



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:19 PM UTC

PDB ID : 3BA0 / pdb_00003ba0
Title : Crystal structure of full-length human MMP-12
Authors : Bertini, I.; Calderone, V.; Fragai, M.; Jaiswal, R.; Luchinat, C.; Melikian, M.;
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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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

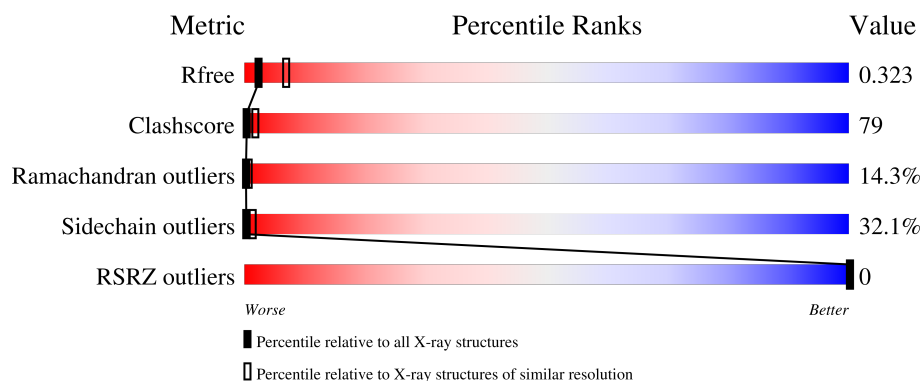
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	

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 mutation	UNP P39900

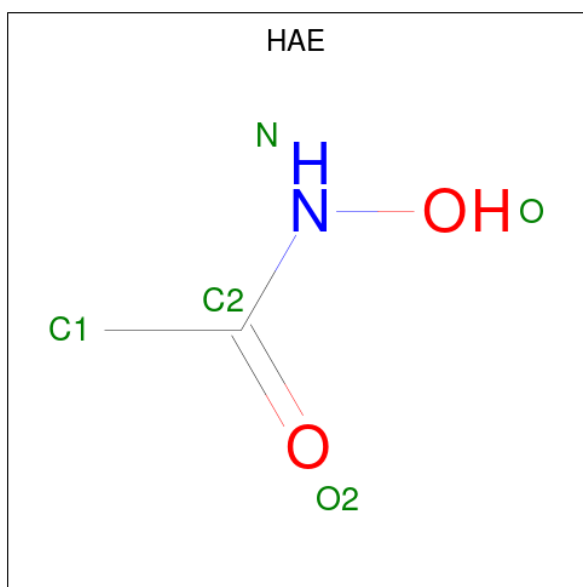
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 4 is ACETOHYDROXAMIC ACID (CCD ID: HAE) (formula: C₂H₅NO₂).



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

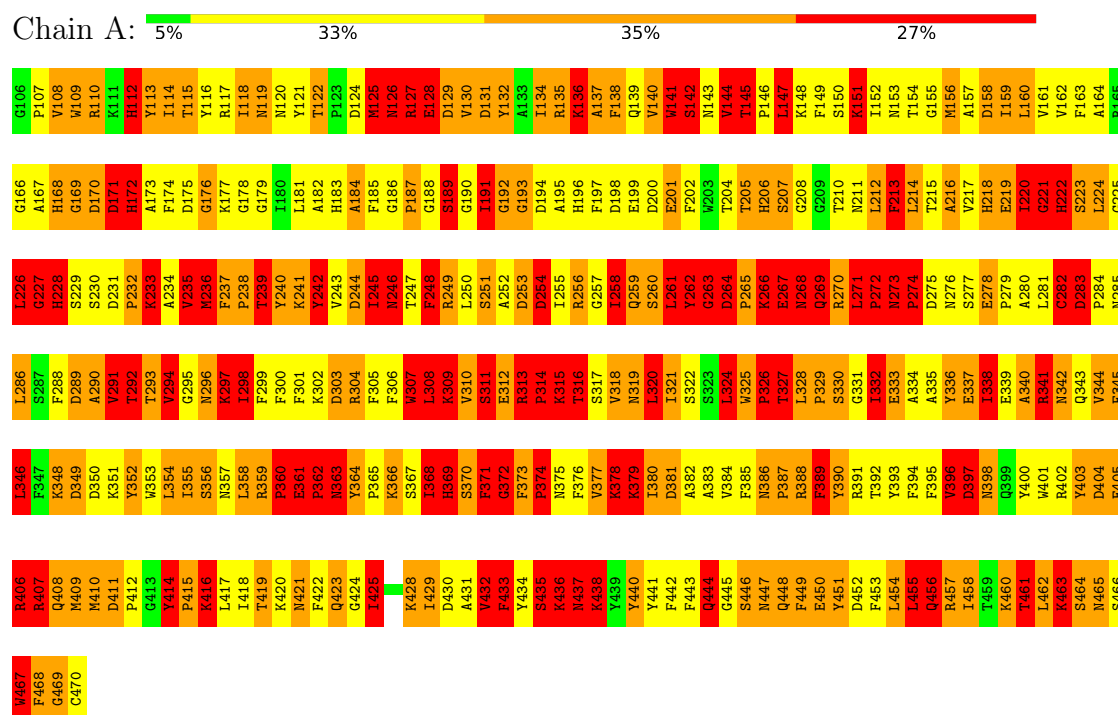
- Molecule 5 is water.

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, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 (9.07%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 18.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.055 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3063	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	2.76	216/3089 (7.0%)	3.04	344/4189 (8.2%)

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 (216) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	167	ALA	CA-CB	-12.86	1.36	1.52
1	A	239	THR	CA-CB	12.17	1.74	1.53
1	A	195	ALA	C-O	-11.37	1.11	1.24
1	A	310	VAL	CA-CB	-10.59	1.40	1.54
1	A	279	PRO	N-CD	10.59	1.62	1.47
1	A	177	LYS	CA-C	-10.53	1.42	1.53
1	A	397	ASP	C-N	-9.75	1.20	1.34
1	A	112	HIS	CA-C	9.74	1.65	1.52
1	A	366	LYS	CA-C	-9.64	1.41	1.52
1	A	310	VAL	CA-C	9.51	1.64	1.52
1	A	125	MET	C-N	9.48	1.47	1.33
1	A	196	HIS	N-CA	-9.32	1.34	1.45
1	A	192	GLY	C-O	9.25	1.36	1.23
1	A	145	THR	C-N	8.90	1.41	1.33
1	A	403	TYR	CA-C	-8.84	1.42	1.52
1	A	216	ALA	CA-CB	-8.77	1.39	1.53
1	A	173	ALA	C-O	-8.68	1.11	1.23
1	A	416	LYS	C-O	-8.67	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	242	TYR	CA-C	8.49	1.64	1.52
1	A	425	ILE	CA-CB	8.48	1.64	1.54
1	A	326	PRO	N-CD	8.43	1.59	1.47
1	A	312	GLU	N-CA	-8.40	1.35	1.46
1	A	396	VAL	C-N	8.38	1.45	1.33
1	A	372	GLY	CA-C	-8.29	1.46	1.52
1	A	233	LYS	CA-C	8.23	1.63	1.52
1	A	223	SER	C-N	-8.20	1.22	1.33
1	A	436	LYS	CD-CE	8.17	1.76	1.52
1	A	219	GLU	N-CA	-8.11	1.34	1.46
1	A	389	PHE	C-O	-8.08	1.14	1.23
1	A	254	ASP	C-O	8.05	1.33	1.24
1	A	377	VAL	CA-CB	8.00	1.63	1.53
1	A	109	TRP	N-CA	7.97	1.56	1.46
1	A	405	GLU	C-N	-7.97	1.21	1.33
1	A	310	VAL	C-O	7.85	1.33	1.24
1	A	406	ARG	C-O	-7.80	1.13	1.24
1	A	363	ASN	N-CA	7.80	1.56	1.46
1	A	395	PHE	CA-C	-7.69	1.43	1.52
1	A	332	ILE	C-O	-7.68	1.15	1.24
1	A	451	TYR	C-O	-7.68	1.15	1.23
1	A	324	LEU	CA-CB	-7.61	1.40	1.53
1	A	273	ASN	CA-C	7.59	1.62	1.52
1	A	311	SER	C-O	-7.48	1.14	1.24
1	A	260	SER	C-N	-7.46	1.22	1.33
1	A	272	PRO	CA-C	7.32	1.67	1.52
1	A	147	LEU	C-O	7.32	1.32	1.23
1	A	138	PHE	C-O	-7.31	1.15	1.24
1	A	278	GLU	C-O	7.30	1.33	1.24
1	A	233	LYS	CE-NZ	7.29	1.71	1.49
1	A	342	ASN	CA-CB	-7.26	1.41	1.53
1	A	292	THR	CA-C	-7.25	1.44	1.52
1	A	434	TYR	CA-CB	-7.24	1.43	1.53
1	A	425	ILE	CA-C	7.24	1.61	1.53
1	A	380	ILE	CA-C	-7.19	1.44	1.52
1	A	247	THR	C-O	7.12	1.33	1.24
1	A	341	ARG	CZ-NH2	7.08	1.42	1.33
1	A	263	GLY	C-N	-7.05	1.23	1.33
1	A	362	PRO	CA-C	7.05	1.62	1.52
1	A	291	VAL	CA-CB	-7.05	1.48	1.55
1	A	208	GLY	C-O	7.04	1.34	1.23
1	A	408	GLN	C-N	-7.04	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	164	ALA	CA-CB	-7.02	1.43	1.53
1	A	378	LYS	CA-C	7.00	1.63	1.52
1	A	212	LEU	C-N	6.99	1.43	1.33
1	A	199	GLU	CA-CB	-6.98	1.41	1.53
1	A	196	HIS	CA-C	-6.98	1.44	1.52
1	A	458	ILE	N-CA	-6.97	1.37	1.46
1	A	352	TYR	C-O	6.97	1.32	1.23
1	A	229	SER	C-O	6.92	1.31	1.24
1	A	314	PRO	C-N	-6.90	1.24	1.33
1	A	348	LYS	C-O	6.90	1.32	1.23
1	A	261	LEU	C-N	-6.85	1.25	1.33
1	A	311	SER	N-CA	6.78	1.54	1.46
1	A	239	THR	C-O	-6.75	1.15	1.24
1	A	307	TRP	CA-C	-6.74	1.44	1.52
1	A	408	GLN	C-O	-6.73	1.15	1.24
1	A	137	ALA	CA-CB	-6.70	1.43	1.53
1	A	227	GLY	C-O	6.70	1.32	1.23
1	A	108	VAL	CB-CG1	6.58	1.74	1.52
1	A	342	ASN	N-CA	-6.58	1.36	1.46
1	A	392	THR	C-O	-6.57	1.15	1.24
1	A	438	LYS	CA-C	6.57	1.61	1.52
1	A	175	ASP	C-O	-6.55	1.15	1.24
1	A	398	ASN	C-O	-6.52	1.15	1.24
1	A	462	LEU	C-O	6.51	1.31	1.23
1	A	324	LEU	C-N	-6.49	1.26	1.33
1	A	197	PHE	N-CA	6.49	1.53	1.46
1	A	324	LEU	N-CA	-6.46	1.37	1.46
1	A	338	ILE	C-O	-6.45	1.16	1.24
1	A	344	VAL	CA-CB	-6.44	1.46	1.54
1	A	118	ILE	CA-CB	-6.43	1.46	1.53
1	A	410	MET	CA-C	6.43	1.60	1.52
1	A	136	LYS	C-O	-6.39	1.16	1.24
1	A	325	TRP	C-O	-6.37	1.17	1.25
1	A	274	PRO	CB-CG	6.33	1.81	1.49
1	A	184	ALA	C-O	-6.31	1.15	1.23
1	A	446	SER	CA-C	-6.31	1.44	1.52
1	A	369	HIS	C-N	-6.30	1.24	1.33
1	A	136	LYS	CA-C	-6.29	1.44	1.52
1	A	304	ARG	C-O	-6.27	1.15	1.24
1	A	436	LYS	CA-CB	6.26	1.64	1.53
1	A	356	SER	C-O	-6.23	1.16	1.23
1	A	144	VAL	C-N	-6.22	1.24	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	297	LYS	CA-C	-6.21	1.45	1.52
1	A	409	MET	CA-C	6.20	1.59	1.52
1	A	416	LYS	CA-C	-6.20	1.45	1.53
1	A	251	SER	C-O	6.20	1.31	1.23
1	A	467	TRP	N-CA	6.17	1.54	1.46
1	A	147	LEU	CG-CD1	6.14	1.72	1.52
1	A	251	SER	N-CA	6.14	1.54	1.46
1	A	275	ASP	CG-OD1	6.13	1.36	1.25
1	A	332	ILE	N-CA	6.12	1.54	1.46
1	A	444	GLN	CD-NE2	6.08	1.46	1.33
1	A	382	ALA	CA-CB	-6.08	1.43	1.53
1	A	228	HIS	C-N	-6.07	1.25	1.33
1	A	210	THR	C-O	-6.02	1.17	1.23
1	A	423	GLN	CA-C	6.02	1.60	1.52
1	A	107	PRO	C-O	6.01	1.31	1.24
1	A	288	PHE	CA-C	-6.01	1.45	1.52
1	A	341	ARG	CZ-NH1	5.99	1.41	1.32
1	A	187	PRO	N-CA	5.98	1.54	1.47
1	A	289	ASP	C-O	5.97	1.31	1.24
1	A	315	LYS	N-CA	-5.95	1.38	1.46
1	A	412	PRO	N-CA	-5.95	1.40	1.47
1	A	417	LEU	C-O	5.95	1.30	1.24
1	A	432	VAL	CA-C	-5.94	1.45	1.52
1	A	135	ARG	C-O	5.94	1.31	1.24
1	A	128	GLU	N-CA	-5.93	1.38	1.46
1	A	328	LEU	C-N	5.90	1.40	1.33
1	A	379	LYS	CD-CE	5.90	1.70	1.52
1	A	127	ARG	CD-NE	5.87	1.54	1.46
1	A	327	THR	N-CA	5.86	1.53	1.46
1	A	440	TYR	C-O	-5.85	1.16	1.23
1	A	279	PRO	CA-CB	-5.81	1.43	1.53
1	A	461	THR	N-CA	5.81	1.53	1.46
1	A	314	PRO	N-CD	-5.81	1.39	1.47
1	A	343	GLN	CB-CG	-5.79	1.35	1.52
1	A	129	ASP	C-O	5.78	1.31	1.24
1	A	362	PRO	N-CA	5.78	1.54	1.47
1	A	421	ASN	N-CA	-5.76	1.38	1.46
1	A	310	VAL	N-CA	5.76	1.53	1.46
1	A	394	PHE	C-O	-5.75	1.16	1.23
1	A	449	PHE	C-O	-5.75	1.17	1.24
1	A	348	LYS	CA-C	5.73	1.59	1.52
1	A	351	LYS	CG-CD	5.73	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	425	ILE	CG1-CD1	5.70	1.74	1.51
1	A	112	HIS	N-CA	-5.70	1.38	1.46
1	A	305	PHE	N-CA	-5.69	1.39	1.45
1	A	131	ASP	CG-OD1	5.68	1.36	1.25
1	A	210	THR	C-N	-5.66	1.25	1.33
1	A	461	THR	C-O	-5.64	1.17	1.24
1	A	259	GLN	N-CA	-5.63	1.39	1.46
1	A	312	GLU	CA-CB	-5.62	1.44	1.53
1	A	113	TYR	CA-C	5.61	1.60	1.52
1	A	293	THR	CA-CB	-5.60	1.44	1.53
1	A	206	HIS	C-O	-5.60	1.18	1.24
1	A	372	GLY	C-N	-5.59	1.22	1.33
1	A	361	GLU	CD-OE2	5.58	1.35	1.25
1	A	325	TRP	C-N	5.54	1.46	1.33
1	A	132	TYR	CA-C	-5.50	1.47	1.53
1	A	109	TRP	CA-CB	5.50	1.61	1.53
1	A	219	GLU	CD-OE2	5.49	1.35	1.25
1	A	345	PHE	C-O	-5.48	1.17	1.24
1	A	320	LEU	N-CA	5.46	1.52	1.45
1	A	167	ALA	N-CA	-5.45	1.39	1.46
1	A	181	LEU	CA-CB	-5.43	1.46	1.54
1	A	127	ARG	CB-CG	-5.42	1.36	1.52
1	A	114	ILE	CA-C	5.42	1.59	1.52
1	A	368	ILE	CA-C	-5.40	1.45	1.52
1	A	158	ASP	N-CA	5.39	1.53	1.46
1	A	290	ALA	CA-CB	5.39	1.63	1.53
1	A	305	PHE	C-O	-5.39	1.17	1.23
1	A	361	GLU	CG-CD	5.37	1.65	1.52
1	A	452	ASP	CA-CB	5.36	1.59	1.53
1	A	120	ASN	N-CA	-5.35	1.39	1.46
1	A	465	ASN	N-CA	5.34	1.53	1.46
1	A	326	PRO	C-O	5.33	1.30	1.24
1	A	248	PHE	N-CA	5.31	1.53	1.46
1	A	356	SER	CA-C	-5.31	1.45	1.52
1	A	309	LYS	C-O	-5.29	1.17	1.24
1	A	114	ILE	CA-CB	-5.29	1.46	1.55
1	A	463	LYS	N-CA	-5.29	1.39	1.46
1	A	336	TYR	CA-C	-5.26	1.46	1.52
1	A	351	LYS	CE-NZ	5.26	1.65	1.49
1	A	458	ILE	CA-C	5.25	1.58	1.52
1	A	147	LEU	N-CA	5.24	1.51	1.45
1	A	276	ASN	N-CA	5.24	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	368	ILE	C-O	5.24	1.30	1.24
1	A	297	LYS	CG-CD	5.24	1.68	1.52
1	A	383	ALA	C-O	5.24	1.30	1.23
1	A	236	MET	C-N	-5.22	1.22	1.33
1	A	308	LEU	CG-CD2	-5.22	1.35	1.52
1	A	373	PHE	C-O	-5.21	1.17	1.24
1	A	361	GLU	N-CA	5.19	1.53	1.46
1	A	301	PHE	C-O	-5.18	1.17	1.23
1	A	272	PRO	CB-CG	5.17	1.71	1.51
1	A	328	LEU	N-CA	5.17	1.55	1.45
1	A	346	LEU	CG-CD2	-5.17	1.35	1.52
1	A	236	MET	N-CA	-5.16	1.39	1.46
1	A	220	ILE	C-N	-5.14	1.25	1.33
1	A	193	GLY	CA-C	-5.13	1.44	1.51
1	A	206	HIS	CA-C	-5.13	1.47	1.53
1	A	285	ASN	CB-CG	5.13	1.64	1.52
1	A	387	PRO	CA-C	5.13	1.60	1.52
1	A	142	SER	C-O	5.12	1.31	1.23
1	A	315	LYS	C-N	-5.12	1.26	1.33
1	A	377	VAL	N-CA	5.09	1.52	1.46
1	A	329	PRO	CA-C	-5.09	1.47	1.52
1	A	266	LYS	C-O	5.08	1.30	1.24
1	A	351	LYS	C-O	5.08	1.30	1.23
1	A	450	GLU	CA-C	-5.08	1.46	1.52
1	A	131	ASP	CA-C	-5.07	1.46	1.52
1	A	146	PRO	C-O	-5.06	1.18	1.23
1	A	317	SER	C-O	-5.06	1.18	1.23
1	A	357	ASN	N-CA	-5.05	1.38	1.46
1	A	419	THR	C-N	-5.03	1.27	1.33
1	A	374	PRO	N-CD	5.02	1.54	1.47

All (344) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	414	TYR	CA-C-N	-33.74	77.67	119.84
1	A	414	TYR	C-N-CA	-33.74	77.67	119.84
1	A	263	GLY	CA-C-N	21.98	161.26	121.70
1	A	263	GLY	C-N-CA	21.98	161.26	121.70
1	A	315	LYS	CA-C-N	18.88	147.44	120.82
1	A	315	LYS	C-N-CA	18.88	147.44	120.82
1	A	406	ARG	CA-C-O	18.53	141.70	119.28
1	A	397	ASP	CA-C-N	17.15	146.38	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	397	ASP	C-N-CA	17.15	146.38	120.31
1	A	368	ILE	O-C-N	-17.09	101.20	122.57
1	A	227	GLY	O-C-N	-17.01	100.58	122.70
1	A	169	GLY	CA-C-N	16.89	145.19	121.71
1	A	169	GLY	C-N-CA	16.89	145.19	121.71
1	A	270	ARG	N-CA-C	16.78	134.92	110.59
1	A	171	ASP	CA-CB-CG	16.58	129.18	112.60
1	A	397	ASP	CA-C-O	-15.56	98.26	120.51
1	A	142	SER	O-C-N	15.47	141.67	122.34
1	A	325	TRP	CA-C-O	15.38	131.59	119.59
1	A	278	GLU	O-C-N	-13.78	105.47	121.32
1	A	245	ILE	N-CA-C	13.04	126.64	113.47
1	A	359	ARG	CA-C-N	12.65	135.66	119.84
1	A	359	ARG	C-N-CA	12.65	135.66	119.84
1	A	386	ASN	CB-CA-C	12.37	122.95	110.33
1	A	435	SER	CA-C-O	-12.36	106.58	120.54
1	A	327	THR	N-CA-C	-12.31	97.00	112.88
1	A	192	GLY	N-CA-C	-12.21	84.23	113.18
1	A	279	PRO	CA-N-CD	-12.05	94.62	111.50
1	A	170	ASP	CA-CB-CG	11.87	124.47	112.60
1	A	369	HIS	CA-C-N	11.66	143.81	121.54
1	A	369	HIS	C-N-CA	11.66	143.81	121.54
1	A	145	THR	CA-C-N	-11.66	108.94	120.83
1	A	145	THR	C-N-CA	-11.66	108.94	120.83
1	A	396	VAL	O-C-N	-11.65	107.60	122.97
1	A	414	TYR	N-CA-C	11.64	135.54	109.81
1	A	328	LEU	N-CA-C	11.58	126.96	110.40
1	A	363	ASN	N-CA-C	11.41	135.10	110.80
1	A	373	PHE	CA-C-N	-11.07	106.01	119.84
1	A	373	PHE	C-N-CA	-11.07	106.01	119.84
1	A	397	ASP	O-C-N	10.80	136.96	122.59
1	A	398	ASN	CA-CB-CG	10.68	123.28	112.60
1	A	435	SER	O-C-N	10.47	135.16	123.22
1	A	444	GLN	N-CA-C	-10.46	91.85	108.90
1	A	327	THR	CA-C-O	10.34	131.79	119.59
1	A	172	HIS	O-C-N	-10.31	107.60	122.87
1	A	406	ARG	O-C-N	-10.26	108.21	122.37
1	A	424	GLY	CA-C-N	-10.23	109.58	122.26
1	A	424	GLY	C-N-CA	-10.23	109.58	122.26
1	A	414	TYR	C-N-CD	10.12	166.51	125.00
1	A	191	ILE	N-CA-C	-9.96	88.62	109.34
1	A	386	ASN	CA-C-O	9.92	128.62	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	378	LYS	N-CA-C	9.88	125.07	112.92
1	A	411	ASP	N-CA-C	-9.78	94.45	109.41
1	A	131	ASP	N-CA-C	-9.74	100.66	111.28
1	A	371	PHE	O-C-N	-9.62	109.80	122.59
1	A	402	ARG	NE-CZ-NH1	-9.61	111.89	121.50
1	A	280	ALA	N-CA-C	9.49	124.23	109.52
1	A	425	ILE	CB-CA-C	9.45	123.05	112.19
1	A	208	GLY	N-CA-C	-9.34	102.06	112.33
1	A	206	HIS	O-C-N	-9.20	113.28	123.13
1	A	146	PRO	CA-C-O	9.19	129.40	118.92
1	A	158	ASP	N-CA-C	9.09	124.80	112.90
1	A	396	VAL	CA-CB-CG2	9.06	125.80	110.40
1	A	222	HIS	CA-CB-CG	9.03	122.83	113.80
1	A	373	PHE	CA-CB-CG	9.02	122.81	113.80
1	A	389	PHE	CA-C-N	9.01	138.75	121.54
1	A	389	PHE	C-N-CA	9.01	138.75	121.54
1	A	124	ASP	CA-C-N	9.01	138.74	121.54
1	A	124	ASP	C-N-CA	9.01	138.74	121.54
1	A	373	PHE	O-C-N	8.98	131.65	121.32
1	A	326	PRO	N-CA-C	8.98	130.97	112.47
1	A	302	LYS	O-C-N	-8.94	115.28	123.50
1	A	279	PRO	N-CA-CB	8.77	112.25	102.60
1	A	246	ASN	N-CA-C	-8.76	101.94	114.12
1	A	206	HIS	CA-C-O	8.72	128.28	119.91
1	A	402	ARG	NE-CZ-NH2	8.68	127.01	119.20
1	A	294	VAL	N-CA-C	-8.65	92.71	107.24
1	A	258	ILE	N-CA-C	-8.65	91.36	109.34
1	A	425	ILE	N-CA-C	8.53	119.50	111.91
1	A	125	MET	CA-C-O	8.49	132.65	120.51
1	A	465	ASN	N-CA-C	8.38	122.33	110.68
1	A	261	LEU	CA-C-O	8.33	129.63	119.31
1	A	173	ALA	O-C-N	-8.31	112.51	122.65
1	A	380	ILE	N-CA-C	-8.26	96.55	108.53
1	A	468	PHE	N-CA-C	-8.17	101.14	112.25
1	A	408	GLN	CA-C-O	8.14	132.15	120.51
1	A	415	PRO	N-CA-C	-8.13	95.72	112.47
1	A	432	VAL	CB-CA-C	-8.08	99.26	110.90
1	A	285	ASN	N-CA-C	-8.05	100.45	111.56
1	A	278	GLU	C-N-CD	8.02	138.25	120.60
1	A	327	THR	CB-CA-C	7.92	124.10	110.72
1	A	292	THR	CB-CA-C	-7.89	95.71	111.17
1	A	327	THR	O-C-N	-7.85	112.91	122.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	HIS	N-CA-C	7.82	123.11	113.50
1	A	126	ASN	N-CA-C	-7.81	94.17	110.80
1	A	142	SER	CA-C-O	-7.80	110.22	119.35
1	A	215	THR	N-CA-C	-7.80	101.61	112.45
1	A	310	VAL	CA-C-N	7.76	136.35	121.54
1	A	310	VAL	C-N-CA	7.76	136.35	121.54
1	A	269	GLN	CA-C-N	7.74	137.60	122.03
1	A	269	GLN	C-N-CA	7.74	137.60	122.03
1	A	278	GLU	CA-C-O	-7.73	109.57	120.16
1	A	153	ASN	CB-CA-C	-7.72	97.67	110.72
1	A	408	GLN	O-C-N	-7.71	112.34	122.59
1	A	409	MET	O-C-N	-7.61	114.23	123.36
1	A	170	ASP	CA-C-N	7.61	136.07	121.54
1	A	170	ASP	C-N-CA	7.61	136.07	121.54
1	A	267	GLU	CA-C-N	7.60	136.05	121.54
1	A	267	GLU	C-N-CA	7.60	136.05	121.54
1	A	113	TYR	CB-CA-C	-7.58	97.48	109.84
1	A	400	TYR	N-CA-C	7.55	119.90	109.18
1	A	326	PRO	O-C-N	-7.54	112.46	122.64
1	A	124	ASP	N-CA-C	-7.52	103.98	113.01
1	A	360	PRO	N-CA-C	7.52	127.96	112.47
1	A	409	MET	N-CA-CB	-7.50	99.42	110.37
1	A	155	GLY	N-CA-C	-7.45	101.10	111.76
1	A	325	TRP	N-CA-C	7.37	123.03	107.91
1	A	206	HIS	CA-CB-CG	7.36	121.16	113.80
1	A	349	ASP	CB-CA-C	-7.35	106.19	115.89
1	A	326	PRO	CA-N-CD	-7.34	101.73	112.00
1	A	275	ASP	N-CA-C	-7.29	99.46	109.95
1	A	263	GLY	CA-C-O	-7.28	107.90	120.57
1	A	316	THR	CA-C-N	7.26	133.40	122.95
1	A	316	THR	C-N-CA	7.26	133.40	122.95
1	A	141	TRP	O-C-N	-7.23	112.48	122.46
1	A	357	ASN	CA-C-N	7.23	133.04	122.63
1	A	357	ASN	C-N-CA	7.23	133.04	122.63
1	A	364	TYR	N-CA-C	7.20	118.41	110.13
1	A	242	TYR	CB-CA-C	7.18	124.70	110.42
1	A	134	ILE	CB-CG1-CD1	-7.18	98.73	113.80
1	A	277	SER	CA-CB-OG	7.16	125.42	111.10
1	A	242	TYR	CA-C-O	7.14	130.72	120.51
1	A	213	PHE	CB-CA-C	-7.13	97.51	110.56
1	A	368	ILE	CA-C-O	-7.12	111.87	120.78
1	A	144	VAL	CA-CB-CG2	7.06	122.39	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	ASP	O-C-N	7.05	134.28	123.00
1	A	396	VAL	CB-CA-C	7.02	120.60	110.98
1	A	177	LYS	N-CA-C	-7.01	95.29	107.20
1	A	341	ARG	NE-CZ-NH1	-6.98	114.52	121.50
1	A	145	THR	CB-CA-C	6.96	119.87	109.63
1	A	406	ARG	CB-CA-C	-6.91	97.56	110.01
1	A	328	LEU	CB-CA-C	-6.87	98.05	108.63
1	A	302	LYS	N-CA-C	6.87	119.30	107.28
1	A	171	ASP	CA-C-N	-6.87	112.07	123.33
1	A	171	ASP	C-N-CA	-6.87	112.07	123.33
1	A	396	VAL	CA-C-N	-6.85	108.45	121.54
1	A	396	VAL	C-N-CA	-6.85	108.45	121.54
1	A	224	LEU	N-CA-C	6.84	121.88	112.04
1	A	396	VAL	N-CA-C	6.80	117.93	107.99
1	A	304	ARG	O-C-N	-6.75	114.23	122.34
1	A	368	ILE	CB-CG1-CD1	6.73	127.93	113.80
1	A	218	HIS	CB-CA-C	-6.71	100.35	110.88
1	A	444	GLN	CA-CB-CG	6.68	127.46	114.10
1	A	332	ILE	N-CA-C	6.68	123.23	109.34
1	A	309	LYS	CA-C-N	6.67	133.97	121.97
1	A	309	LYS	C-N-CA	6.67	133.97	121.97
1	A	202	PHE	N-CA-C	-6.64	97.59	108.41
1	A	222	HIS	ND1-CG-CD2	-6.63	99.47	106.10
1	A	381	ASP	N-CA-C	6.62	121.49	113.41
1	A	279	PRO	O-C-N	-6.60	108.57	121.10
1	A	142	SER	CB-CA-C	6.58	121.07	110.09
1	A	125	MET	CA-C-N	6.57	134.09	121.54
1	A	125	MET	C-N-CA	6.57	134.09	121.54
1	A	265	PRO	CA-C-N	6.56	134.07	121.54
1	A	265	PRO	C-N-CA	6.56	134.07	121.54
1	A	335	ALA	N-CA-C	6.52	119.07	108.76
1	A	397	ASP	CB-CA-C	-6.52	97.45	110.42
1	A	237	PHE	N-CA-C	-6.51	95.43	109.81
1	A	366	LYS	CA-C-N	-6.50	109.00	122.07
1	A	366	LYS	C-N-CA	-6.50	109.00	122.07
1	A	433	PHE	CA-C-O	-6.50	114.27	121.23
1	A	308	LEU	CA-C-N	6.49	133.93	121.54
1	A	308	LEU	C-N-CA	6.49	133.93	121.54
1	A	288	PHE	N-CA-C	6.48	119.74	109.50
1	A	259	GLN	O-C-N	-6.46	115.11	122.09
1	A	270	ARG	CA-C-O	6.44	129.42	121.89
1	A	269	GLN	O-C-N	6.38	130.90	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	ARG	NH1-CZ-NH2	6.36	127.57	119.30
1	A	192	GLY	O-C-N	6.35	130.96	122.70
1	A	291	VAL	N-CA-C	6.35	116.64	107.88
1	A	147	LEU	O-C-N	6.34	130.20	123.03
1	A	371	PHE	CA-CB-CG	6.33	120.13	113.80
1	A	265	PRO	N-CA-C	6.32	125.49	112.47
1	A	303	ASP	CA-CB-CG	6.29	118.89	112.60
1	A	312	GLU	CA-C-N	6.29	137.14	121.80
1	A	312	GLU	C-N-CA	6.29	137.14	121.80
1	A	272	PRO	N-CA-C	6.26	128.39	112.10
1	A	325	TRP	CB-CA-C	6.23	120.41	110.62
1	A	447	ASN	CA-C-O	6.23	128.08	120.60
1	A	259	GLN	CB-CA-C	6.22	120.74	110.90
1	A	147	LEU	N-CA-C	6.21	120.05	110.42
1	A	278	GLU	N-CA-C	6.21	123.53	109.81
1	A	113	TYR	CA-CB-CG	6.20	125.05	113.90
1	A	315	LYS	N-CA-CB	6.20	120.96	110.49
1	A	393	TYR	CA-C-O	-6.19	114.10	120.54
1	A	421	ASN	N-CA-CB	-6.18	101.66	110.81
1	A	244	ASP	CA-C-N	-6.18	115.28	122.14
1	A	244	ASP	C-N-CA	-6.18	115.28	122.14
1	A	460	LYS	N-CA-C	-6.17	98.19	108.75
1	A	261	LEU	CA-C-N	-6.14	112.33	122.39
1	A	261	LEU	C-N-CA	-6.14	112.33	122.39
1	A	230	SER	N-CA-C	-6.12	104.67	111.71
1	A	264	ASP	CA-CB-CG	6.12	118.72	112.60
1	A	407	ARG	CD-NE-CZ	6.07	132.90	124.40
1	A	370	SER	CA-C-O	6.07	129.19	120.51
1	A	451	TYR	N-CA-C	6.06	119.56	107.62
1	A	135	ARG	NE-CZ-NH1	-6.04	115.46	121.50
1	A	294	VAL	CB-CA-C	6.03	117.91	110.73
1	A	266	LYS	N-CA-C	6.01	123.59	110.80
1	A	282	CYS	N-CA-C	6.00	119.89	112.03
1	A	262	TYR	O-C-N	-5.99	113.20	122.61
1	A	241	LYS	N-CA-CB	5.98	117.83	110.53
1	A	325	TRP	CA-CB-CG	5.96	124.92	113.60
1	A	373	PHE	C-N-CD	5.92	149.26	125.00
1	A	220	ILE	O-C-N	-5.91	115.18	122.57
1	A	269	GLN	N-CA-C	5.89	118.50	108.90
1	A	370	SER	O-C-N	-5.86	114.79	122.59
1	A	396	VAL	CA-CB-CG1	5.86	120.36	110.40
1	A	307	TRP	N-CA-C	-5.85	99.87	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	ILE	CB-CA-C	5.84	119.55	111.49
1	A	312	GLU	CB-CG-CD	5.83	122.52	112.60
1	A	374	PRO	CA-C-N	5.83	131.83	120.99
1	A	374	PRO	C-N-CA	5.83	131.83	120.99
1	A	359	ARG	CD-NE-CZ	5.82	132.55	124.40
1	A	141	TRP	N-CA-CB	5.82	119.88	110.40
1	A	224	LEU	N-CA-CB	5.79	119.17	110.19
1	A	437	ASN	N-CA-C	5.79	123.14	110.80
1	A	313	ARG	CA-C-N	-5.79	112.60	119.84
1	A	313	ARG	C-N-CA	-5.79	112.60	119.84
1	A	277	SER	CA-C-N	5.79	135.92	121.80
1	A	277	SER	C-N-CA	5.79	135.92	121.80
1	A	277	SER	N-CA-C	5.79	118.82	109.79
1	A	225	GLY	CA-C-N	5.77	128.90	120.71
1	A	225	GLY	C-N-CA	5.77	128.90	120.71
1	A	327	THR	OG1-CB-CG2	-5.74	97.81	109.30
1	A	279	PRO	CB-CA-C	5.74	126.34	112.00
1	A	308	LEU	N-CA-C	5.72	117.73	108.34
1	A	171	ASP	O-C-N	-5.71	115.00	122.59
1	A	260	SER	CA-C-N	5.69	131.10	121.14
1	A	260	SER	C-N-CA	5.69	131.10	121.14
1	A	432	VAL	CA-C-O	-5.68	115.05	121.75
1	A	110	ARG	CB-CA-C	5.67	119.52	111.74
1	A	298	ILE	CB-CA-C	-5.67	103.98	110.73
1	A	340	ALA	N-CA-C	5.66	119.72	113.21
1	A	345	PHE	CA-C-N	5.65	130.28	122.77
1	A	345	PHE	C-N-CA	5.65	130.28	122.77
1	A	374	PRO	CA-N-CD	-5.64	104.10	112.00
1	A	303	ASP	CB-CA-C	5.63	121.63	110.42
1	A	341	ARG	CG-CD-NE	-5.63	99.62	112.00
1	A	261	LEU	O-C-N	-5.61	114.72	122.46
1	A	461	THR	CA-C-O	-5.60	114.31	120.36
1	A	112	HIS	N-CA-CB	-5.59	101.04	110.49
1	A	120	ASN	CA-C-N	5.59	130.71	123.00
1	A	120	ASN	C-N-CA	5.59	130.71	123.00
1	A	359	ARG	NE-CZ-NH1	5.55	127.05	121.50
1	A	301	PHE	N-CA-C	5.55	119.28	109.96
1	A	258	ILE	O-C-N	5.55	129.50	122.57
1	A	332	ILE	O-C-N	-5.55	115.64	122.57
1	A	171	ASP	CB-CA-C	5.53	121.43	110.42
1	A	239	THR	N-CA-C	-5.53	99.02	110.80
1	A	176	GLY	CA-C-N	-5.52	113.60	121.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	GLY	C-N-CA	-5.52	113.60	121.33
1	A	309	LYS	N-CA-CB	5.52	119.82	110.49
1	A	158	ASP	CB-CG-OD1	5.51	131.07	118.40
1	A	455	LEU	CB-CG-CD2	5.51	127.22	110.70
1	A	271	LEU	CB-CA-C	5.51	121.02	110.17
1	A	141	TRP	CA-C-N	-5.50	113.47	122.54
1	A	141	TRP	C-N-CA	-5.50	113.47	122.54
1	A	326	PRO	N-CA-CB	5.49	109.02	103.25
1	A	447	ASN	N-CA-C	5.49	118.39	109.06
1	A	371	PHE	N-CA-C	-5.48	99.13	110.80
1	A	316	THR	N-CA-CB	5.47	118.06	109.69
1	A	377	VAL	CB-CA-C	-5.47	103.59	111.19
1	A	273	ASN	N-CA-CB	-5.47	100.64	110.37
1	A	317	SER	O-C-N	-5.46	114.69	122.99
1	A	421	ASN	CA-C-O	5.45	125.87	119.06
1	A	220	ILE	CA-C-O	5.44	127.58	120.78
1	A	283	ASP	N-CA-C	-5.43	100.07	109.58
1	A	190	GLY	CA-C-N	5.43	131.74	121.97
1	A	190	GLY	C-N-CA	5.43	131.74	121.97
1	A	294	VAL	N-CA-CB	5.43	119.05	112.10
1	A	375	ASN	CA-CB-CG	5.41	118.01	112.60
1	A	449	PHE	N-CA-C	5.37	117.16	108.41
1	A	402	ARG	CD-NE-CZ	-5.36	116.89	124.40
1	A	258	ILE	CG1-CB-CG2	-5.36	94.63	110.70
1	A	235	VAL	O-C-N	5.35	129.26	122.57
1	A	236	MET	N-CA-C	5.35	122.20	110.80
1	A	315	LYS	CB-CG-CD	5.34	123.59	111.30
1	A	370	SER	CA-C-N	-5.34	111.34	121.54
1	A	370	SER	C-N-CA	-5.34	111.34	121.54
1	A	192	GLY	CA-C-N	5.33	131.00	122.25
1	A	192	GLY	C-N-CA	5.33	131.00	122.25
1	A	380	ILE	CA-C-O	-5.33	114.64	120.72
1	A	312	GLU	N-CA-CB	-5.33	101.48	110.49
1	A	440	TYR	N-CA-C	-5.33	100.34	109.24
1	A	353	TRP	N-CA-C	5.33	117.08	108.34
1	A	370	SER	CB-CA-C	5.32	121.01	110.42
1	A	172	HIS	CA-CB-CG	5.32	119.12	113.80
1	A	270	ARG	N-CA-CB	-5.31	102.35	110.42
1	A	371	PHE	CA-C-O	-5.30	112.93	120.51
1	A	267	GLU	CB-CA-C	-5.30	99.88	110.42
1	A	351	LYS	CB-CG-CD	5.29	123.46	111.30
1	A	304	ARG	N-CA-C	-5.28	106.43	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	382	ALA	O-C-N	-5.27	117.37	123.33
1	A	316	THR	CB-CA-C	5.27	118.13	109.90
1	A	449	PHE	CA-C-O	-5.25	114.68	120.30
1	A	268	ASN	N-CA-C	5.25	121.99	110.80
1	A	308	LEU	CA-C-O	-5.25	114.67	120.24
1	A	419	THR	CA-C-O	5.25	125.74	119.60
1	A	140	VAL	CB-CA-C	5.22	119.85	111.29
1	A	212	LEU	N-CA-C	-5.22	106.50	112.92
1	A	112	HIS	CA-C-O	-5.20	113.07	120.51
1	A	140	VAL	CA-CB-CG2	5.20	119.24	110.40
1	A	145	THR	C-N-CD	5.20	146.30	125.00
1	A	146	PRO	CA-N-CD	-5.18	104.75	112.00
1	A	461	THR	N-CA-C	-5.18	100.46	108.90
1	A	326	PRO	CA-CB-CG	-5.18	94.67	104.50
1	A	110	ARG	NE-CZ-NH2	5.17	123.85	119.20
1	A	158	ASP	CB-CG-OD2	-5.16	106.52	118.40
1	A	236	MET	CB-CA-C	5.13	120.64	110.42
1	A	226	LEU	CA-C-N	5.12	131.45	121.41
1	A	226	LEU	C-N-CA	5.12	131.45	121.41
1	A	317	SER	CA-C-O	5.12	127.63	120.52
1	A	462	LEU	CA-C-O	5.12	127.18	121.40
1	A	215	THR	OG1-CB-CG2	-5.11	99.08	109.30
1	A	151	LYS	CA-C-N	-5.09	114.26	121.85
1	A	151	LYS	C-N-CA	-5.09	114.26	121.85
1	A	389	PHE	N-CA-C	5.09	122.38	114.64
1	A	152	ILE	CA-C-O	-5.09	115.54	121.80
1	A	242	TYR	N-CA-CB	-5.08	101.91	110.49
1	A	204	THR	O-C-N	5.07	129.15	123.27
1	A	160	LEU	CD1-CG-CD2	-5.07	99.65	110.80
1	A	333	GLU	N-CA-C	5.04	119.56	113.41
1	A	425	ILE	CA-C-O	5.04	125.17	120.14
1	A	118	ILE	CG1-CB-CG2	-5.03	95.60	110.70
1	A	394	PHE	N-CA-C	5.03	118.41	109.96
1	A	301	PHE	CA-C-N	5.02	128.74	121.26
1	A	301	PHE	C-N-CA	5.02	128.74	121.26
1	A	112	HIS	CA-C-N	5.02	128.68	121.50
1	A	112	HIS	C-N-CA	5.02	128.68	121.50
1	A	266	LYS	O-C-N	-5.02	115.92	122.59
1	A	311	SER	N-CA-CB	5.02	118.97	110.49
1	A	266	LYS	CA-C-N	5.01	131.11	121.54
1	A	266	LYS	C-N-CA	5.01	131.11	121.54
1	A	146	PRO	O-C-N	-5.01	113.11	122.33

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
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	2848	464	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	2853	464	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 79.

All (464) 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:CE	1:A:436:LYS:CD	1.77	1.54
1:A:233:LYS:CE	1:A:233:LYS:NZ	1.71	1.51
1:A:274:PRO:CB	1:A:274:PRO:CG	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:HB3	1:A:256:ARG:HH21	1.04	1.15
1:A:241:LYS:O	1:A:243:VAL:HG13	1.47	1.13
1:A:378:LYS:HB2	1:A:378:LYS:NZ	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:310:VAL:HG13	1:A:311:SER:N	1.52	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:HB3	1:A:249:ARG:HH11	1.20	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:141:TRP:O	1:A:145:THR:HG22	1.61	1.00
1:A:310:VAL:HG13	1:A:311:SER:H	0.84	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:435:SER:HG	1:A:441:TYR:HE2	1.04	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:HB3	1:A:256:ARG:NH2	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: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:234:ALA:C	1:A:236:MET:H	1.73	0.91
1:A:156:MET:HB2	5:A:30:HOH:O	1.68	0.90
1:A:406:ARG:HG2	1:A:406:ARG:HH11	1.35	0.90
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:HB2	1:A:378:LYS:HZ2	1.28	0.89
1:A:220:ILE:O	1:A:221:GLY:C	2.09	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:246:ASN:N	1:A:246:ASN:HD22	1.72	0.87
1:A:271:LEU:N	1:A:272:PRO:O	2.07	0.87
1:A:338:ILE:HG23	1:A:385:PHE:CE2	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:378:LYS:NZ	1:A:378:LYS:CB	2.39	0.84
1:A:228:HIS:CG	1:A:238:PRO:HG3	2.13	0.83
1:A:378:LYS:O	1:A:379:LYS:CG	2.26	0.83
1:A:138:PHE:HB3	1:A:149:PHE:CD2	2.14	0.83
1:A:340:ALA:C	1:A:341:ARG:HG3	2.04	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:306:PHE:C	1:A:307:TRP:HD1	1.88	0.81
1:A:438:LYS:O	1:A:438:LYS:HG3	1.78	0.81
1:A:116:TYR:CG	1:A:138:PHE:CE1	2.69	0.80
1:A:310:VAL:CG1	1:A:311:SER:N	2.22	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:281:LEU:HD21	1:A:316:THR:HB	1.64	0.79
1:A:297:LYS:CG	1:A:308:LEU:HD11	2.02	0.79
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:234:ALA:HB1	1:A:254:ASP:OD2	1.82	0.78
1:A:465:ASN:O	1:A:465:ASN:OD1	2.04	0.76
1:A:249:ARG:HB3	1:A:249:ARG:NH1	1.97	0.76
1:A:231:ASP:HB2	1:A:253:ASP:OD2	1.85	0.76
1:A:234:ALA:C	1:A:236:MET:N	2.44	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:432:VAL:HG13	1:A:442:PHE:CE1	2.20	0.75
1:A:437:ASN:OD1	1:A:437:ASN:N	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:THR:HG22	1:A:298:ILE:HG23	1.70	0.74
1:A:463:LYS:O	1:A:464:SER:C	2.31	0.73
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:436:LYS:C	1:A:437:ASN:OD1	2.32	0.73
1:A:156:MET:HG3	1:A:156:MET:O	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:303:ASP:O	1:A:321:ILE:HD11	1.89	0.72
1:A:378:LYS:O	1:A:379:LYS:HG2	1.90	0.72
1:A:159:ILE:HG23	1:A:193:GLY:O	1.90	0.71
1:A:218:HIS:CE1	1:A:236:MET:HB3	2.25	0.71
1:A:248:PHE:C	1:A:249:ARG:HG3	2.15	0.71
1:A:127:ARG:HG2	1:A:127:ARG:HH11	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:228:HIS:CG	1:A:238:PRO:CG	2.74	0.70
1:A:292:THR:HG22	1:A:293:THR:H	1.56	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
1:A:266:LYS:O	1:A:267:GLU:HB2	1.92	0.69
1:A:307:TRP:N	1:A:307:TRP:CD1	2.59	0.69
1:A:388:ARG:HH21	1:A:454:LEU:HD21	1.56	0.69
1:A:249:ARG:HH22	1:A:271:LEU:HD22	1.58	0.69
1:A:246:ASN:ND2	1:A:246:ASN:H	1.91	0.68
1:A:368:ILE:O	1:A:369:HIS:CG	2.45	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:HZ3	1:A:378:LYS:CB	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:LYS:CE	1:A:309:LYS:HB2	2.25	0.65
1:A:468:PHE:CD1	1:A:468:PHE:N	2.61	0.65
1:A:241:LYS:HG2	1:A:243:VAL:CG1	2.27	0.64
1:A:340:ALA:C	1:A:341:ARG:CG	2.68	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:248:PHE:C	1:A:248:PHE:CD2	2.73	0.64
1:A:435:SER:C	1:A:437:ASN:H	2.06	0.64
1:A:119:ASN:HB2	1:A:161:VAL:O	1.97	0.63
1:A:297:LYS:HE2	1:A:309:LYS:CB	2.23	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:243:VAL:HG23	1:A:244:ASP:O	1.99	0.63
1:A:307:TRP:HD1	1:A:307:TRP:N	1.96	0.63
1:A:445:GLY:C	1:A:447:ASN:H	2.05	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: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
1:A:222:HIS:C	1:A:224:LEU:H	2.08	0.61
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:134:ILE:C	1:A:136:LYS:N	2.57	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:368:ILE:O	1:A:369:HIS:CD2	2.54	0.61
1:A:438:LYS:O	1:A:438:LYS:CG	2.48	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:143:ASN:C	1:A:144:VAL:HG13	2.27	0.59
1:A:372:GLY:O	1:A:410:MET:HE2	2.01	0.59
1:A:364:TYR:HE2	1:A:366:LYS:CE	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:HIS:HD2	1:A:373:PHE:HB2	1.67	0.59
1:A:433:PHE:CD1	1:A:433:PHE:C	2.80	0.59
1:A:465:ASN:O	1:A:465:ASN:CG	2.42	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:446:SER:C	1:A:464:SER:HB2	2.28	0.58
1:A:281:LEU:CD2	1:A:316:THR:HB	2.34	0.58
1:A:309:LYS:HD3	1:A:309:LYS:N	2.18	0.58
1:A:340:ALA:O	1:A:341:ARG:CG	2.51	0.58
1:A:248:PHE:C	1:A:249:ARG:CG	2.77	0.58
1:A:174:PHE:HE2	1:A:183:HIS:HD1	1.48	0.58
1:A:109:TRP:CD1	1:A:224:LEU:HD23	2.38	0.58
1:A:308:LEU:O	1:A:309:LYS:HD2	2.04	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:211:ASN:OD1	1:A:214:LEU:HB2	2.04	0.57
1:A:298:ILE:HD11	1:A:310:VAL:HB	1.85	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:188:GLY:C	1:A:189:SER:O	2.47	0.57
1:A:449:PHE:HD2	1:A:461:THR:HG22	1.63	0.57
1:A:271:LEU:HA	1:A:272:PRO:C	2.30	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
1:A:408:GLN:O	1:A:409:MET:HG2	2.05	0.57
1:A:174:PHE:CE2	1:A:183:HIS:ND1	2.71	0.57
1:A:291:VAL:HG13	1:A:431:ALA:HB1	1.86	0.57
1:A:118:ILE:HD12	1:A:151:LYS:HD2	1.87	0.56
1:A:137:ALA:HA	1:A:217:VAL:CG1	2.35	0.56
1:A:248:PHE:CG	1:A:249:ARG:N	2.72	0.56
1:A:292:THR:HG23	1:A:336:TYR:HA	1.88	0.56
1:A:396:VAL:O	1:A:397:ASP:C	2.48	0.56
1:A:139:GLN:O	1:A:140:VAL:C	2.48	0.56
1:A:134:ILE:HG22	1:A:135:ARG:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ARG:HH12	1:A:271:LEU:HD13	1.71	0.56
1:A:290:ALA:HB2	1:A:333:GLU:C	2.31	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:311:SER:C	1:A:313:ARG:H	2.14	0.56
1:A:358:LEU:O	1:A:359:ARG:HG2	2.06	0.56
1:A:451:TYR:HD1	1:A:458:ILE:HD12	1.71	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:467:TRP:C	1:A:468:PHE:HD1	2.14	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:403:TYR:HD1	1:A:410:MET:SD	2.30	0.55
1:A:142:SER:HA	1:A:145:THR:CG2	2.32	0.55
1:A:293:THR:O	1:A:337:GLU:HG2	2.06	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:281:LEU:C	1:A:282:CYS:SG	2.90	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: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:308:LEU:O	1:A:309:LYS:CD	2.56	0.54
1:A:281:LEU:O	1:A:470:CYS:SG	2.66	0.54
1:A:337:GLU:C	1:A:338:ILE:HG13	2.33	0.54
1:A:259:GLN:O	1:A:262:TYR:O	2.24	0.53
1:A:310:VAL:HG12	1:A:311:SER:H	1.63	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
1:A:401:TRP:CZ2	1:A:415:PRO:HG3	2.43	0.53
1:A:418:ILE:HG21	1:A:425:ILE:HD11	1.90	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:432:VAL:HG13	1:A:442:PHE:CD1	2.44	0.53
1:A:460:LYS:HE3	1:A:462:LEU:CD2	2.14	0.53
1:A:116:TYR:CD2	1:A:138:PHE:CE1	2.96	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:TRP:CD1	1:A:318:VAL:HB	2.44	0.53
1:A:291:VAL:HG23	1:A:292:THR:N	2.24	0.52
1:A:117:ARG:HB2	1:A:157:ALA:HB2	1.92	0.52
1:A:213:PHE:CD2	1:A:214:LEU:HD13	2.43	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:125:MET:HG2	1:A:127:ARG:NH1	2.25	0.52
1:A:384:VAL:HG11	1:A:432:VAL:HG11	1.91	0.52
1:A:414:TYR:CE2	1:A:416:LYS:HE3	2.44	0.52
1:A:467:TRP:H	1:A:467:TRP:CD1	2.28	0.52
1:A:130:VAL:HG22	1:A:212:LEU:HD21	1.91	0.52
1:A:143:ASN:O	1:A:144:VAL:CG1	2.57	0.52
1:A:438:LYS:CA	1:A:453:PHE:CE2	2.86	0.52
1:A:162:VAL:HG12	1:A:163:PHE:N	2.24	0.52
1:A:211:ASN:OD1	1:A:213:PHE:HB3	2.10	0.52
1:A:456:GLN:O	1:A:457:ARG:HG3	2.10	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:435:SER:C	1:A:437:ASN:N	2.68	0.51
1:A:231:ASP:O	1:A:237:PHE:HB2	2.11	0.51
1:A:252:ALA:HA	1:A:255:ILE:CD1	2.30	0.51
1:A:430:ASP:HB2	1:A:443:PHE:O	2.10	0.51
1:A:162:VAL:CG1	1:A:163:PHE:N	2.73	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:213:PHE:O	1:A:217:VAL:HG22	2.10	0.51
1:A:378:LYS:C	1:A:379:LYS:CG	2.84	0.51
1:A:442:PHE:O	1:A:448:GLN:CA	2.58	0.51
1:A:228:HIS:CD2	1:A:238:PRO:CG	2.89	0.50
1:A:408:GLN:C	1:A:409:MET:HG2	2.36	0.50
1:A:134:ILE:C	1:A:136:LYS:H	2.19	0.50
1:A:127:ARG:O	1:A:128:GLU:C	2.53	0.50
1:A:221:GLY:O	1:A:224:LEU:CA	2.60	0.50
1:A:356:SER:O	1:A:359:ARG:N	2.45	0.50
1:A:418:ILE:CG2	1:A:425:ILE:HD11	2.41	0.50
1:A:451:TYR:CD1	1:A:458:ILE:HD12	2.46	0.50
1:A:130:VAL:HG23	1:A:212:LEU:HD21	1.94	0.50
1:A:369:HIS:CD2	1:A:373:PHE:HB2	2.47	0.50
1:A:306:PHE:C	1:A:307:TRP:CD1	2.78	0.50
1:A:154:THR:O	1:A:154:THR:CG2	2.60	0.50
1:A:311:SER:O	1:A:313:ARG:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:GLY:O	1:A:179:GLY:C	2.54	0.49
1:A:463:LYS:O	1:A:465:ASN:N	2.44	0.49
1:A:467:TRP:CD1	1:A:467:TRP:N	2.79	0.49
1:A:409:MET:O	1:A:410:MET:C	2.53	0.49
1:A:241:LYS:CG	1:A:243:VAL:CG1	2.91	0.49
1:A:318:VAL:HG23	1:A:319:ASN:N	2.26	0.49
1:A:346:LEU:HD23	1:A:355:ILE:CD1	2.43	0.49
1:A:446:SER:C	1:A:464:SER:CB	2.86	0.49
1:A:113:TYR:CD2	1:A:148:LYS:HG3	2.47	0.49
1:A:218:HIS:C	1:A:218:HIS:CD2	2.90	0.49
1:A:245:ILE:HG12	1:A:246:ASN:ND2	2.27	0.49
1:A:345:PHE:CE2	1:A:354:LEU:HD11	2.48	0.49
1:A:283:ASP:O	1:A:286:LEU:HB2	2.13	0.49
1:A:436:LYS:CE	1:A:436:LYS:CG	2.79	0.48
1:A:132:TYR:CZ	1:A:136:LYS:CD	2.96	0.48
1:A:134:ILE:O	1:A:135:ARG:C	2.55	0.48
1:A:352:TYR:HE2	1:A:354:LEU:CD1	2.26	0.48
1:A:453:PHE:C	1:A:453:PHE:CD1	2.91	0.48
1:A:460:LYS:NZ	1:A:462:LEU:HD21	2.28	0.48
1:A:116:TYR:CE1	1:A:151:LYS:HB2	2.48	0.48
1:A:245:ILE:HG12	1:A:246:ASN:HD22	1.78	0.48
1:A:127:ARG:O	1:A:129:ASP:N	2.47	0.48
1:A:329:PRO:CB	1:A:348:LYS:NZ	2.76	0.48
1:A:333:GLU:OE2	1:A:379:LYS:HD2	2.14	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:438:LYS:C	1:A:453:PHE:CE2	2.92	0.48
1:A:134:ILE:O	1:A:136:LYS:N	2.46	0.48
1:A:170:ASP:OD1	1:A:185:PHE:CE2	2.67	0.48
1:A:295:GLY:O	1:A:296:ASN:HB2	2.03	0.48
1:A:222:HIS:C	1:A:224:LEU:N	2.66	0.47
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:113:TYR:HD2	1:A:148:LYS:HG3	1.79	0.47
1:A:248:PHE:O	1:A:249:ARG:CG	2.62	0.47
1:A:271:LEU:CA	1:A:272:PRO:O	2.63	0.47
1:A:454:LEU:HA	1:A:454:LEU:HD13	1.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:326:PRO:CG	1:A:360:PRO:HG2	2.45	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:228:HIS:CE1	1:A:238:PRO:CG	2.90	0.46
1:A:221:GLY:O	1:A:224:LEU:N	2.45	0.46
1:A:182:ALA:HB1	1:A:219:GLU:HG3	1.97	0.46
1:A:231:ASP:OD2	1:A:253:ASP:HB2	2.15	0.46
1:A:455:LEU:C	1:A:455:LEU:HD12	2.39	0.46
1:A:232:PRO:HA	1:A:237:PHE:CD1	2.50	0.46
1:A:304:ARG:HA	1:A:321:ILE:HD11	1.97	0.46
1:A:440:TYR:CE1	1:A:453:PHE:CB	2.98	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:214:LEU:O	1:A:217:VAL:HG23	2.16	0.46
1:A:318:VAL:CG2	1:A:319:ASN:N	2.75	0.46
1:A:188:GLY:O	1:A:189:SER:C	2.59	0.46
1:A:466:SER:O	1:A:469:GLY:HA2	2.16	0.46
1:A:232:PRO:C	1:A:234:ALA:H	2.24	0.46
1:A:256:ARG:CG	1:A:257:GLY:N	2.79	0.45
1:A:436:LYS:C	1:A:437:ASN:CG	2.84	0.45
1:A:136:LYS:HE3	1:A:136:LYS:HB3	1.80	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:237:PHE:CD2	1:A:239:THR:HB	2.51	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:109:TRP:HD1	1:A:224:LEU:HD23	1.80	0.45
1:A:290:ALA:HB2	1:A:334:ALA:N	2.31	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
1:A:121:TYR:CD1	1:A:130:VAL:HG11	2.52	0.45
1:A:251:SER:O	1:A:252:ALA:C	2.60	0.45
1:A:271:LEU:CA	1:A:272:PRO:C	2.90	0.45
1:A:273:ASN:CB	1:A:274:PRO:CD	2.94	0.45
1:A:231:ASP:HB3	1:A:234:ALA:HB2	1.98	0.44
1:A:436:LYS:N	1:A:437:ASN:OD1	2.50	0.44
1:A:142:SER:CB	1:A:147:LEU:O	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:LEU:HD12	5:A:59:HOH:O	2.18	0.44
1:A:391:ARG:NE	1:A:411:ASP:OD2	2.51	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:160:LEU:HB2	1:A:194:ASP:OD2	2.17	0.44
1:A:352:TYR:O	1:A:365:PRO:HA	2.17	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:386:ASN:OD1	1:A:388:ARG:HB2	2.17	0.44
1:A:468:PHE:O	1:A:469:GLY:C	2.60	0.44
1:A:349:ASP:HB3	1:A:350:ASP:H	1.56	0.43
1:A:396:VAL:O	1:A:398:ASN:N	2.50	0.43
1:A:428:LYS:HG3	1:A:429:ILE:N	2.30	0.43
1:A:297:LYS:CG	1:A:309:LYS:HB3	2.47	0.43
1:A:130:VAL:HG12	1:A:131:ASP:N	2.32	0.43
1:A:345:PHE:CE2	1:A:354:LEU:HG	2.54	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:137:ALA:O	1:A:138:PHE:C	2.61	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:236:MET:SD	1:A:240:TYR:HA	2.59	0.43
1:A:241:LYS:CG	1:A:243:VAL:HG13	2.49	0.43
1:A:265:PRO:HB2	1:A:274:PRO:HB3	2.01	0.43
1:A:309:LYS:HZ3	1:A:309:LYS:HG2	1.43	0.43
1:A:340:ALA:O	1:A:341:ARG:HG3	2.16	0.43
1:A:294:VAL:HG11	1:A:344:VAL:HG21	2.01	0.42
1:A:406:ARG:HH11	1:A:406:ARG:CG	2.18	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:443:PHE:HA	1:A:447:ASN:O	2.20	0.42
1:A:122:THR:H	1:A:122:THR:HG22	1.37	0.42
1:A:259:GLN:HA	1:A:263:GLY:O	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CD2	1:A:248:PHE:O	2.73	0.42
1:A:159:ILE:HG22	1:A:160:LEU:N	2.35	0.42
1:A:198:ASP:O	1:A:201:GLU:HG2	2.19	0.41
1:A:228:HIS:ND1	1:A:238:PRO:CG	2.82	0.41
1:A:293:THR:HB	1:A:297:LYS:O	2.20	0.41
1:A:326:PRO:HG3	1:A:360:PRO:HG2	2.02	0.41
1:A:368:ILE:HD13	1:A:380:ILE:HD11	2.02	0.41
1:A:378:LYS:HZ2	1:A:378:LYS:CB	2.11	0.41
1:A:455:LEU:O	1:A:456:GLN:C	2.62	0.41
1:A:109:TRP:CE2	1:A:187:PRO:HB3	2.55	0.41
1:A:121:TYR:CE1	1:A:130:VAL:HG11	2.55	0.41
1:A:168:HIS:CE1	1:A:183:HIS:CE1	3.06	0.41
1:A:249:ARG:NH2	1:A:271:LEU:HD22	2.31	0.41
1:A:344:VAL:O	1:A:355:ILE:HB	2.20	0.41
1:A:432:VAL:CG1	1:A:442:PHE:CE1	3.00	0.41
1:A:245:ILE:O	1:A:245:ILE:HG13	2.08	0.41
1:A:273:ASN:ND2	1:A:273:ASN:H	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:116:TYR:HA	1:A:159:ILE:O	2.21	0.41
1:A:176:GLY:O	1:A:200:ASP:HB2	2.20	0.41
1:A:193:GLY:O	1:A:223:SER:HB3	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:401:TRP:CE3	1:A:410:MET:HE3	2.56	0.41
1:A:212:LEU:O	1:A:212:LEU:HG	2.21	0.40
1:A:444:GLN:O	1:A:447:ASN:CB	2.69	0.40
1:A:345:PHE:HE2	1:A:354:LEU:HD11	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

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

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
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

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Mol	Chain	Res	Type
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%)	216 (68%)	102 (32%)	0 1

All (102) 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

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Mol	Chain	Res	Type
1	A	130	VAL
1	A	136	LYS
1	A	145	THR
1	A	147	LEU
1	A	150	SER
1	A	151	LYS
1	A	156	MET
1	A	159	ILE
1	A	171	ASP
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	254	ASP
1	A	256	ARG
1	A	258	ILE
1	A	261	LEU
1	A	266	LYS
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	294	VAL
1	A	297	LYS
1	A	298	ILE
1	A	307	TRP

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Mol	Chain	Res	Type
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	324	LEU
1	A	327	THR
1	A	328	LEU
1	A	330	SER
1	A	332	ILE
1	A	337	GLU
1	A	338	ILE
1	A	339	GLU
1	A	346	LEU
1	A	354	LEU
1	A	355	ILE
1	A	358	LEU
1	A	361	GLU
1	A	363	ASN
1	A	368	ILE
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	396	VAL
1	A	406	ARG
1	A	407	ARG
1	A	416	LYS
1	A	419	THR
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

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Mol	Chain	Res	Type
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	ASN
1	A	153	ASN
1	A	228	HIS
1	A	246	ASN
1	A	259	GLN
1	A	269	GLN
1	A	343	GLN
1	A	369	HIS
1	A	421	ASN
1	A	456	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 ⓘ

There are no oligosaccharides 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	4.37	3 (75%)	2,4,4	2.45	1 (50%)

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	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	477	HAE	C2-N	6.40	1.42	1.33
4	A	477	HAE	C1-C2	4.46	1.59	1.50
4	A	477	HAE	O2-C2	3.52	1.31	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	477	HAE	C1-C2-N	3.08	121.22	116.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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, 95th 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 ²)	Q<0.9
1	A	365/365 (100%)	-1.58	0 100 100	2, 3, 18, 27	0

There are no RSRZ outliers to report.

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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th 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(Å ²)	Q<0.9
4	HAE	A	477	5/5	0.99	0.05	9,14,16,17	0
2	ZN	A	472	1/1	1.00	0.01	2,2,2,2	0
3	CA	A	473	1/1	1.00	0.03	2,2,2,2	0
3	CA	A	474	1/1	1.00	0.03	2,2,2,2	0
3	CA	A	475	1/1	1.00	0.01	2,2,2,2	0
3	CA	A	476	1/1	1.00	0.02	15,15,15,15	0
2	ZN	A	471	1/1	1.00	0.01	11,11,11,11	0

6.5 Other polymers [i](#)

There are no such residues in this entry.