-CZ-NH2	-9.81	115.40	120.30
1	A	135	ARG	NE-CZ-NH1	-9.68	115.46	120.30
1	A	170	ASP	CB-CG-OD1	9.59	126.93	118.30
1	A	455	LEU	CB-CG-CD2	9.54	127.22	111.00
1	A	125	MET	CA-C-N	-9.46	96.39	117.20
1	A	396	VAL	O-C-N	-9.44	107.60	122.70
1	A	172	HIS	O-C-N	-9.44	107.60	122.70
1	A	169	GLY	C-N-CA	9.39	145.19	121.70
1	A	142	SER	CA-C-N	-9.15	97.06	117.20
1	A	278	GLU	CA-C-N	9.13	142.68	117.10
1	A	414	TYR	N-CA-C	9.09	135.54	111.00
1	A	406	ARG	O-C-N	-9.05	108.21	122.70
1	A	363	ASN	N-CA-C	8.93	135.10	111.00
1	A	397	ASP	O-C-N	8.91	136.96	122.70
1	A	270	ARG	N-CA-C	8.86	134.92	111.00
1	A	369	HIS	C-N-CA	8.84	143.81	121.70
1	A	279	PRO	O-C-N	-8.83	108.57	122.70
1	A	145	THR	C-N-CD	8.53	146.30	128.40
1	A	191	ILE	N-CA-C	-8.29	88.62	111.00
1	A	278	GLU	O-C-N	-8.23	105.47	121.10
1	A	231	ASP	CB-CG-OD2	8.05	125.54	118.30
1	A	200	ASP	CB-CG-OD2	7.97	125.47	118.30
1	A	358	LEU	CA-CB-CG	7.93	133.54	115.30
1	A	371	PHE	O-C-N	-7.88	109.80	123.20
1	A	275	ASP	CB-CG-OD1	7.83	125.35	118.30
1	A	435	SER	O-C-N	7.79	135.16	122.70
1	A	144	VAL	CA-CB-CG2	7.66	122.39	110.90
1	A	258	ILE	CG1-CB-CG2	-7.62	94.63	111.40
1	A	279	PRO	N-CA-CB	7.46	112.25	103.30
1	A	341	ARG	NH1-CZ-NH2	7.43	127.57	119.40
1	A	264	ASP	CA-C-N	-7.43	96.31	117.10
1	A	275	ASP	CB-CG-OD2	-7.40	111.64	118.30
1	A	388	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	A	124	ASP	CB-CG-OD2	7.33	124.90	118.30
1	A	213	PHE	CA-C-N	-7.32	101.09	117.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	258	ILE	N-CA-C	-7.28	91.36	111.00
1	A	129	ASP	CB-CG-OD1	-7.26	111.76	118.30
1	A	326	PRO	N-CA-C	7.26	130.97	112.10
1	A	368	ILE	CA-C-N	7.21	133.06	117.20
1	A	118	ILE	CG1-CB-CG2	-7.18	95.60	111.40
1	A	171	ASP	CA-CB-CG	7.17	129.18	113.40
1	A	242	TYR	CB-CA-C	7.15	124.70	110.40
1	A	110	ARG	NE-CZ-NH2	7.10	123.85	120.30
1	A	444	GLN	N-CA-C	-7.09	91.85	111.00
1	A	263	GLY	CA-C-O	-7.06	107.90	120.60
1	A	326	PRO	CA-N-CD	-6.98	101.73	111.50
1	A	264	ASP	O-C-N	6.94	134.28	121.10
1	A	389	PHE	C-N-CA	6.82	138.75	121.70
1	A	124	ASP	C-N-CA	6.82	138.74	121.70
1	A	294	VAL	N-CA-C	-6.78	92.71	111.00
1	A	407	ARG	CD-NE-CZ	6.65	132.90	123.60
1	A	308	LEU	CA-CB-CG	6.59	130.45	115.30
1	A	408	GLN	O-C-N	-6.48	112.34	122.70
1	A	397	ASP	CB-CA-C	-6.47	97.45	110.40
1	A	113	TYR	CB-CA-C	-6.46	97.48	110.40
1	A	213	PHE	CB-CA-C	-6.45	97.51	110.40
1	A	435	SER	CA-C-O	-6.44	106.58	120.10
1	A	406	ARG	CB-CA-C	-6.42	97.56	110.40
1	A	326	PRO	O-C-N	-6.40	112.46	122.70
1	A	328	LEU	CB-CA-C	-6.40	98.05	110.20
1	A	444	GLN	CA-CB-CG	6.39	127.46	113.40
1	A	359	ARG	CD-NE-CZ	6.39	132.55	123.60
1	A	432	VAL	CB-CA-C	-6.39	99.26	111.40
1	A	141	TRP	O-C-N	-6.39	112.48	122.70
1	A	156	MET	CG-SD-CE	6.38	110.41	100.20
1	A	173	ALA	O-C-N	-6.37	112.51	122.70
1	A	153	ASN	CB-CA-C	-6.37	97.67	110.40
1	A	269	GLN	C-N-CA	6.36	137.60	121.70
1	A	212	LEU	CA-CB-CG	6.34	129.89	115.30
1	A	396	VAL	CA-CB-CG1	6.30	120.36	110.90
1	A	415	PRO	N-CA-C	-6.30	95.72	112.10
1	A	324	LEU	CB-CG-CD2	-6.30	100.30	111.00
1	A	386	ASN	CB-CA-C	6.28	122.95	110.40
1	A	272	PRO	N-CA-C	6.26	128.39	112.10
1	A	126	ASN	N-CA-C	-6.24	94.17	111.00
1	A	462	LEU	CB-CG-CD2	6.22	121.57	111.00
1	A	409	MET	N-CA-CB	-6.21	99.42	110.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	312	GLU	C-N-CA	6.18	137.14	121.70
1	A	263	GLY	CA-C-N	6.14	130.70	117.20
1	A	113	TYR	CA-CB-CG	6.13	125.05	113.40
1	A	411	ASP	N-CA-C	-6.13	94.45	111.00
1	A	327	THR	O-C-N	-6.12	112.91	122.70
1	A	269	GLN	CA-C-N	-6.11	103.76	117.20
1	A	360	PRO	N-CA-C	6.10	127.96	112.10
1	A	308	LEU	CB-CG-CD1	-6.04	100.74	111.00
1	A	146	PRO	O-C-N	-5.99	113.11	122.70
1	A	125	MET	CA-C-O	5.97	132.65	120.10
1	A	328	LEU	N-CA-C	5.91	126.96	111.00
1	A	325	TRP	CA-CB-CG	5.91	124.92	113.70
1	A	206	HIS	O-C-N	-5.88	113.28	122.70
1	A	292	THR	CB-CA-C	-5.88	95.71	111.60
1	A	262	TYR	O-C-N	-5.88	113.20	123.20
1	A	310	VAL	C-N-CA	5.86	136.35	121.70
1	A	283	ASP	CB-CG-OD2	-5.84	113.04	118.30
1	A	177	LYS	N-CA-C	-5.82	95.29	111.00
1	A	341	ARG	CG-CD-NE	-5.80	99.62	111.80
1	A	245	ILE	N-CA-C	5.79	126.64	111.00
1	A	142	SER	CB-CA-C	5.78	121.07	110.10
1	A	237	PHE	N-CA-C	-5.77	95.43	111.00
1	A	321	ILE	CG1-CB-CG2	-5.76	98.72	111.40
1	A	265	PRO	CA-C-N	-5.76	104.52	117.20
1	A	315	LYS	N-CA-CB	5.75	120.96	110.60
1	A	170	ASP	C-N-CA	5.75	136.07	121.70
1	A	370	SER	CB-CA-C	5.74	121.01	110.10
1	A	267	GLU	C-N-CA	5.74	136.05	121.70
1	A	279	PRO	CB-CA-C	5.74	126.34	112.00
1	A	408	GLN	CA-C-O	5.74	132.15	120.10
1	A	425	ILE	CB-CA-C	5.73	123.05	111.60
1	A	271	LEU	CB-CA-C	5.69	121.02	110.20
1	A	277	SER	C-N-CA	5.69	135.92	121.70
1	A	270	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	177	LYS	CD-CE-NZ	5.68	124.77	111.70
1	A	171	ASP	CB-CG-OD1	5.67	123.40	118.30
1	A	181	LEU	CB-CG-CD1	-5.67	101.36	111.00
1	A	371	PHE	CA-C-N	-5.66	104.87	116.20
1	A	311	SER	N-CA-CB	5.65	118.97	110.50
1	A	279	PRO	CA-C-N	5.62	129.55	117.20
1	A	303	ASP	CB-CA-C	5.62	121.63	110.40
1	A	348	LYS	CD-CE-NZ	-5.61	98.80	111.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	258	ILE	CA-C-N	-5.58	104.93	117.20
1	A	200	ASP	CB-CG-OD1	-5.57	113.28	118.30
1	A	327	THR	CA-C-O	5.57	131.79	120.10
1	A	140	VAL	CA-CB-CG2	5.56	119.24	110.90
1	A	373	PHE	O-C-N	5.55	131.65	121.10
1	A	454	LEU	CB-CG-CD2	5.54	120.42	111.00
1	A	181	LEU	CB-CG-CD2	-5.54	101.59	111.00
1	A	273	ASN	N-CA-CB	-5.53	100.64	110.60
1	A	171	ASP	CB-CA-C	5.51	121.43	110.40
1	A	325	TRP	CA-C-O	5.47	131.59	120.10
1	A	181	LEU	CA-CB-CG	5.46	127.86	115.30
1	A	222	HIS	CA-CB-CG	5.43	122.83	113.60
1	A	134	ILE	CB-CG1-CD1	-5.42	98.73	113.90
1	A	380	ILE	N-CA-C	-5.35	96.55	111.00
1	A	337	GLU	CB-CA-C	5.32	121.03	110.40
1	A	112	HIS	N-CA-CB	-5.31	101.04	110.60
1	A	452	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	327	THR	OG1-CB-CG2	-5.30	97.81	110.00
1	A	396	VAL	C-N-CA	-5.30	108.45	121.70
1	A	409	MET	O-C-N	-5.30	114.23	122.70
1	A	270	ARG	CA-C-N	-5.29	105.56	117.20
1	A	304	ARG	O-C-N	-5.29	114.23	122.70
1	A	449	PHE	CG-CD2-CE2	-5.29	114.98	120.80
1	A	374	PRO	CA-N-CD	-5.29	104.10	111.50
1	A	147	LEU	CB-CG-CD1	5.27	119.96	111.00
1	A	235	VAL	CA-C-N	-5.27	105.60	117.20
1	A	277	SER	CA-CB-OG	5.27	125.42	111.20
1	A	267	GLU	CB-CA-C	-5.26	99.88	110.40
1	A	378	LYS	N-CA-C	5.21	125.07	111.00
1	A	327	THR	N-CA-C	-5.19	97.00	111.00
1	A	259	GLN	CB-CA-C	5.17	120.74	110.40
1	A	404	ASP	CB-CG-OD2	5.16	122.95	118.30
1	A	141	TRP	N-CA-CB	5.16	119.88	110.60
1	A	265	PRO	N-CA-C	5.15	125.49	112.10
1	A	269	GLN	O-C-N	5.12	130.90	122.70
1	A	309	LYS	N-CA-CB	5.12	119.82	110.60
1	A	236	MET	CB-CA-C	5.12	120.64	110.40
1	A	328	LEU	CB-CG-CD2	-5.12	102.30	111.00
1	A	158	ASP	N-CA-C	5.11	124.80	111.00
1	A	325	TRP	CA-C-N	-5.10	102.81	117.10
1	A	366	LYS	C-N-CA	-5.08	109.00	121.70
1	A	220	ILE	C-N-CA	-5.08	111.64	122.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	312	GLU	N-CA-CB	-5.07	101.48	110.60
1	A	242	TYR	CA-C-O	5.06	130.72	120.10
1	A	283	ASP	CB-CG-OD1	5.05	122.84	118.30
1	A	170	ASP	CA-CB-CG	5.03	124.47	113.40
1	A	218	HIS	CB-CA-C	-5.03	100.35	110.40
1	A	237	PHE	N-CA-CB	-5.02	101.56	110.60
1	A	354	LEU	CB-CG-CD2	-5.02	102.47	111.00
1	A	278	GLU	CA-C-O	-5.01	109.57	120.10
1	A	368	ILE	CB-CG1-CD1	5.01	127.93	113.90
1	A	317	SER	O-C-N	-5.00	114.69	122.70
1	A	325	TRP	CB-CA-C	5.00	120.41	110.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	236	MET	CA

All (40) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	141	TRP	Mainchain
1	A	142	SER	Mainchain
1	A	145	THR	Mainchain
1	A	169	GLY	Peptide
1	A	171	ASP	Mainchain
1	A	172	HIS	Mainchain
1	A	191	ILE	Mainchain
1	A	205	THR	Mainchain
1	A	213	PHE	Mainchain
1	A	220	ILE	Mainchain
1	A	221	GLY	Mainchain
1	A	227	GLY	Mainchain
1	A	228	HIS	Mainchain
1	A	236	MET	Peptide
1	A	262	TYR	Mainchain
1	A	263	GLY	Mainchain
1	A	264	ASP	Mainchain
1	A	267	GLU	Mainchain
1	A	269	GLN	Peptide
1	A	278	GLU	Mainchain
1	A	308	LEU	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	A	314	PRO	Mainchain
1	A	315	LYS	Mainchain
1	A	316	THR	Mainchain
1	A	326	PRO	Mainchain,Peptide
1	A	331	GLY	Peptide
1	A	367	SER	Mainchain
1	A	368	ILE	Mainchain
1	A	369	HIS	Peptide
1	A	371	PHE	Mainchain,Peptide
1	A	372	GLY	Mainchain
1	A	390	TYR	Mainchain
1	A	396	VAL	Mainchain,Peptide
1	A	404	ASP	Mainchain
1	A	405	GLU	Mainchain
1	A	406	ARG	Sidechain
1	A	435	SER	Mainchain

## 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	2990	0	2843	456	0
2	A	2	0	0	0	0
3	A	4	0	0	1	0
4	A	5	0	5	0	0
5	A	62	0	0	8	0
All	All	3063	0	2848	456	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 78.

All (456) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:LYS:CD	1:A:436:LYS:CE	1.77	1.54
1:A:233:LYS:CE	1:A:233:LYS:NZ	1.71	1.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:PRO:CG	1:A:274:PRO:CB	1.81	1.46
1:A:218:HIS:ND1	1:A:236:MET:HB2	1.45	1.28
1:A:297:LYS:HG2	1:A:308:LEU:CD1	1.69	1.23
1:A:310:VAL:CG1	1:A:311:SER:H	1.50	1.20
1:A:142:SER:HB2	1:A:147:LEU:O	1.40	1.18
1:A:256:ARG:HH21	1:A:256:ARG:HB3	1.04	1.15
1:A:310:VAL:HG13	1:A:311:SER:N	1.52	1.13
1:A:241:LYS:O	1:A:243:VAL:HG13	1.47	1.13
1:A:378:LYS:NZ	1:A:378:LYS:HB2	1.62	1.13
1:A:253:ASP:O	1:A:256:ARG:HG2	1.48	1.13
1:A:295:GLY:O	1:A:296:ASN:HB3	1.36	1.12
1:A:438:LYS:HD2	1:A:454:LEU:HD23	1.21	1.11
1:A:460:LYS:HE3	1:A:462:LEU:HD21	1.21	1.09
1:A:216:ALA:O	1:A:220:ILE:HG13	1.54	1.06
1:A:295:GLY:O	1:A:296:ASN:CB	1.98	1.05
1:A:235:VAL:HG11	1:A:248:PHE:HE1	1.19	1.04
1:A:218:HIS:HD1	1:A:236:MET:HB2	0.92	1.02
1:A:297:LYS:HG2	1:A:308:LEU:HD11	1.06	1.02
1:A:374:PRO:HD2	1:A:377:VAL:HG23	1.42	1.02
1:A:249:ARG:HH11	1:A:249:ARG:HB3	1.20	1.01
1:A:364:TYR:CD2	1:A:366:LYS:HE2	1.95	1.01
1:A:218:HIS:HD1	1:A:236:MET:CB	1.74	1.01
1:A:310:VAL:HG13	1:A:311:SER:H	0.84	1.00
1:A:141:TRP:O	1:A:145:THR:HG22	1.61	1.00
1:A:297:LYS:HE2	1:A:309:LYS:HB2	1.46	0.98
1:A:218:HIS:ND1	1:A:236:MET:CB	2.27	0.97
1:A:259:GLN:HE22	1:A:270:ARG:NH2	1.62	0.96
1:A:460:LYS:CE	1:A:462:LEU:HD21	1.94	0.96
1:A:374:PRO:HD2	1:A:377:VAL:CG2	1.94	0.95
1:A:438:LYS:CD	1:A:454:LEU:HD23	1.96	0.95
1:A:252:ALA:HA	1:A:255:ILE:HD12	1.45	0.95
1:A:364:TYR:CE2	1:A:366:LYS:HE2	2.01	0.95
1:A:256:ARG:NH2	1:A:256:ARG:HB3	1.81	0.95
1:A:438:LYS:HA	1:A:453:PHE:CE2	2.01	0.95
1:A:435:SER:OG	1:A:441:TYR:CE2	2.22	0.94
1:A:259:GLN:HE22	1:A:270:ARG:HH22	1.12	0.93
1:A:234:ALA:C	1:A:236:MET:H	1.73	0.92
1:A:142:SER:HA	1:A:145:THR:HG22	1.52	0.92
1:A:228:HIS:CD2	1:A:238:PRO:HG3	2.06	0.91
1:A:156:MET:HB2	5:A:30:HOH:O	1.68	0.90
1:A:406:ARG:HH11	1:A:406:ARG:HG2	1.35	0.90

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:HIS:CE1	1:A:238:PRO:HG3	2.06	0.90
1:A:364:TYR:CE2	1:A:366:LYS:CE	2.54	0.90
1:A:235:VAL:HG11	1:A:248:PHE:CE1	2.07	0.90
1:A:228:HIS:NE2	1:A:238:PRO:HG3	1.87	0.90
1:A:451:TYR:OH	1:A:456:GLN:HB3	1.72	0.90
1:A:188:GLY:O	1:A:192:GLY:HA3	1.72	0.89
1:A:378:LYS:HZ2	1:A:378:LYS:HB2	1.28	0.89
1:A:362:PRO:O	1:A:363:ASN:HB2	1.71	0.89
1:A:256:ARG:HH21	1:A:256:ARG:CB	1.85	0.88
1:A:218:HIS:CE1	1:A:236:MET:CB	2.56	0.88
1:A:449:PHE:CD2	1:A:461:THR:HG22	2.09	0.88
1:A:338:ILE:HG23	1:A:385:PHE:CE2	2.10	0.87
1:A:271:LEU:N	1:A:272:PRO:O	2.07	0.87
1:A:246:ASN:HD22	1:A:246:ASN:N	1.72	0.87
1:A:450:GLU:OE1	1:A:460:LYS:HG3	1.73	0.87
1:A:141:TRP:O	1:A:145:THR:CG2	2.23	0.87
1:A:378:LYS:HB2	1:A:378:LYS:HZ3	1.37	0.86
1:A:325:TRP:HD1	1:A:326:PRO:HD2	1.37	0.86
1:A:218:HIS:CE1	1:A:236:MET:HB2	2.12	0.84
1:A:435:SER:OG	1:A:441:TYR:HE2	1.59	0.84
1:A:220:ILE:O	1:A:221:GLY:C	2.09	0.84
1:A:378:LYS:NZ	1:A:378:LYS:CB	2.39	0.84
1:A:378:LYS:O	1:A:379:LYS:CG	2.26	0.83
1:A:228:HIS:CG	1:A:238:PRO:HG3	2.13	0.83
1:A:138:PHE:HB3	1:A:149:PHE:CD2	2.14	0.83
1:A:374:PRO:HG2	1:A:376:PHE:HB2	1.61	0.82
1:A:258:ILE:O	1:A:262:TYR:HB2	1.80	0.81
1:A:297:LYS:CD	1:A:309:LYS:HB3	2.10	0.81
1:A:116:TYR:CD1	1:A:138:PHE:HE1	1.99	0.81
1:A:438:LYS:O	1:A:438:LYS:HG3	1.78	0.81
1:A:310:VAL:CG1	1:A:311:SER:N	2.22	0.80
1:A:116:TYR:CG	1:A:138:PHE:CE1	2.69	0.80
1:A:273:ASN:HB3	1:A:274:PRO:HD3	1.64	0.80
1:A:259:GLN:NE2	1:A:270:ARG:HH22	1.79	0.80
1:A:226:LEU:HD11	1:A:257:GLY:O	1.80	0.80
1:A:345:PHE:CZ	1:A:354:LEU:HD21	2.16	0.80
1:A:404:ASP:OD1	1:A:407:ARG:HB2	1.80	0.80
1:A:431:ALA:HB3	1:A:443:PHE:HB2	1.64	0.80
1:A:297:LYS:HD3	1:A:309:LYS:HB3	1.62	0.79
1:A:297:LYS:CG	1:A:308:LEU:HD11	2.02	0.79
1:A:281:LEU:HD21	1:A:316:THR:HB	1.64	0.79

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:ASN:N	1:A:246:ASN:ND2	2.31	0.79
1:A:442:PHE:O	1:A:448:GLN:HA	1.83	0.79
1:A:108:VAL:HG11	1:A:261:LEU:HB3	1.64	0.78
1:A:438:LYS:HD2	1:A:454:LEU:CD2	2.10	0.78
1:A:340:ALA:C	1:A:341:ARG:HG3	2.04	0.78
1:A:234:ALA:HB1	1:A:254:ASP:OD2	1.82	0.78
1:A:306:PHE:C	1:A:307:TRP:HD1	1.88	0.76
1:A:465:ASN:O	1:A:465:ASN:OD1	2.04	0.76
1:A:249:ARG:NH1	1:A:249:ARG:HB3	1.97	0.76
1:A:231:ASP:HB2	1:A:253:ASP:OD2	1.85	0.76
1:A:325:TRP:CD1	1:A:326:PRO:HD2	2.21	0.76
1:A:112:HIS:O	1:A:147:LEU:HD23	1.86	0.75
1:A:437:ASN:N	1:A:437:ASN:OD1	2.17	0.75
1:A:432:VAL:HG13	1:A:442:PHE:CE1	2.20	0.75
1:A:364:TYR:CE2	1:A:366:LYS:NZ	2.53	0.75
1:A:255:ILE:O	1:A:259:GLN:HB2	1.86	0.75
1:A:468:PHE:O	1:A:470:CYS:N	2.21	0.74
1:A:127:ARG:NH1	1:A:127:ARG:HG2	2.02	0.74
1:A:293:THR:HG22	1:A:298:ILE:HG23	1.70	0.74
1:A:182:ALA:HB3	1:A:219:GLU:HG3	1.69	0.73
1:A:327:THR:HG22	5:A:61:HOH:O	1.87	0.73
1:A:404:ASP:HB2	1:A:411:ASP:OD1	1.88	0.73
1:A:268:ASN:OD1	1:A:269:GLN:NE2	2.21	0.73
1:A:156:MET:O	1:A:156:MET:HG3	1.87	0.72
1:A:182:ALA:CB	1:A:219:GLU:HG3	2.18	0.72
1:A:297:LYS:HG2	1:A:308:LEU:HD12	1.70	0.72
1:A:428:LYS:O	1:A:444:GLN:NE2	2.22	0.72
1:A:378:LYS:O	1:A:379:LYS:HG2	1.90	0.72
1:A:303:ASP:O	1:A:321:ILE:HD11	1.89	0.72
1:A:218:HIS:CE1	1:A:236:MET:HB3	2.25	0.71
1:A:159:ILE:HG23	1:A:193:GLY:O	1.90	0.71
1:A:234:ALA:C	1:A:236:MET:N	2.44	0.71
1:A:127:ARG:HH11	1:A:127:ARG:HG2	1.53	0.71
1:A:143:ASN:O	1:A:144:VAL:HG13	1.89	0.71
1:A:172:HIS:NE2	5:A:32:HOH:O	2.21	0.70
1:A:292:THR:HG22	1:A:293:THR:H	1.56	0.70
1:A:228:HIS:CG	1:A:238:PRO:CG	2.74	0.70
1:A:360:PRO:O	1:A:361:GLU:O	2.08	0.70
1:A:248:PHE:HA	5:A:13:HOH:O	1.90	0.70
1:A:293:THR:HA	1:A:298:ILE:HA	1.75	0.69
1:A:320:LEU:HD12	1:A:320:LEU:N	2.08	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:LYS:O	1:A:267:GLU:HB2	1.92	0.69
1:A:307:TRP:CD1	1:A:307:TRP:N	2.59	0.69
1:A:388:ARG:HH21	1:A:454:LEU:HD21	1.56	0.69
1:A:463:LYS:O	1:A:464:SER:C	2.31	0.69
1:A:249:ARG:HH22	1:A:271:LEU:HD22	1.58	0.69
1:A:246:ASN:H	1:A:246:ASN:ND2	1.91	0.68
1:A:368:ILE:O	1:A:369:HIS:CG	2.45	0.68
1:A:436:LYS:C	1:A:437:ASN:OD1	2.32	0.68
1:A:450:GLU:CB	1:A:460:LYS:HB2	2.23	0.68
1:A:378:LYS:O	1:A:379:LYS:HG3	1.92	0.68
1:A:198:ASP:OD2	3:A:475:CA:CA	1.71	0.67
1:A:450:GLU:HB3	1:A:460:LYS:HB2	1.76	0.67
1:A:378:LYS:CB	1:A:378:LYS:HZ3	2.04	0.67
1:A:248:PHE:C	1:A:249:ARG:HG3	2.15	0.67
1:A:329:PRO:HB2	1:A:348:LYS:NZ	2.10	0.67
1:A:132:TYR:CZ	1:A:136:LYS:HD3	2.31	0.66
1:A:172:HIS:CE1	5:A:32:HOH:O	2.47	0.66
1:A:449:PHE:CE2	1:A:461:THR:HG22	2.30	0.66
1:A:352:TYR:HE2	1:A:354:LEU:HD12	1.61	0.65
1:A:297:LYS:CE	1:A:309:LYS:HB2	2.25	0.65
1:A:468:PHE:N	1:A:468:PHE:CD1	2.61	0.65
1:A:435:SER:HG	1:A:441:TYR:HE2	0.76	0.64
1:A:241:LYS:HG2	1:A:243:VAL:CG1	2.27	0.64
1:A:374:PRO:CD	1:A:377:VAL:HG23	2.23	0.64
1:A:226:LEU:CD1	1:A:257:GLY:O	2.46	0.64
1:A:297:LYS:HE2	1:A:309:LYS:CB	2.23	0.63
1:A:119:ASN:HB2	1:A:161:VAL:O	1.97	0.63
1:A:257:GLY:HA2	1:A:260:SER:HB3	1.81	0.63
1:A:213:PHE:HD2	1:A:214:LEU:HD13	1.62	0.63
1:A:307:TRP:HD1	1:A:307:TRP:N	1.96	0.63
1:A:243:VAL:HG23	1:A:244:ASP:O	1.99	0.63
1:A:435:SER:OG	1:A:441:TYR:CD2	2.52	0.63
1:A:468:PHE:N	1:A:468:PHE:HD1	1.95	0.62
1:A:226:LEU:HD21	1:A:257:GLY:O	1.99	0.62
1:A:125:MET:HG2	1:A:127:ARG:HH12	1.65	0.62
1:A:130:VAL:CG2	1:A:212:LEU:HD21	2.30	0.62
1:A:211:ASN:OD1	1:A:214:LEU:HD22	2.00	0.62
1:A:340:ALA:C	1:A:341:ARG:CG	2.68	0.62
1:A:435:SER:O	1:A:437:ASN:N	2.25	0.62
1:A:304:ARG:O	1:A:321:ILE:HG12	2.00	0.61
1:A:312:GLU:O	1:A:314:PRO:HD3	1.99	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:PHE:CE1	1:A:391:ARG:HB2	2.35	0.61
1:A:232:PRO:O	1:A:234:ALA:N	2.33	0.61
1:A:256:ARG:HG3	1:A:257:GLY:N	2.14	0.61
1:A:384:VAL:HB	1:A:432:VAL:HB	1.81	0.61
1:A:297:LYS:CG	1:A:308:LEU:CD1	2.63	0.61
1:A:342:ASN:O	1:A:356:SER:HA	2.00	0.61
1:A:241:LYS:O	1:A:243:VAL:CG1	2.38	0.61
1:A:438:LYS:O	1:A:438:LYS:CG	2.48	0.61
1:A:368:ILE:O	1:A:369:HIS:CD2	2.54	0.61
1:A:406:ARG:HG2	1:A:406:ARG:NH1	2.11	0.60
1:A:440:TYR:CE1	1:A:453:PHE:HB3	2.35	0.60
1:A:116:TYR:CD1	1:A:138:PHE:CE1	2.85	0.60
1:A:445:GLY:C	1:A:447:ASN:H	2.05	0.60
1:A:369:HIS:HD2	1:A:373:PHE:HB2	1.67	0.59
1:A:364:TYR:HE2	1:A:366:LYS:CE	2.15	0.59
1:A:248:PHE:CD2	1:A:248:PHE:C	2.73	0.59
1:A:435:SER:C	1:A:437:ASN:H	2.06	0.59
1:A:234:ALA:O	1:A:236:MET:N	2.36	0.59
1:A:364:TYR:HB3	1:A:365:PRO:HA	1.84	0.59
1:A:376:PHE:HA	5:A:1:HOH:O	2.01	0.59
1:A:222:HIS:CE1	1:A:227:GLY:O	2.56	0.58
1:A:321:ILE:HD12	1:A:330:SER:HA	1.85	0.58
1:A:228:HIS:ND1	1:A:238:PRO:HG3	2.17	0.58
1:A:297:LYS:CE	1:A:309:LYS:CB	2.81	0.58
1:A:438:LYS:HA	1:A:453:PHE:CZ	2.37	0.58
1:A:438:LYS:HA	1:A:453:PHE:HE2	1.64	0.58
1:A:309:LYS:N	1:A:309:LYS:HD3	2.18	0.58
1:A:281:LEU:CD2	1:A:316:THR:HB	2.34	0.58
1:A:340:ALA:O	1:A:341:ARG:CG	2.51	0.58
1:A:174:PHE:HE2	1:A:183:HIS:HD1	1.48	0.58
1:A:308:LEU:O	1:A:309:LYS:HD2	2.04	0.58
1:A:109:TRP:CD1	1:A:224:LEU:HD23	2.38	0.58
1:A:232:PRO:HG2	1:A:233:LYS:HD2	1.86	0.58
1:A:388:ARG:HH21	1:A:454:LEU:CD2	2.17	0.58
1:A:298:ILE:HD11	1:A:310:VAL:HB	1.85	0.57
1:A:211:ASN:OD1	1:A:214:LEU:HB2	2.04	0.57
1:A:132:TYR:CE1	1:A:136:LYS:HD3	2.38	0.57
1:A:291:VAL:CG1	1:A:431:ALA:HB1	2.34	0.57
1:A:449:PHE:HD2	1:A:461:THR:HG22	1.63	0.57
1:A:291:VAL:CG2	1:A:292:THR:N	2.68	0.57
1:A:144:VAL:HG11	1:A:250:LEU:HD12	1.87	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:GLN:O	1:A:409:MET:HG2	2.05	0.57
1:A:291:VAL:HG13	1:A:431:ALA:HB1	1.86	0.57
1:A:174:PHE:CE2	1:A:183:HIS:ND1	2.71	0.57
1:A:118:ILE:HD12	1:A:151:LYS:HD2	1.87	0.56
1:A:134:ILE:C	1:A:136:LYS:N	2.57	0.56
1:A:292:THR:HG23	1:A:336:TYR:HA	1.88	0.56
1:A:248:PHE:CG	1:A:249:ARG:N	2.72	0.56
1:A:137:ALA:HA	1:A:217:VAL:CG1	2.35	0.56
1:A:249:ARG:HH12	1:A:271:LEU:HD13	1.71	0.56
1:A:134:ILE:HG22	1:A:135:ARG:N	2.20	0.56
1:A:185:PHE:O	1:A:193:GLY:HA2	2.06	0.56
1:A:266:LYS:HE3	1:A:470:CYS:O	2.05	0.56
1:A:286:LEU:HD11	1:A:307:TRP:CZ3	2.41	0.56
1:A:451:TYR:HD1	1:A:458:ILE:HD12	1.71	0.56
1:A:358:LEU:O	1:A:359:ARG:HG2	2.06	0.56
1:A:273:ASN:CB	1:A:274:PRO:HD3	2.36	0.55
1:A:307:TRP:CE3	1:A:468:PHE:HE2	2.25	0.55
1:A:403:TYR:HD1	1:A:410:MET:SD	2.30	0.55
1:A:115:THR:OG1	1:A:158:ASP:OD1	2.21	0.55
1:A:154:THR:HG23	1:A:154:THR:O	2.06	0.55
1:A:293:THR:O	1:A:337:GLU:HG2	2.06	0.55
1:A:142:SER:HA	1:A:145:THR:CG2	2.32	0.55
1:A:292:THR:HG22	1:A:293:THR:N	2.20	0.55
1:A:307:TRP:CG	1:A:318:VAL:HB	2.42	0.55
1:A:168:HIS:CE1	1:A:183:HIS:HE1	2.24	0.55
1:A:444:GLN:O	1:A:447:ASN:HB2	2.06	0.54
1:A:240:TYR:CZ	1:A:242:TYR:HB3	2.42	0.54
1:A:433:PHE:CD1	1:A:433:PHE:C	2.80	0.54
1:A:465:ASN:CG	1:A:465:ASN:O	2.42	0.54
1:A:116:TYR:CZ	1:A:151:LYS:HB2	2.42	0.54
1:A:142:SER:O	1:A:145:THR:O	2.24	0.54
1:A:143:ASN:C	1:A:144:VAL:HG13	2.27	0.54
1:A:308:LEU:O	1:A:309:LYS:CD	2.56	0.54
1:A:446:SER:C	1:A:464:SER:HB2	2.28	0.54
1:A:281:LEU:O	1:A:470:CYS:SG	2.66	0.54
1:A:310:VAL:HG12	1:A:311:SER:H	1.63	0.53
1:A:259:GLN:O	1:A:262:TYR:O	2.24	0.53
1:A:248:PHE:C	1:A:249:ARG:CG	2.77	0.53
1:A:418:ILE:HG21	1:A:425:ILE:HD11	1.90	0.53
1:A:329:PRO:HB2	1:A:348:LYS:HZ2	1.72	0.53
1:A:136:LYS:O	1:A:139:GLN:HB2	2.08	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:TRP:CZ2	1:A:415:PRO:HG3	2.43	0.53
1:A:418:ILE:O	1:A:422:PHE:HB2	2.08	0.53
1:A:447:ASN:N	1:A:464:SER:HB2	2.23	0.53
1:A:450:GLU:OE1	1:A:460:LYS:CG	2.52	0.53
1:A:297:LYS:CD	1:A:309:LYS:CB	2.83	0.53
1:A:297:LYS:CE	1:A:311:SER:HB3	2.39	0.53
1:A:460:LYS:HE3	1:A:462:LEU:CD2	2.14	0.53
1:A:432:VAL:HG13	1:A:442:PHE:CD1	2.44	0.53
1:A:116:TYR:CD2	1:A:138:PHE:CE1	2.96	0.53
1:A:307:TRP:CD1	1:A:318:VAL:HB	2.44	0.53
1:A:271:LEU:HA	1:A:272:PRO:C	2.30	0.52
1:A:188:GLY:C	1:A:189:SER:O	2.47	0.52
1:A:291:VAL:HG23	1:A:292:THR:N	2.24	0.52
1:A:309:LYS:NZ	1:A:313:ARG:O	2.35	0.52
1:A:352:TYR:CE2	1:A:354:LEU:HD12	2.41	0.52
1:A:213:PHE:CD2	1:A:214:LEU:HD13	2.43	0.52
1:A:117:ARG:HB2	1:A:157:ALA:HB2	1.92	0.52
1:A:384:VAL:HG11	1:A:432:VAL:HG11	1.91	0.52
1:A:125:MET:HG2	1:A:127:ARG:NH1	2.25	0.52
1:A:414:TYR:CE2	1:A:416:LYS:HE3	2.44	0.52
1:A:130:VAL:HG22	1:A:212:LEU:HD21	1.91	0.52
1:A:438:LYS:CA	1:A:453:PHE:CE2	2.86	0.52
1:A:143:ASN:O	1:A:144:VAL:CG1	2.57	0.52
1:A:456:GLN:O	1:A:457:ARG:HG3	2.10	0.52
1:A:211:ASN:OD1	1:A:213:PHE:HB3	2.10	0.52
1:A:162:VAL:HG12	1:A:163:PHE:N	2.24	0.52
1:A:396:VAL:O	1:A:397:ASP:C	2.48	0.52
1:A:125:MET:CG	1:A:127:ARG:HH12	2.23	0.52
1:A:130:VAL:HG23	1:A:212:LEU:CD2	2.40	0.51
1:A:231:ASP:O	1:A:237:PHE:HB2	2.11	0.51
1:A:430:ASP:HB2	1:A:443:PHE:O	2.10	0.51
1:A:252:ALA:HA	1:A:255:ILE:CD1	2.30	0.51
1:A:139:GLN:O	1:A:140:VAL:C	2.48	0.51
1:A:256:ARG:O	1:A:260:SER:N	2.32	0.51
1:A:281:LEU:CD1	1:A:315:LYS:NZ	2.73	0.51
1:A:162:VAL:CG1	1:A:163:PHE:N	2.73	0.51
1:A:213:PHE:O	1:A:217:VAL:HG22	2.10	0.51
1:A:311:SER:C	1:A:313:ARG:H	2.14	0.51
1:A:442:PHE:O	1:A:448:GLN:CA	2.58	0.51
1:A:467:TRP:C	1:A:468:PHE:HD1	2.14	0.50
1:A:228:HIS:CD2	1:A:238:PRO:CG	2.89	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:ALA:HB2	1:A:333:GLU:C	2.31	0.50
1:A:418:ILE:CG2	1:A:425:ILE:HD11	2.41	0.50
1:A:221:GLY:O	1:A:224:LEU:CA	2.60	0.50
1:A:451:TYR:CD1	1:A:458:ILE:HD12	2.46	0.50
1:A:356:SER:O	1:A:359:ARG:N	2.45	0.50
1:A:463:LYS:O	1:A:465:ASN:N	2.44	0.50
1:A:130:VAL:HG23	1:A:212:LEU:HD21	1.94	0.50
1:A:281:LEU:C	1:A:282:CYS:SG	2.90	0.50
1:A:369:HIS:CD2	1:A:373:PHE:HB2	2.47	0.50
1:A:311:SER:O	1:A:313:ARG:N	2.45	0.50
1:A:154:THR:CG2	1:A:154:THR:O	2.60	0.50
1:A:467:TRP:N	1:A:467:TRP:CD1	2.79	0.49
1:A:221:GLY:O	1:A:224:LEU:N	2.45	0.49
1:A:318:VAL:HG23	1:A:319:ASN:N	2.26	0.49
1:A:241:LYS:CG	1:A:243:VAL:CG1	2.91	0.49
1:A:346:LEU:HD23	1:A:355:ILE:CD1	2.43	0.49
1:A:222:HIS:C	1:A:224:LEU:N	2.66	0.49
1:A:337:GLU:C	1:A:338:ILE:HG13	2.33	0.49
1:A:113:TYR:CD2	1:A:148:LYS:HG3	2.47	0.49
1:A:318:VAL:CG2	1:A:319:ASN:N	2.75	0.49
1:A:345:PHE:CE2	1:A:354:LEU:HD11	2.48	0.49
1:A:245:ILE:HG12	1:A:246:ASN:ND2	2.27	0.49
1:A:283:ASP:O	1:A:286:LEU:HB2	2.13	0.49
1:A:436:LYS:CG	1:A:436:LYS:CE	2.79	0.48
1:A:460:LYS:NZ	1:A:462:LEU:HD21	2.28	0.48
1:A:352:TYR:HE2	1:A:354:LEU:CD1	2.26	0.48
1:A:132:TYR:CZ	1:A:136:LYS:CD	2.96	0.48
1:A:245:ILE:HG12	1:A:246:ASN:HD22	1.78	0.48
1:A:116:TYR:CE1	1:A:151:LYS:HB2	2.48	0.48
1:A:127:ARG:O	1:A:129:ASP:N	2.47	0.48
1:A:333:GLU:OE2	1:A:379:LYS:HD2	2.14	0.48
1:A:329:PRO:CB	1:A:348:LYS:NZ	2.76	0.48
1:A:116:TYR:O	1:A:151:LYS:HA	2.13	0.48
1:A:184:ALA:HB1	1:A:194:ASP:O	2.14	0.48
1:A:295:GLY:O	1:A:296:ASN:HB2	2.03	0.48
1:A:170:ASP:OD1	1:A:185:PHE:CE2	2.67	0.48
1:A:134:ILE:O	1:A:136:LYS:N	2.46	0.48
1:A:255:ILE:O	1:A:259:GLN:CB	2.61	0.47
1:A:258:ILE:HD13	1:A:258:ILE:HA	1.64	0.47
1:A:455:LEU:O	1:A:456:GLN:O	2.31	0.47
1:A:248:PHE:O	1:A:249:ARG:CG	2.62	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:TYR:HD2	1:A:148:LYS:HG3	1.79	0.47
1:A:454:LEU:HD13	1:A:454:LEU:HA	1.41	0.47
1:A:271:LEU:CA	1:A:272:PRO:O	2.63	0.47
1:A:281:LEU:O	1:A:282:CYS:SG	2.73	0.47
1:A:377:VAL:HG13	1:A:396:VAL:HG11	1.96	0.47
1:A:232:PRO:HA	1:A:237:PHE:CG	2.50	0.47
1:A:299:PHE:CE2	1:A:308:LEU:HD22	2.50	0.47
1:A:226:LEU:CD2	1:A:257:GLY:O	2.62	0.47
1:A:425:ILE:O	1:A:444:GLN:HG3	2.15	0.47
1:A:440:TYR:HE1	1:A:453:PHE:CB	2.28	0.47
1:A:326:PRO:CG	1:A:360:PRO:HG2	2.45	0.47
1:A:428:LYS:HG3	1:A:429:ILE:N	2.30	0.47
1:A:228:HIS:CE1	1:A:238:PRO:CG	2.90	0.46
1:A:231:ASP:OD2	1:A:253:ASP:HB2	2.15	0.46
1:A:182:ALA:HB1	1:A:219:GLU:HG3	1.97	0.46
1:A:435:SER:C	1:A:437:ASN:N	2.68	0.46
1:A:232:PRO:HA	1:A:237:PHE:CD1	2.50	0.46
1:A:440:TYR:CE1	1:A:453:PHE:CB	2.98	0.46
1:A:304:ARG:HA	1:A:321:ILE:HD11	1.97	0.46
1:A:408:GLN:C	1:A:409:MET:HG2	2.36	0.46
1:A:199:GLU:O	1:A:199:GLU:HG3	2.15	0.46
1:A:127:ARG:HH11	1:A:127:ARG:CG	2.26	0.46
1:A:237:PHE:O	1:A:239:THR:N	2.48	0.46
1:A:428:LYS:O	1:A:444:GLN:HG2	2.16	0.46
1:A:378:LYS:C	1:A:379:LYS:CG	2.84	0.46
1:A:214:LEU:O	1:A:217:VAL:HG23	2.16	0.46
1:A:134:ILE:C	1:A:136:LYS:H	2.19	0.46
1:A:466:SER:O	1:A:469:GLY:HA2	2.16	0.46
1:A:256:ARG:CG	1:A:257:GLY:N	2.79	0.45
1:A:127:ARG:O	1:A:128:GLU:C	2.53	0.45
1:A:136:LYS:HB3	1:A:136:LYS:HE3	1.80	0.45
1:A:237:PHE:CD2	1:A:239:THR:HB	2.51	0.45
1:A:108:VAL:CG1	1:A:261:LEU:HB3	2.39	0.45
1:A:226:LEU:HD22	1:A:261:LEU:HD11	1.98	0.45
1:A:300:PHE:O	1:A:306:PHE:HA	2.16	0.45
1:A:403:TYR:CZ	1:A:408:GLN:HA	2.52	0.45
1:A:450:GLU:HB2	1:A:460:LYS:HB2	1.96	0.45
1:A:290:ALA:HB2	1:A:334:ALA:N	2.31	0.45
1:A:109:TRP:HD1	1:A:224:LEU:HD23	1.80	0.45
1:A:293:THR:HG22	1:A:298:ILE:CG2	2.42	0.45
1:A:403:TYR:OH	1:A:408:GLN:HA	2.15	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:GLY:O	1:A:179:GLY:C	2.54	0.45
1:A:121:TYR:CD1	1:A:130:VAL:HG11	2.52	0.45
1:A:273:ASN:CB	1:A:274:PRO:CD	2.94	0.45
1:A:409:MET:O	1:A:410:MET:C	2.53	0.45
1:A:436:LYS:N	1:A:437:ASN:OD1	2.50	0.44
1:A:231:ASP:HB3	1:A:234:ALA:HB2	1.98	0.44
1:A:446:SER:C	1:A:464:SER:CB	2.86	0.44
1:A:218:HIS:CD2	1:A:218:HIS:C	2.90	0.44
1:A:142:SER:CB	1:A:147:LEU:O	2.35	0.44
1:A:391:ARG:NE	1:A:411:ASP:OD2	2.51	0.44
1:A:324:LEU:HD12	5:A:59:HOH:O	2.18	0.44
1:A:218:HIS:HE1	1:A:236:MET:HB3	1.77	0.44
1:A:252:ALA:O	1:A:255:ILE:HB	2.17	0.44
1:A:384:VAL:HG11	1:A:432:VAL:CG1	2.48	0.44
1:A:185:PHE:O	1:A:193:GLY:CA	2.66	0.44
1:A:352:TYR:O	1:A:365:PRO:HA	2.17	0.44
1:A:160:LEU:HB2	1:A:194:ASP:OD2	2.17	0.44
1:A:453:PHE:C	1:A:453:PHE:CD1	2.91	0.44
1:A:125:MET:HB3	1:A:126:ASN:H	1.00	0.44
1:A:348:LYS:O	1:A:349:ASP:HB2	2.16	0.44
1:A:134:ILE:O	1:A:135:ARG:C	2.55	0.44
1:A:386:ASN:OD1	1:A:388:ARG:HB2	2.17	0.44
1:A:396:VAL:O	1:A:398:ASN:N	2.50	0.43
1:A:349:ASP:HB3	1:A:350:ASP:H	1.56	0.43
1:A:297:LYS:CG	1:A:309:LYS:HB3	2.47	0.43
1:A:345:PHE:CE2	1:A:354:LEU:HG	2.54	0.43
1:A:130:VAL:HG12	1:A:131:ASP:N	2.32	0.43
1:A:141:TRP:CE3	1:A:258:ILE:HG13	2.53	0.43
1:A:216:ALA:O	1:A:220:ILE:CG1	2.45	0.43
1:A:170:ASP:O	1:A:171:ASP:HB3	2.18	0.43
1:A:438:LYS:C	1:A:453:PHE:CE2	2.92	0.43
1:A:373:PHE:HB3	1:A:377:VAL:HG21	2.00	0.43
1:A:273:ASN:HB3	1:A:274:PRO:CD	2.42	0.43
1:A:386:ASN:HA	1:A:387:PRO:HD2	1.83	0.43
1:A:245:ILE:HG13	1:A:245:ILE:O	2.08	0.43
1:A:236:MET:SD	1:A:240:TYR:HA	2.59	0.43
1:A:265:PRO:HB2	1:A:274:PRO:HB3	2.01	0.43
1:A:309:LYS:HG2	1:A:309:LYS:HZ3	1.43	0.43
1:A:241:LYS:CG	1:A:243:VAL:HG13	2.49	0.43
1:A:340:ALA:O	1:A:341:ARG:HG3	2.16	0.43
1:A:406:ARG:HH11	1:A:406:ARG:CG	2.18	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:VAL:HG11	1:A:344:VAL:HG21	2.01	0.42
1:A:443:PHE:HA	1:A:447:ASN:O	2.20	0.42
1:A:142:SER:CA	1:A:145:THR:HG22	2.34	0.42
1:A:174:PHE:CD1	1:A:198:ASP:HA	2.53	0.42
1:A:206:HIS:HB2	1:A:207:SER:H	1.66	0.42
1:A:259:GLN:HA	1:A:263:GLY:O	2.20	0.42
1:A:122:THR:H	1:A:122:THR:HG22	1.37	0.42
1:A:455:LEU:HD12	1:A:455:LEU:C	2.39	0.42
1:A:451:TYR:OH	1:A:456:GLN:CB	2.56	0.42
1:A:291:VAL:HG23	1:A:292:THR:H	1.84	0.42
1:A:374:PRO:HD2	1:A:377:VAL:HG21	1.93	0.42
1:A:231:ASP:OD2	1:A:253:ASP:CB	2.68	0.42
1:A:297:LYS:CG	1:A:308:LEU:HD12	2.43	0.42
1:A:416:LYS:HD3	1:A:421:ASN:ND2	2.34	0.42
1:A:248:PHE:O	1:A:248:PHE:CD2	2.73	0.42
1:A:159:ILE:HG22	1:A:160:LEU:N	2.35	0.42
1:A:228:HIS:ND1	1:A:238:PRO:CG	2.82	0.41
1:A:198:ASP:O	1:A:201:GLU:HG2	2.19	0.41
1:A:293:THR:HB	1:A:297:LYS:O	2.20	0.41
1:A:378:LYS:HZ2	1:A:378:LYS:CB	2.11	0.41
1:A:368:ILE:HD13	1:A:380:ILE:HD11	2.02	0.41
1:A:326:PRO:HG3	1:A:360:PRO:HG2	2.02	0.41
1:A:109:TRP:CE2	1:A:187:PRO:HB3	2.55	0.41
1:A:249:ARG:NH2	1:A:271:LEU:HD22	2.31	0.41
1:A:432:VAL:CG1	1:A:442:PHE:CE1	3.00	0.41
1:A:168:HIS:CE1	1:A:183:HIS:CE1	3.06	0.41
1:A:121:TYR:CE1	1:A:130:VAL:HG11	2.55	0.41
1:A:344:VAL:O	1:A:355:ILE:HB	2.20	0.41
1:A:273:ASN:H	1:A:273:ASN:ND2	2.18	0.41
1:A:309:LYS:HE2	1:A:315:LYS:O	2.21	0.41
1:A:292:THR:CG2	1:A:336:TYR:HA	2.50	0.41
1:A:440:TYR:CD1	1:A:453:PHE:HB3	2.55	0.41
1:A:188:GLY:O	1:A:189:SER:C	2.59	0.41
1:A:116:TYR:HA	1:A:159:ILE:O	2.21	0.41
1:A:193:GLY:O	1:A:223:SER:HB3	2.20	0.41
1:A:176:GLY:O	1:A:200:ASP:HB2	2.20	0.41
1:A:271:LEU:HA	1:A:271:LEU:HD23	1.65	0.41
1:A:388:ARG:HG2	5:A:2:HOH:O	2.20	0.41
1:A:414:TYR:C	1:A:415:PRO:O	2.49	0.41
1:A:444:GLN:O	1:A:447:ASN:CB	2.69	0.40
1:A:212:LEU:HG	1:A:212:LEU:O	2.21	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:PHE:HE2	1:A:354:LEU:HD11	1.87	0.40
1:A:329:PRO:CG	1:A:348:LYS:HZ3	2.34	0.40
1:A:232:PRO:C	1:A:234:ALA:H	2.24	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	363/365 (100%)	241 (66%)	70 (19%)	52 (14%)	<b>0</b> <b>1</b>

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	MET
1	A	144	VAL
1	A	191	ILE
1	A	233	LYS
1	A	235	VAL
1	A	236	MET
1	A	239	THR
1	A	242	TYR
1	A	248	PHE
1	A	264	ASP
1	A	266	LYS
1	A	267	GLU
1	A	268	ASN
1	A	272	PRO
1	A	273	ASN
1	A	296	ASN
1	A	309	LYS
1	A	311	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	315	LYS
1	A	332	ILE
1	A	361	GLU
1	A	363	ASN
1	A	370	SER
1	A	397	ASP
1	A	437	ASN
1	A	456	GLN
1	A	469	GLY
1	A	171	ASP
1	A	258	ILE
1	A	362	PRO
1	A	436	LYS
1	A	128	GLU
1	A	166	GLY
1	A	189	SER
1	A	238	PRO
1	A	274	PRO
1	A	360	PRO
1	A	464	SER
1	A	126	ASN
1	A	127	ARG
1	A	222	HIS
1	A	232	PRO
1	A	371	PHE
1	A	457	ARG
1	A	326	PRO
1	A	341	ARG
1	A	379	LYS
1	A	438	LYS
1	A	186	GLY
1	A	221	GLY
1	A	368	ILE
1	A	414	TYR

### 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	318/318 (100%)	221 (70%)	97 (30%)	<b>0</b> <b>2</b>

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	ARG
1	A	112	HIS
1	A	114	ILE
1	A	115	THR
1	A	119	ASN
1	A	122	THR
1	A	127	ARG
1	A	128	GLU
1	A	130	VAL
1	A	136	LYS
1	A	139	GLN
1	A	145	THR
1	A	147	LEU
1	A	150	SER
1	A	156	MET
1	A	171	ASP
1	A	174	PHE
1	A	189	SER
1	A	191	ILE
1	A	201	GLU
1	A	205	THR
1	A	207	SER
1	A	214	LEU
1	A	226	LEU
1	A	233	LYS
1	A	235	VAL
1	A	240	TYR
1	A	242	TYR
1	A	245	ILE
1	A	246	ASN
1	A	248	PHE
1	A	249	ARG
1	A	253	ASP
1	A	256	ARG
1	A	258	ILE
1	A	260	SER
1	A	261	LEU
1	A	266	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	271	LEU
1	A	282	CYS
1	A	283	ASP
1	A	284	PRO
1	A	286	LEU
1	A	289	ASP
1	A	291	VAL
1	A	292	THR
1	A	297	LYS
1	A	298	ILE
1	A	304	ARG
1	A	307	TRP
1	A	309	LYS
1	A	313	ARG
1	A	315	LYS
1	A	316	THR
1	A	318	VAL
1	A	319	ASN
1	A	320	LEU
1	A	321	ILE
1	A	322	SER
1	A	327	THR
1	A	330	SER
1	A	332	ILE
1	A	337	GLU
1	A	339	GLU
1	A	346	LEU
1	A	354	LEU
1	A	355	ILE
1	A	358	LEU
1	A	368	ILE
1	A	371	PHE
1	A	374	PRO
1	A	378	LYS
1	A	381	ASP
1	A	388	ARG
1	A	389	PHE
1	A	390	TYR
1	A	406	ARG
1	A	407	ARG
1	A	416	LYS
1	A	419	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	420	LYS
1	A	423	GLN
1	A	425	ILE
1	A	428	LYS
1	A	429	ILE
1	A	432	VAL
1	A	433	PHE
1	A	437	ASN
1	A	438	LYS
1	A	444	GLN
1	A	448	GLN
1	A	454	LEU
1	A	455	LEU
1	A	456	GLN
1	A	461	THR
1	A	463	LYS
1	A	467	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	ASN
1	A	228	HIS
1	A	246	ASN
1	A	259	GLN
1	A	269	GLN
1	A	296	ASN
1	A	369	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

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 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	477	-	4,4,4	4.35	4 (100%)	4,4,4	2.75	3 (75%)

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	477	-	-	0/1/2/2	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	477	HAE	O-N	2.41	1.44	1.39
4	A	477	HAE	O2-C2	3.41	1.31	1.23
4	A	477	HAE	C1-C2	4.61	1.59	1.50
4	A	477	HAE	C2-N	6.08	1.42	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	477	HAE	O2-C2-N	-3.10	119.54	123.42
4	A	477	HAE	C1-C2-N	2.68	121.22	116.09
4	A	477	HAE	O-N-C2	3.33	124.58	119.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	365/365 (100%)	-0.55	2 (0%) 91 76	2, 3, 18, 27	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	271	LEU	2.8
1	A	277	SER	2.7

### 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
4	HAE	A	477	5/5	0.93	0.16	-0.44	9,14,16,17	0
3	CA	A	473	1/1	0.98	0.10	-1.33	2,2,2,2	0
3	CA	A	474	1/1	0.98	0.10	-1.65	2,2,2,2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CA	A	475	1/1	0.99	0.05	-2.76	2,2,2,2	0
3	CA	A	476	1/1	0.98	0.07	-2.82	15,15,15,15	0
2	ZN	A	472	1/1	0.99	0.06	-3.63	2,2,2,2	0
2	ZN	A	471	1/1	0.98	0.06	-	11,11,11,11	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.