



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 3, 2026 – 11:39 PM UTC

PDB ID : 1I6Q / pdb_00001i6q
Title : Formation of a protein intermediate and its trapping by the simultaneous crystallization process: Crystal structure of an iron-saturated intermediate in the FE3+ binding pathway of camel lactoferrin at 2.7 resolution
Authors : Khan, J.A.; Kumar, P.; Srinivasan, A.; Singh, T.P.
Deposited on : 2001-03-03
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

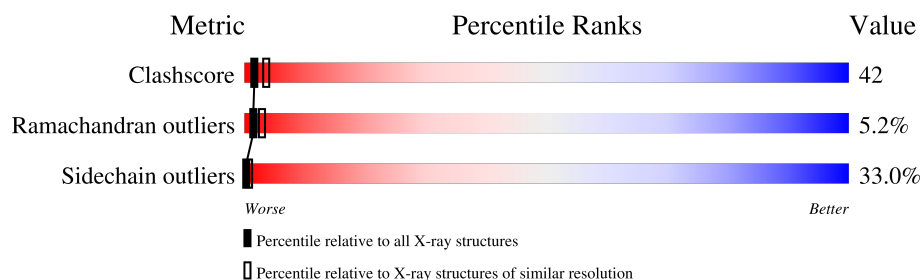
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	689	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5527 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 LACTOFERRIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	689	Total	C	N	O	S	15	0	0
			5284	3318	934	994	38			

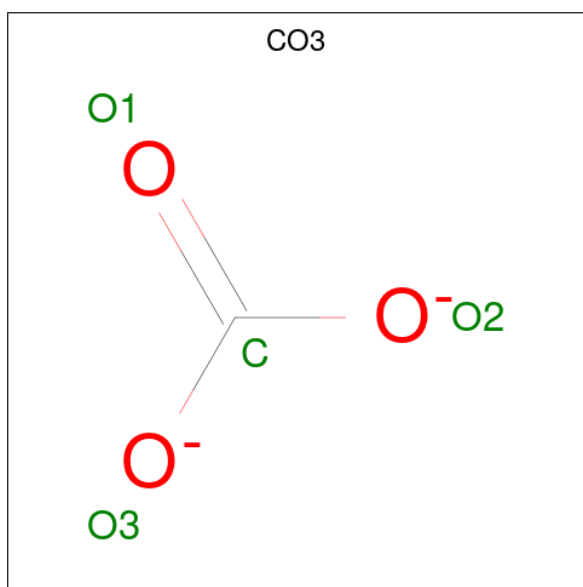
There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	LYS	SER	SEE REMARK 999	UNP Q9TUM0
A	87	GLN	ASN	SEE REMARK 999	UNP Q9TUM0
A	242	PHE	SER	SEE REMARK 999	UNP Q9TUM0
A	312	LYS	SER	SEE REMARK 999	UNP Q9TUM0
A	477	ASP	ASN	SEE REMARK 999	UNP Q9TUM0
A	513	LEU	ASN	SEE REMARK 999	UNP Q9TUM0
A	523	LEU	TYR	SEE REMARK 999	UNP Q9TUM0
A	556	GLY	ASN	SEE REMARK 999	UNP Q9TUM0
A	608	ARG	GLU	SEE REMARK 999	UNP Q9TUM0
A	623	GLU	GLN	SEE REMARK 999	UNP Q9TUM0
A	658	ASP	GLU	SEE REMARK 999	UNP Q9TUM0

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 3 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	1	3		
3	A	1	Total	C	O	0	0
			4	1	3		

- Molecule 4 is water.

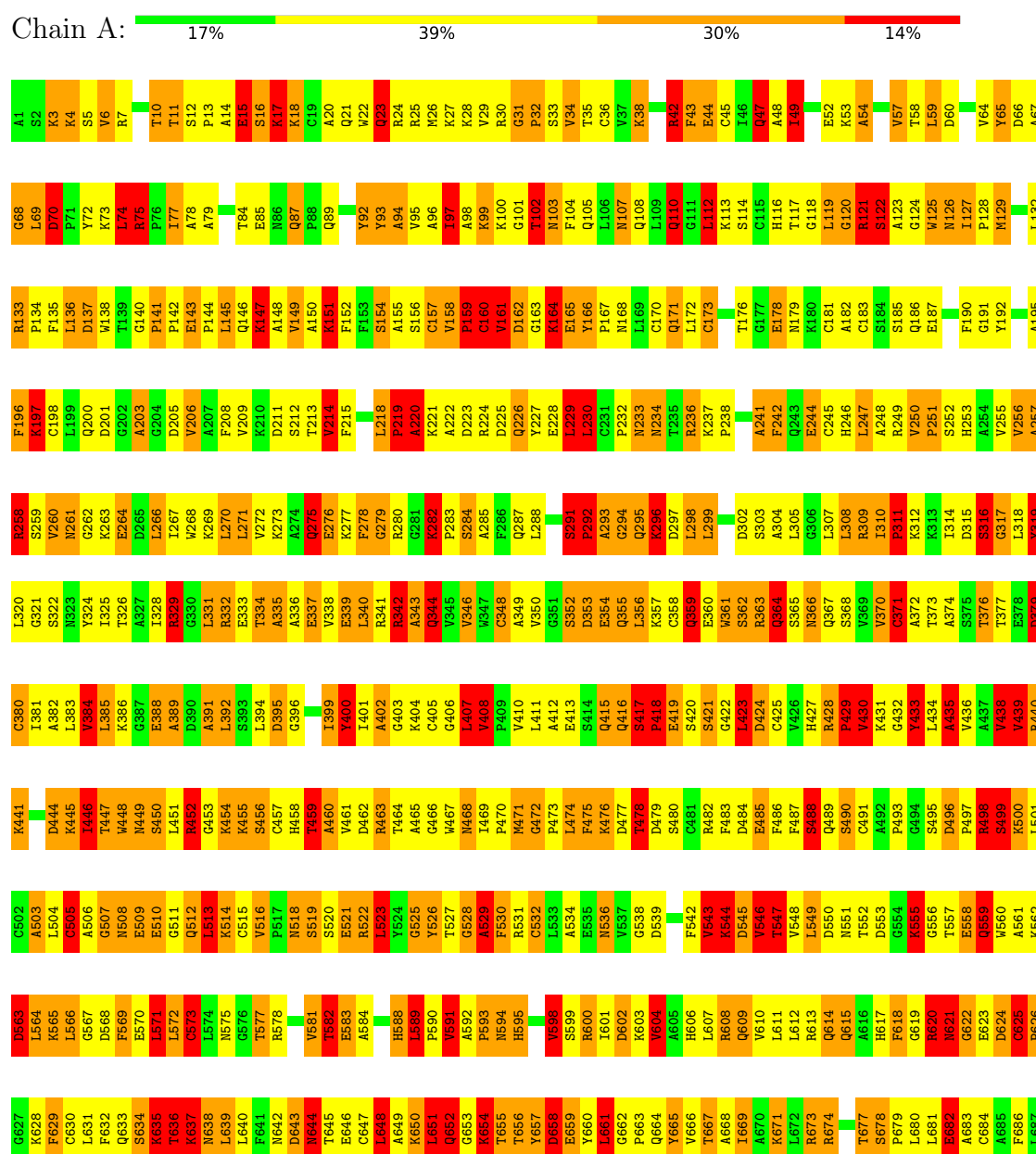
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	233	Total	O	0	0
			233	233		

3 Residue-property plots

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

Note EDS was not executed.

• Molecule 1: LACTOFERRIN





4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	175.91Å 80.62Å 56.29Å 90.00° 92.37° 90.00°	Depositor
Resolution (Å)	25.00 – 2.70	Depositor
% Data completeness (in resolution range)	94.1 (25.00-2.70)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.188 , 0.255	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5527	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CO3, FE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.72	40/5392 (0.7%)	2.99	602/7293 (8.3%)

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	16

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	430	VAL	C-N	-56.09	0.55	1.33
1	A	526	TYR	CA-C	-37.85	1.02	1.52
1	A	526	TYR	N-CA	36.52	1.93	1.46
1	A	569	PHE	C-N	-28.48	0.94	1.33
1	A	572	LEU	C-N	-28.47	0.93	1.33
1	A	570	GLU	CB-CG	-27.83	0.69	1.52
1	A	571	LEU	CB-CG	-21.01	1.11	1.53
1	A	92	TYR	CA-CB	16.21	1.80	1.53
1	A	427	HIS	CB-CG	13.54	1.69	1.50
1	A	572	LEU	CB-CG	11.85	1.77	1.53
1	A	293	ALA	C-N	-8.57	1.21	1.33
1	A	595	HIS	CB-CG	8.12	1.61	1.50
1	A	395	ASP	CA-CB	-8.05	1.40	1.53
1	A	294	GLY	CA-C	7.67	1.62	1.51
1	A	121	ARG	N-CA	6.96	1.55	1.46
1	A	427	HIS	CA-CB	6.94	1.63	1.54
1	A	294	GLY	C-N	6.93	1.43	1.33
1	A	293	ALA	CA-C	-6.84	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	432	GLY	C-N	-6.83	1.24	1.33
1	A	292	PRO	N-CA	6.79	1.56	1.47
1	A	432	GLY	CA-C	-6.75	1.42	1.51
1	A	120	GLY	N-CA	6.54	1.54	1.45
1	A	11	THR	N-CA	6.15	1.53	1.45
1	A	164	LYS	N-CA	-6.08	1.39	1.47
1	A	10	THR	CA-C	6.08	1.60	1.52
1	A	122	SER	C-N	6.00	1.42	1.33
1	A	427	HIS	CA-C	5.91	1.60	1.52
1	A	10	THR	C-N	5.76	1.42	1.33
1	A	135	PHE	N-CA	-5.62	1.38	1.46
1	A	420	SER	CA-C	5.56	1.59	1.52
1	A	342	ARG	CA-C	5.43	1.59	1.52
1	A	421	SER	N-CA	5.40	1.52	1.46
1	A	213	THR	C-N	5.38	1.40	1.34
1	A	331	LEU	N-CA	5.34	1.52	1.46
1	A	431	LYS	C-N	-5.29	1.25	1.33
1	A	294	GLY	N-CA	5.27	1.53	1.45
1	A	160	CYS	CA-C	5.08	1.59	1.52
1	A	428	ARG	C-N	5.06	1.45	1.33
1	A	162	ASP	N-CA	5.04	1.52	1.46
1	A	157	CYS	C-N	5.02	1.39	1.33

All (602) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	395	ASP	CA-CB-CG	29.38	141.98	112.60
1	A	682	GLU	CB-CG-CD	26.53	157.70	112.60
1	A	141	PRO	N-CA-C	24.70	140.83	110.70
1	A	569	PHE	O-C-N	-22.27	88.74	122.81
1	A	571	LEU	CB-CG-CD2	-21.07	47.50	110.70
1	A	253	HIS	CA-CB-CG	20.63	134.43	113.80
1	A	329	ARG	CD-NE-CZ	20.00	152.40	124.40
1	A	563	ASP	CA-CB-CG	19.87	132.47	112.60
1	A	508	ASN	CA-CB-CG	19.32	131.92	112.60
1	A	526	TYR	CA-C-N	17.35	142.99	120.44
1	A	526	TYR	C-N-CA	17.35	142.99	120.44
1	A	429	PRO	O-C-N	-16.76	100.02	122.64
1	A	444	ASP	CA-CB-CG	16.56	129.16	112.60
1	A	107	ASN	CA-CB-CG	15.89	128.49	112.60
1	A	617	HIS	CA-CB-CG	15.55	129.35	113.80
1	A	60	ASP	CA-CB-CG	15.41	128.01	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	572	LEU	CA-C-N	-15.22	92.47	121.54
1	A	572	LEU	C-N-CA	-15.22	92.47	121.54
1	A	624	ASP	CA-CB-CG	14.50	127.10	112.60
1	A	432	GLY	CA-C-N	-14.49	103.00	123.00
1	A	432	GLY	C-N-CA	-14.49	103.00	123.00
1	A	567	GLY	CA-C-N	13.71	147.56	122.06
1	A	567	GLY	C-N-CA	13.71	147.56	122.06
1	A	122	SER	CA-C-N	13.67	139.70	120.29
1	A	122	SER	C-N-CA	13.67	139.70	120.29
1	A	280	ARG	CD-NE-CZ	13.29	143.01	124.40
1	A	464	THR	N-CA-CB	-13.11	91.01	110.01
1	A	57	VAL	CA-C-O	-12.73	108.99	120.96
1	A	572	LEU	CB-CG-CD1	-12.65	72.73	110.70
1	A	96	ALA	CA-C-O	-12.46	107.32	120.40
1	A	625	CYS	N-CA-CB	12.39	132.43	110.37
1	A	250	VAL	CB-CA-C	12.18	124.86	110.85
1	A	317	GLY	N-CA-C	11.97	127.09	112.73
1	A	352	SER	N-CA-C	11.78	125.48	111.82
1	A	162	ASP	CA-CB-CG	11.74	124.34	112.60
1	A	43	PHE	CA-CB-CG	-11.69	102.11	113.80
1	A	293	ALA	CA-C-O	-11.54	111.48	119.68
1	A	293	ALA	CA-C-N	-11.53	98.81	121.41
1	A	293	ALA	C-N-CA	-11.53	98.81	121.41
1	A	287	GLN	OE1-CD-NE2	-11.25	111.35	122.60
1	A	464	THR	CB-CA-C	11.12	128.33	110.88
1	A	354	GLU	CB-CG-CD	11.11	131.48	112.60
1	A	673	ARG	CA-CB-CG	11.02	136.13	114.10
1	A	253	HIS	CB-CA-C	11.01	127.42	109.70
1	A	595	HIS	CA-CB-CG	10.99	124.79	113.80
1	A	212	SER	N-CA-C	10.78	124.11	111.71
1	A	148	ALA	CA-C-O	-10.78	107.57	119.97
1	A	651	LEU	N-CA-CB	10.77	126.98	110.28
1	A	664	GLN	CB-CG-CD	10.71	130.81	112.60
1	A	186	GLN	OE1-CD-NE2	-10.52	112.08	122.60
1	A	649	ALA	CA-C-O	10.51	131.38	120.24
1	A	23	GLN	OE1-CD-NE2	-10.50	112.10	122.60
1	A	295	GLN	OE1-CD-NE2	-10.45	112.15	122.60
1	A	508	ASN	OD1-CG-ND2	-10.43	112.17	122.60
1	A	105	GLN	OE1-CD-NE2	-10.42	112.18	122.60
1	A	275	GLN	OE1-CD-NE2	-10.29	112.31	122.60
1	A	344	GLN	OE1-CD-NE2	-10.29	112.31	122.60
1	A	21	GLN	OE1-CD-NE2	-10.27	112.33	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	482	ARG	CD-NE-CZ	10.25	138.75	124.40
1	A	284	SER	N-CA-C	10.18	124.40	110.35
1	A	42	ARG	CD-NE-CZ	10.12	138.56	124.40
1	A	309	ARG	CA-C-N	10.12	129.88	122.59
1	A	309	ARG	C-N-CA	10.12	129.88	122.59
1	A	644	ASN	CA-CB-CG	10.10	122.69	112.60
1	A	65	TYR	O-C-N	10.05	132.43	122.07
1	A	682	GLU	CA-CB-CG	10.05	134.21	114.10
1	A	448	TRP	CA-C-O	-9.99	110.17	121.15
1	A	110	GLN	OE1-CD-NE2	-9.98	112.62	122.60
1	A	570	GLU	CB-CG-CD	-9.95	95.68	112.60
1	A	146	GLN	OE1-CD-NE2	-9.91	112.69	122.60
1	A	431	LYS	CA-C-N	-9.87	102.07	121.41
1	A	431	LYS	C-N-CA	-9.87	102.07	121.41
1	A	367	GLN	N-CA-C	9.87	124.96	111.54
1	A	364	GLN	OE1-CD-NE2	-9.85	112.75	122.60
1	A	651	LEU	CA-C-O	-9.85	108.64	119.97
1	A	653	GLY	CA-C-O	9.82	131.05	119.46
1	A	355	GLN	OE1-CD-NE2	-9.77	112.83	122.60
1	A	423	LEU	N-CA-C	9.74	128.67	112.99
1	A	433	TYR	CB-CA-C	9.72	126.55	109.72
1	A	75	ARG	CA-CB-CG	9.72	133.54	114.10
1	A	415	GLN	OE1-CD-NE2	-9.71	112.89	122.60
1	A	684	CYS	N-CA-C	9.71	122.76	111.11
1	A	359	GLN	OE1-CD-NE2	-9.69	112.91	122.60
1	A	637	LYS	CA-CB-CG	9.55	133.20	114.10
1	A	487	PHE	CA-C-O	-9.52	110.49	121.72
1	A	229	LEU	CA-C-O	-9.51	110.37	121.11
1	A	391	ALA	CA-C-O	9.47	131.56	121.33
1	A	394	LEU	CA-C-O	-9.46	110.46	121.16
1	A	171	GLN	OE1-CD-NE2	-9.43	113.17	122.60
1	A	87	GLN	OE1-CD-NE2	-9.40	113.20	122.60
1	A	291	SER	CA-C-N	9.29	131.45	119.84
1	A	291	SER	C-N-CA	9.29	131.45	119.84
1	A	89	GLN	OE1-CD-NE2	-9.26	113.34	122.60
1	A	567	GLY	CA-C-O	9.22	136.61	120.57
1	A	427	HIS	CA-CB-CG	9.21	123.01	113.80
1	A	673	ARG	CD-NE-CZ	9.21	137.29	124.40
1	A	244	GLU	CA-C-O	9.18	130.25	119.32
1	A	654	LYS	CA-C-O	9.03	129.15	121.02
1	A	47	GLN	CA-C-O	-9.02	110.98	120.55
1	A	102	THR	CA-C-O	9.02	133.41	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	GLY	CA-C-N	8.98	129.63	120.38
1	A	140	GLY	C-N-CA	8.98	129.63	120.38
1	A	509	GLU	CB-CG-CD	8.96	127.83	112.60
1	A	195	ALA	N-CA-C	-8.76	101.81	111.36
1	A	348	CYS	N-CA-CB	8.70	123.00	109.69
1	A	251	PRO	CA-C-O	-8.66	111.38	122.12
1	A	652	GLN	CA-CB-CG	8.65	131.41	114.10
1	A	143	GLU	CA-C-O	8.64	128.05	119.49
1	A	371	CYS	N-CA-C	8.63	123.13	108.02
1	A	523	LEU	CB-CA-C	8.61	121.90	111.22
1	A	159	PRO	CB-CA-C	8.60	125.76	111.56
1	A	671	LYS	CA-C-O	8.57	130.50	121.07
1	A	618	PHE	CA-CB-CG	8.54	122.34	113.80
1	A	430	VAL	CA-C-N	-8.54	105.23	121.54
1	A	430	VAL	C-N-CA	-8.54	105.23	121.54
1	A	349	ALA	CA-C-O	-8.50	111.51	121.11
1	A	136	LEU	N-CA-C	8.48	121.59	111.33
1	A	221	LYS	N-CA-C	-8.48	103.11	113.97
1	A	381	ILE	N-CA-CB	8.47	120.45	110.55
1	A	427	HIS	CB-CA-C	8.46	123.29	109.07
1	A	363	ARG	CD-NE-CZ	8.43	136.20	124.40
1	A	569	PHE	CA-C-N	8.42	134.54	121.99
1	A	569	PHE	C-N-CA	8.42	134.54	121.99
1	A	519	SER	CA-C-N	8.40	133.07	120.31
1	A	519	SER	C-N-CA	8.40	133.07	120.31
1	A	70	ASP	CA-CB-CG	-8.35	104.25	112.60
1	A	343	ALA	N-CA-C	8.32	121.92	111.69
1	A	564	LEU	N-CA-CB	8.31	124.30	110.59
1	A	689	ARG	CD-NE-CZ	8.30	136.02	124.40
1	A	250	VAL	CA-CB-CG1	8.26	124.44	110.40
1	A	664	GLN	CA-C-O	8.24	130.06	120.00
1	A	526	TYR	CB-CA-C	8.17	126.67	110.42
1	A	293	ALA	O-C-N	-8.15	111.37	120.58
1	A	544	LYS	N-CA-CB	8.13	123.25	110.56
1	A	255	VAL	O-C-N	-8.12	113.73	122.83
1	A	571	LEU	CB-CG-CD1	8.08	134.93	110.70
1	A	623	GLU	CA-C-N	8.07	136.96	121.54
1	A	623	GLU	C-N-CA	8.07	136.96	121.54
1	A	95	VAL	CG1-CB-CG2	-8.04	93.11	110.80
1	A	42	ARG	CA-CB-CG	7.99	130.08	114.10
1	A	120	GLY	CA-C-N	7.96	136.74	121.54
1	A	120	GLY	C-N-CA	7.96	136.74	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	661	LEU	CA-C-O	7.96	129.18	119.79
1	A	664	GLN	OE1-CD-NE2	-7.92	114.68	122.60
1	A	280	ARG	NE-CZ-NH1	7.88	129.38	121.50
1	A	417	SER	CA-C-N	7.86	129.66	119.84
1	A	417	SER	C-N-CA	7.86	129.66	119.84
1	A	594	ASN	OD1-CG-ND2	-7.84	114.76	122.60
1	A	418	PRO	N-CA-C	7.82	128.59	112.47
1	A	201	ASP	CA-CB-CG	7.81	120.41	112.60
1	A	214	VAL	CB-CA-C	-7.78	101.84	112.04
1	A	381	ILE	CA-C-O	-7.78	112.92	121.17
1	A	282	LYS	O-C-N	7.75	128.18	121.20
1	A	167	PRO	N-CA-C	7.74	124.94	114.18
1	A	621	ASN	CA-C-O	7.74	130.13	120.15
1	A	567	GLY	O-C-N	-7.72	112.66	122.70
1	A	170	CYS	N-CA-CB	7.69	121.87	110.49
1	A	350	VAL	CA-CB-CG2	7.69	123.47	110.40
1	A	141	PRO	CA-C-N	7.69	127.40	119.56
1	A	141	PRO	C-N-CA	7.69	127.40	119.56
1	A	559	GLN	N-CA-C	7.67	127.13	110.80
1	A	510	GLU	N-CA-C	-7.62	101.99	110.91
1	A	543	VAL	CA-CB-CG2	7.61	123.34	110.40
1	A	495	SER	CA-C-O	-7.61	112.61	121.82
1	A	354	GLU	N-CA-C	-7.60	103.07	111.36
1	A	451	LEU	N-CA-C	7.58	122.62	113.23
1	A	555	LYS	N-CA-C	7.56	126.14	114.64
1	A	7	ARG	NH1-CZ-NH2	-7.56	109.48	119.30
1	A	468	ASN	N-CA-C	7.52	120.43	111.33
1	A	219	PRO	CA-N-CD	-7.50	101.50	112.00
1	A	485	GLU	CA-CB-CG	7.48	129.06	114.10
1	A	340	LEU	CA-C-N	7.48	130.91	120.29
1	A	340	LEU	C-N-CA	7.48	130.91	120.29
1	A	573	CYS	CA-C-N	7.46	130.89	120.29
1	A	573	CYS	C-N-CA	7.46	130.89	120.29
1	A	653	GLY	CA-C-N	7.42	132.88	121.53
1	A	653	GLY	C-N-CA	7.42	132.88	121.53
1	A	677	THR	N-CA-C	7.37	121.19	110.28
1	A	42	ARG	CA-C-O	7.35	128.43	119.97
1	A	652	GLN	OE1-CD-NE2	-7.34	115.26	122.60
1	A	190	PHE	CA-CB-CG	7.33	121.13	113.80
1	A	404	LYS	N-CA-CB	7.33	121.59	110.30
1	A	297	ASP	CA-CB-CG	7.32	119.92	112.60
1	A	171	GLN	CA-C-N	-7.31	111.20	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	GLN	C-N-CA	-7.31	111.20	122.60
1	A	487	PHE	CA-CB-CG	-7.31	106.49	113.80
1	A	364	GLN	CG-CD-NE2	7.30	127.35	116.40
1	A	584	ALA	N-CA-C	-7.28	104.00	113.17
1	A	529	ALA	CB-CA-C	7.27	123.86	110.56
1	A	241	ALA	N-CA-C	-7.26	103.98	112.92
1	A	222	ALA	CA-C-N	7.25	130.00	120.28
1	A	222	ALA	C-N-CA	7.25	130.00	120.28
1	A	371	CYS	N-CA-CB	-7.24	99.21	110.65
1	A	594	ASN	CA-CB-CG	7.23	119.83	112.60
1	A	416	GLN	CA-C-O	7.22	128.31	119.79
1	A	465	ALA	O-C-N	7.21	131.87	122.42
1	A	471	MET	N-CA-C	7.21	121.18	112.38
1	A	532	CYS	CA-CB-SG	7.20	130.96	114.40
1	A	215	PHE	CA-C-O	7.17	128.16	120.55
1	A	280	ARG	NH1-CZ-NH2	-7.17	109.98	119.30
1	A	444	ASP	CB-CA-C	7.16	118.80	109.28
1	A	572	LEU	O-C-N	-7.16	113.07	122.59
1	A	302	ASP	CA-CB-CG	-7.14	105.46	112.60
1	A	604	VAL	CA-CB-CG1	7.14	122.54	110.40
1	A	620	ARG	CD-NE-CZ	7.13	134.38	124.40
1	A	508	ASN	CA-C-N	7.12	132.72	122.40
1	A	508	ASN	C-N-CA	7.12	132.72	122.40
1	A	639	LEU	CA-C-O	7.08	128.79	120.58
1	A	440	ARG	NE-CZ-NH2	7.07	125.56	119.20
1	A	295	GLN	CG-CD-NE2	7.07	127.00	116.40
1	A	396	GLY	N-CA-C	7.05	122.48	113.24
1	A	227	TYR	N-CA-C	7.05	120.64	109.50
1	A	70	ASP	N-CA-CB	7.05	122.91	110.37
1	A	275	GLN	CG-CD-NE2	7.04	126.96	116.40
1	A	396	GLY	O-C-N	-7.04	114.78	122.24
1	A	344	GLN	CG-CD-NE2	7.01	126.91	116.40
1	A	507	GLY	N-CA-C	-7.00	103.86	112.68
1	A	220	ALA	CA-C-N	-6.99	110.65	122.11
1	A	220	ALA	C-N-CA	-6.99	110.65	122.11
1	A	509	GLU	CA-C-O	6.99	129.47	120.81
1	A	446	ILE	CA-C-O	6.97	129.49	120.78
1	A	310	ILE	CB-CA-C	-6.96	103.26	110.71
1	A	296	LYS	N-CA-C	6.96	120.24	108.90
1	A	366	ASN	CA-C-N	6.93	131.99	122.07
1	A	366	ASN	C-N-CA	6.93	131.99	122.07
1	A	529	ALA	N-CA-C	-6.93	102.06	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	TYR	CA-C-N	6.93	132.86	122.68
1	A	72	TYR	C-N-CA	6.93	132.86	122.68
1	A	532	CYS	CB-CA-C	6.93	123.59	109.67
1	A	433	TYR	N-CA-CB	-6.92	99.70	110.57
1	A	400	TYR	CA-C-O	-6.92	113.55	120.82
1	A	146	GLN	CG-CD-NE2	6.92	126.78	116.40
1	A	94	ALA	N-CA-CB	6.92	120.15	109.85
1	A	478	THR	N-CA-CB	6.91	120.25	110.36
1	A	171	GLN	CG-CD-NE2	6.91	126.76	116.40
1	A	287	GLN	CG-CD-NE2	6.91	126.76	116.40
1	A	142	PRO	CA-C-O	6.90	129.04	119.18
1	A	582	THR	CA-CB-CG2	6.89	122.21	110.50
1	A	329	ARG	CA-CB-CG	6.87	127.84	114.10
1	A	642	ASN	CA-C-O	6.87	128.75	120.92
1	A	553	ASP	CA-C-O	6.86	125.86	119.00
1	A	435	ALA	CA-C-O	-6.84	113.25	121.05
1	A	683	ALA	CA-C-O	-6.83	113.64	120.82
1	A	7	ARG	NE-CZ-NH1	6.82	128.32	121.50
1	A	267	ILE	O-C-N	6.82	128.59	121.91
1	A	23	GLN	CG-CD-NE2	6.81	126.62	116.40
1	A	339	GLU	CB-CG-CD	6.81	124.18	112.60
1	A	575	ASN	CA-CB-CG	6.80	119.40	112.60
1	A	75	ARG	NE-CZ-NH2	6.80	125.32	119.20
1	A	519	SER	CA-C-O	6.77	127.63	119.10
1	A	546	VAL	N-CA-C	6.75	117.54	110.72
1	A	42	ARG	O-C-N	-6.74	113.98	122.27
1	A	319	TYR	N-CA-CB	6.74	119.79	110.01
1	A	203	ALA	O-C-N	-6.74	115.08	122.09
1	A	549	LEU	CA-C-N	6.74	132.13	121.08
1	A	549	LEU	C-N-CA	6.74	132.13	121.08
1	A	352	SER	CA-C-O	-6.73	112.23	119.97
1	A	64	VAL	O-C-N	6.72	128.39	121.87
1	A	261	ASN	CA-C-O	-6.72	113.80	122.14
1	A	657	TYR	N-CA-CB	6.71	120.20	110.20
1	A	74	LEU	O-C-N	6.68	130.50	122.68
1	A	148	ALA	N-CA-C	-6.68	104.07	111.82
1	A	279	GLY	CA-C-O	-6.67	115.28	122.76
1	A	21	GLN	CG-CD-NE2	6.67	126.40	116.40
1	A	515	CYS	CA-C-O	6.65	131.09	122.45
1	A	652	GLN	N-CA-C	6.64	124.95	110.80
1	A	528	GLY	CA-C-O	6.64	132.12	120.57
1	A	525	GLY	CA-C-O	-6.62	114.83	122.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	LYS	CB-CA-C	6.61	121.33	109.29
1	A	355	GLN	CG-CD-NE2	6.58	126.27	116.40
1	A	396	GLY	CA-C-N	6.58	128.63	120.34
1	A	396	GLY	C-N-CA	6.58	128.63	120.34
1	A	475	PHE	CA-CB-CG	-6.58	107.22	113.80
1	A	105	GLN	CG-CD-NE2	6.56	126.24	116.40
1	A	252	SER	N-CA-CB	6.55	119.73	110.36
1	A	523	LEU	CA-C-N	6.55	133.82	122.81
1	A	523	LEU	C-N-CA	6.55	133.82	122.81
1	A	391	ALA	N-CA-C	6.54	119.00	109.07
1	A	276	GLU	CA-CB-CG	6.53	127.16	114.10
1	A	659	GLU	N-CA-C	-6.53	104.25	111.82
1	A	512	GLN	CB-CG-CD	6.53	123.69	112.60
1	A	31	GLY	N-CA-C	-6.51	99.06	112.34
1	A	433	TYR	CA-CB-CG	6.51	125.62	113.90
1	A	103	ASN	N-CA-C	-6.50	102.70	111.87
1	A	391	ALA	CA-C-N	6.50	133.96	121.54
1	A	391	ALA	C-N-CA	6.50	133.96	121.54
1	A	462	ASP	CA-CB-CG	-6.50	106.10	112.60
1	A	658	ASP	CA-CB-CG	6.48	119.08	112.60
1	A	449	ASN	CA-CB-CG	6.48	119.08	112.60
1	A	89	GLN	CG-CD-NE2	6.47	126.10	116.40
1	A	309	ARG	NH1-CZ-NH2	6.46	127.70	119.30
1	A	415	GLN	CG-CD-NE2	6.46	126.09	116.40
1	A	656	THR	CA-CB-OG1	6.45	119.27	109.60
1	A	233	ASN	N-CA-CB	6.44	120.29	110.44
1	A	526	TYR	N-CA-CB	-6.43	99.62	110.49
1	A	651	LEU	N-CA-C	6.43	119.28	111.82
1	A	110	GLN	CG-CD-NE2	6.43	126.04	116.40
1	A	686	PHE	CA-C-O	6.42	127.35	120.10
1	A	317	GLY	O-C-N	-6.42	116.03	122.19
1	A	49	ILE	CB-CA-C	-6.40	103.69	111.88
1	A	536	ASN	CA-CB-CG	-6.40	106.20	112.60
1	A	108	GLN	OE1-CD-NE2	6.38	128.98	122.60
1	A	503	ALA	CA-C-O	-6.38	114.12	120.82
1	A	151	LYS	CG-CD-CE	6.38	125.96	111.30
1	A	285	ALA	N-CA-C	-6.37	105.52	113.55
1	A	491	CYS	N-CA-CB	6.37	120.88	110.37
1	A	87	GLN	CG-CD-NE2	6.37	125.95	116.40
1	A	93	TYR	CA-CB-CG	-6.37	102.44	113.90
1	A	392	LEU	CA-C-O	6.37	129.61	120.51
1	A	417	SER	CB-CA-C	6.36	122.70	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	LYS	CA-C-O	-6.35	114.26	122.14
1	A	455	LYS	N-CA-CB	6.35	120.76	110.41
1	A	441	LYS	CA-C-O	6.34	127.43	119.12
1	A	482	ARG	NE-CZ-NH1	6.34	127.84	121.50
1	A	598	VAL	CB-CA-C	6.33	119.46	110.84
1	A	686	PHE	CA-CB-CG	-6.33	107.47	113.80
1	A	664	GLN	N-CA-C	-6.33	103.66	112.45
1	A	17	LYS	CA-C-O	-6.31	114.13	121.07
1	A	592	ALA	CA-C-O	-6.30	113.33	119.51
1	A	638	ASN	CA-C-N	6.30	130.31	121.24
1	A	638	ASN	C-N-CA	6.30	130.31	121.24
1	A	523	LEU	CA-CB-CG	6.28	138.28	116.30
1	A	593	PRO	N-CA-C	6.28	122.25	111.77
1	A	505	CYS	CB-CA-C	6.26	122.87	110.42
1	A	264	GLU	CA-C-O	6.25	127.95	121.07
1	A	435	ALA	N-CA-C	-6.24	100.34	110.20
1	A	458	HIS	CA-C-O	6.23	128.63	121.28
1	A	406	GLY	CA-C-N	6.23	133.44	122.67
1	A	406	GLY	C-N-CA	6.23	133.44	122.67
1	A	638	ASN	CA-CB-CG	6.23	118.83	112.60
1	A	294	GLY	CA-C-N	6.20	131.01	122.77
1	A	294	GLY	C-N-CA	6.20	131.01	122.77
1	A	66	ASP	N-CA-C	6.19	118.83	111.71
1	A	542	PHE	CB-CA-C	6.18	120.68	110.78
1	A	338	VAL	CA-C-O	-6.17	114.31	120.85
1	A	65	TYR	CA-C-O	-6.17	114.34	120.82
1	A	545	ASP	CA-C-N	6.17	129.18	120.42
1	A	545	ASP	C-N-CA	6.17	129.18	120.42
1	A	625	CYS	CA-CB-SG	6.17	128.58	114.40
1	A	359	GLN	CG-CD-NE2	6.16	125.64	116.40
1	A	465	ALA	CA-C-O	-6.16	112.13	119.15
1	A	340	LEU	O-C-N	-6.15	115.14	122.15
1	A	224	ARG	N-CA-CB	6.13	120.56	110.39
1	A	683	ALA	N-CA-CB	6.12	118.89	110.01
1	A	584	ALA	CA-C-N	6.11	133.28	121.18
1	A	584	ALA	C-N-CA	6.11	133.28	121.18
1	A	644	ASN	N-CA-CB	6.10	120.17	110.22
1	A	97	ILE	CB-CA-C	-6.10	102.58	112.03
1	A	634	SER	CA-C-N	6.08	131.20	122.08
1	A	634	SER	C-N-CA	6.08	131.20	122.08
1	A	36	CYS	N-CA-C	6.08	119.73	109.76
1	A	523	LEU	O-C-N	-6.08	112.97	121.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	456	SER	CA-C-O	6.07	127.97	121.11
1	A	655	THR	N-CA-C	6.05	120.74	113.23
1	A	54	ALA	CA-C-N	-6.05	112.03	122.79
1	A	54	ALA	C-N-CA	-6.05	112.03	122.79
1	A	366	ASN	N-CA-C	-6.04	103.06	111.52
1	A	438	VAL	CA-CB-CG1	6.04	120.67	110.40
1	A	452	ARG	CA-C-O	-6.01	114.57	121.19
1	A	385	LEU	CA-C-O	-6.01	114.18	120.55
1	A	48	ALA	O-C-N	-6.01	115.78	122.03
1	A	418	PRO	CA-C-N	6.00	133.01	121.54
1	A	418	PRO	C-N-CA	6.00	133.01	121.54
1	A	127	ILE	CA-C-O	-5.99	111.92	119.95
1	A	461	VAL	CA-C-N	5.99	131.09	122.35
1	A	461	VAL	C-N-CA	5.99	131.09	122.35
1	A	211	ASP	CA-C-N	5.98	128.89	120.28
1	A	211	ASP	C-N-CA	5.98	128.89	120.28
1	A	224	ARG	NE-CZ-NH1	-5.98	115.52	121.50
1	A	496	ASP	CA-CB-CG	5.96	118.56	112.60
1	A	488	SER	CB-CA-C	-5.96	101.49	110.90
1	A	536	ASN	CB-CG-ND2	-5.96	107.47	116.40
1	A	614	GLN	CA-C-N	5.94	128.55	120.54
1	A	614	GLN	C-N-CA	5.94	128.55	120.54
1	A	649	ALA	O-C-N	-5.92	116.34	123.27
1	A	498	ARG	CD-NE-CZ	5.91	132.68	124.40
1	A	455	LYS	CB-CA-C	-5.91	99.41	109.51
1	A	632	PHE	CA-C-N	5.90	132.81	121.54
1	A	632	PHE	C-N-CA	5.90	132.81	121.54
1	A	337	GLU	CA-CB-CG	5.88	125.85	114.10
1	A	418	PRO	CB-CA-C	5.87	121.25	111.56
1	A	439	VAL	CB-CA-C	-5.87	102.14	110.82
1	A	3	LYS	CB-CA-C	-5.86	107.07	114.40
1	A	126	ASN	CA-CB-CG	5.85	118.45	112.60
1	A	107	ASN	OD1-CG-ND2	-5.84	116.76	122.60
1	A	112	LEU	CD1-CG-CD2	-5.83	97.98	110.80
1	A	20	ALA	CA-C-O	-5.82	114.67	121.07
1	A	152	PHE	CA-C-O	-5.81	114.91	120.90
1	A	260	VAL	CB-CA-C	-5.81	103.60	111.15
1	A	17	LYS	N-CA-CB	5.80	118.63	109.82
1	A	309	ARG	CG-CD-NE	-5.80	99.25	112.00
1	A	256	VAL	N-CA-C	5.79	118.09	109.17
1	A	278	PHE	CB-CA-C	-5.79	99.80	109.75
1	A	372	ALA	CA-C-O	-5.77	114.43	121.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	GLN	CG-CD-NE2	5.76	125.04	116.40
1	A	95	VAL	O-C-N	-5.76	116.84	123.00
1	A	482	ARG	CA-C-O	5.76	128.03	121.58
1	A	280	ARG	CB-CG-CD	5.75	124.52	111.30
1	A	114	SER	CA-C-O	5.75	127.65	121.16
1	A	242	PHE	CB-CA-C	-5.74	100.00	110.63
1	A	269	LYS	N-CA-CB	5.72	118.62	110.16
1	A	233	ASN	OD1-CG-ND2	-5.72	116.88	122.60
1	A	257	ALA	CA-C-N	-5.71	112.75	120.87
1	A	257	ALA	C-N-CA	-5.71	112.75	120.87
1	A	229	LEU	CA-CB-CG	5.71	136.29	116.30
1	A	77	ILE	CB-CA-C	5.71	116.08	111.06
1	A	280	ARG	N-CA-CB	5.67	118.99	109.92
1	A	350	VAL	N-CA-C	5.67	116.10	108.17
1	A	536	ASN	CA-C-O	5.66	128.60	120.51
1	A	598	VAL	N-CA-CB	-5.66	104.20	110.99
1	A	147	LYS	CB-CA-C	5.65	119.58	109.29
1	A	176	THR	CA-CB-OG1	-5.65	101.12	109.60
1	A	645	THR	CA-C-N	5.65	128.12	120.44
1	A	645	THR	C-N-CA	5.65	128.12	120.44
1	A	196	PHE	CA-CB-CG	5.64	119.44	113.80
1	A	355	GLN	CA-CB-CG	-5.64	102.81	114.10
1	A	244	GLU	O-C-N	-5.64	115.42	122.24
1	A	418	PRO	O-C-N	-5.64	115.03	122.64
1	A	684	CYS	O-C-N	-5.63	116.23	122.09
1	A	218	LEU	N-CA-CB	-5.63	100.86	110.43
1	A	339	GLU	CB-CA-C	5.63	121.15	109.95
1	A	656	THR	O-C-N	-5.63	115.22	122.20
1	A	361	TRP	CA-C-N	5.63	128.61	120.79
1	A	361	TRP	C-N-CA	5.63	128.61	120.79
1	A	223	ASP	CA-C-O	5.62	126.51	120.55
1	A	530	PHE	N-CA-C	5.62	119.98	113.18
1	A	476	LYS	CA-C-O	5.62	126.49	120.70
1	A	485	GLU	CB-CG-CD	5.61	122.13	112.60
1	A	326	THR	N-CA-C	5.60	117.39	111.28
1	A	181	CYS	N-CA-C	-5.60	106.40	113.23
1	A	591	VAL	CB-CA-C	5.59	118.96	111.19
1	A	584	ALA	N-CA-CB	5.59	118.76	110.49
1	A	264	GLU	CB-CA-C	-5.58	102.04	110.92
1	A	497	PRO	N-CA-C	5.58	123.97	112.47
1	A	264	GLU	N-CA-C	5.57	117.82	111.02
1	A	267	ILE	CB-CA-C	-5.56	104.85	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	ILE	N-CA-CB	5.56	118.99	111.21
1	A	448	TRP	N-CA-C	-5.55	102.41	110.24
1	A	47	GLN	OE1-CD-NE2	5.55	128.15	122.60
1	A	242	PHE	CA-C-N	5.55	127.72	120.28
1	A	242	PHE	C-N-CA	5.55	127.72	120.28
1	A	211	ASP	O-C-N	-5.54	115.49	122.20
1	A	384	VAL	N-CA-CB	5.54	118.08	110.54
1	A	643	ASP	CA-C-O	-5.54	114.65	120.63
1	A	68	GLY	CA-C-N	5.53	132.48	122.02
1	A	68	GLY	C-N-CA	5.53	132.48	122.02
1	A	74	LEU	CA-C-O	-5.53	115.42	121.89
1	A	440	ARG	NH1-CZ-NH2	-5.53	112.11	119.30
1	A	433	TYR	N-CA-C	5.53	117.97	109.07
1	A	629	PHE	CA-C-O	-5.52	114.98	121.44
1	A	572	LEU	CB-CG-CD2	5.52	127.26	110.70
1	A	459	THR	CA-C-N	5.51	131.23	121.80
1	A	459	THR	C-N-CA	5.51	131.23	121.80
1	A	408	VAL	N-CA-C	5.49	120.74	108.88
1	A	53	LYS	N-CA-CB	5.49	119.34	110.40
1	A	224	ARG	NE-CZ-NH2	5.49	124.14	119.20
1	A	542	PHE	CA-C-O	5.48	126.24	120.54
1	A	683	ALA	N-CA-C	-5.48	105.21	111.07
1	A	280	ARG	CG-CD-NE	5.47	124.03	112.00
1	A	152	PHE	CB-CA-C	5.46	119.42	110.95
1	A	380	CYS	CB-CA-C	-5.46	102.56	110.96
1	A	595	HIS	N-CA-C	-5.45	101.09	109.76
1	A	186	GLN	CA-CB-CG	-5.45	103.21	114.10
1	A	103	ASN	CB-CA-C	5.44	119.88	111.28
1	A	211	ASP	CA-C-O	5.44	127.38	121.02
1	A	647	CYS	N-CA-C	5.43	115.71	108.38
1	A	119	LEU	CA-C-N	5.43	132.05	121.41
1	A	119	LEU	C-N-CA	5.43	132.05	121.41
1	A	367	GLN	CB-CG-CD	5.42	121.82	112.60
1	A	344	GLN	N-CA-C	5.42	118.89	110.17
1	A	208	PHE	CA-CB-CG	5.40	119.20	113.80
1	A	680	LEU	CA-C-O	5.39	126.17	119.97
1	A	163	GLY	N-CA-C	-5.39	106.87	115.66
1	A	536	ASN	N-CA-C	5.39	122.28	110.80
1	A	348	CYS	CA-C-O	-5.38	114.78	120.92
1	A	620	ARG	CB-CG-CD	5.38	123.68	111.30
1	A	654	LYS	N-CA-C	-5.38	104.06	110.41
1	A	665	TYR	CA-C-N	5.38	127.54	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	665	TYR	C-N-CA	5.38	127.54	120.60
1	A	684	CYS	CA-C-N	5.38	128.49	120.31
1	A	684	CYS	C-N-CA	5.38	128.49	120.31
1	A	460	ALA	N-CA-CB	5.37	119.73	111.46
1	A	400	TYR	CB-CA-C	5.37	119.31	110.88
1	A	42	ARG	N-CA-C	-5.37	105.59	111.82
1	A	649	ALA	CA-C-N	5.36	131.77	121.54
1	A	649	ALA	C-N-CA	5.36	131.77	121.54
1	A	416	GLN	CB-CG-CD	5.35	121.69	112.60
1	A	170	CYS	N-CA-C	-5.34	106.44	113.17
1	A	366	ASN	CA-CB-CG	5.33	117.93	112.60
1	A	547	THR	O-C-N	-5.33	115.50	122.59
1	A	663	PRO	N-CA-C	5.33	121.01	114.35
1	A	74	LEU	N-CA-C	-5.33	102.87	110.59
1	A	42	ARG	CA-C-N	5.32	127.36	120.44
1	A	42	ARG	C-N-CA	5.32	127.36	120.44
1	A	79	ALA	N-CA-CB	-5.32	101.61	110.23
1	A	4	LYS	CA-CB-CG	5.31	124.71	114.10
1	A	42	ARG	NE-CZ-NH1	5.30	126.80	121.50
1	A	125	TRP	CA-CB-CG	5.30	123.67	113.60
1	A	255	VAL	CA-C-O	5.29	126.99	120.74
1	A	635	LYS	CB-CA-C	-5.29	104.42	111.88
1	A	602	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	558	GLU	O-C-N	-5.28	117.20	123.11
1	A	563	ASP	CB-CA-C	5.28	120.92	110.42
1	A	322	SER	CA-C-O	5.27	126.43	120.00
1	A	555	LYS	CA-C-O	-5.27	111.84	118.43
1	A	127	ILE	CA-C-N	5.26	124.77	119.19
1	A	127	ILE	C-N-CA	5.26	124.77	119.19
1	A	617	HIS	N-CA-CB	5.26	117.58	110.59
1	A	636	THR	CA-CB-OG1	5.25	117.48	109.60
1	A	523	LEU	CB-CG-CD1	5.24	126.43	110.70
1	A	565	LYS	CA-CB-CG	5.24	124.58	114.10
1	A	258	ARG	N-CA-CB	5.23	117.66	109.97
1	A	316	SER	CA-C-N	5.23	125.79	119.98
1	A	316	SER	C-N-CA	5.23	125.79	119.98
1	A	321	GLY	CA-C-O	-5.23	117.08	122.26
1	A	648	LEU	CB-CA-C	5.23	118.96	110.22
1	A	191	GLY	O-C-N	-5.23	117.09	122.68
1	A	652	GLN	CB-CG-CD	5.22	121.47	112.60
1	A	116	HIS	CA-CB-CG	5.22	119.02	113.80
1	A	191	GLY	CA-C-O	5.21	129.32	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	422	GLY	CA-C-N	-5.21	111.53	120.23
1	A	422	GLY	C-N-CA	-5.21	111.53	120.23
1	A	462	ASP	N-CA-C	5.21	118.90	111.92
1	A	310	ILE	N-CA-CB	-5.21	104.52	111.08
1	A	253	HIS	CA-C-O	-5.20	115.43	121.15
1	A	642	ASN	CA-C-N	5.20	127.51	120.38
1	A	642	ASN	C-N-CA	5.20	127.51	120.38
1	A	259	SER	CB-CA-C	-5.20	102.69	110.90
1	A	149	VAL	CA-C-N	5.19	127.49	120.38
1	A	149	VAL	C-N-CA	5.19	127.49	120.38
1	A	635	LYS	CA-C-O	5.19	130.11	122.38
1	A	536	ASN	CB-CG-OD1	5.19	131.18	120.80
1	A	304	ALA	N-CA-C	5.19	118.16	110.48
1	A	200	GLN	CB-CG-CD	5.18	121.40	112.60
1	A	232	PRO	CB-CA-C	5.18	119.20	111.85
1	A	277	LYS	CA-C-N	5.17	130.06	121.99
1	A	277	LYS	C-N-CA	5.17	130.06	121.99
1	A	18	LYS	CA-C-O	5.17	125.94	120.10
1	A	661	LEU	N-CA-CB	-5.17	102.34	110.30
1	A	269	LYS	CG-CD-CE	5.17	123.18	111.30
1	A	315	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	402	ALA	O-C-N	-5.16	116.72	122.09
1	A	478	THR	CA-CB-CG2	5.16	119.28	110.50
1	A	498	ARG	CA-C-N	5.16	130.27	121.29
1	A	498	ARG	C-N-CA	5.16	130.27	121.29
1	A	404	LYS	CB-CG-CD	5.16	123.16	111.30
1	A	452	ARG	N-CA-C	-5.16	102.75	110.23
1	A	513	LEU	N-CA-C	5.16	121.78	110.80
1	A	496	ASP	CA-C-N	5.15	126.28	119.84
1	A	496	ASP	C-N-CA	5.15	126.28	119.84
1	A	459	THR	O-C-N	-5.15	116.67	122.03
1	A	544	LYS	N-CA-C	-5.15	102.44	110.42
1	A	261	ASN	N-CA-CB	-5.15	103.52	111.65
1	A	491	CYS	CA-CB-SG	5.15	126.24	114.40
1	A	626	PRO	CA-C-N	5.15	131.50	121.41
1	A	626	PRO	C-N-CA	5.15	131.50	121.41
1	A	297	ASP	CB-CA-C	-5.15	104.58	111.89
1	A	400	TYR	O-C-N	-5.15	116.77	122.07
1	A	488	SER	CA-CB-OG	-5.15	100.81	111.10
1	A	178	GLU	CB-CA-C	-5.14	104.90	111.22
1	A	487	PHE	O-C-N	5.14	128.70	122.94
1	A	604	VAL	N-CA-C	5.14	120.03	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	TYR	CB-CA-C	-5.14	102.81	110.88
1	A	292	PRO	CA-N-CD	-5.13	104.82	112.00
1	A	577	THR	CB-CA-C	5.12	120.61	110.42
1	A	588	HIS	CA-CB-CG	5.11	118.91	113.80
1	A	197	LYS	O-C-N	-5.11	116.70	122.12
1	A	609	GLN	CA-C-O	5.11	125.97	120.55
1	A	407	LEU	N-CA-C	5.10	118.01	110.46
1	A	419	GLU	N-CA-C	5.10	121.66	110.80
1	A	689	ARG	NE-CZ-NH1	5.10	126.60	121.50
1	A	674	ARG	CA-C-O	5.09	125.80	119.79
1	A	267	ILE	CA-C-O	-5.09	115.78	121.17
1	A	341	ARG	CD-NE-CZ	5.08	131.51	124.40
1	A	18	LYS	CA-C-N	5.08	129.26	120.58
1	A	18	LYS	C-N-CA	5.08	129.26	120.58
1	A	380	CYS	CA-C-O	-5.08	115.67	121.00
1	A	309	ARG	NE-CZ-NH1	-5.07	116.43	121.50
1	A	632	PHE	CA-C-O	5.07	125.78	119.79
1	A	15	GLU	CB-CA-C	5.07	118.91	110.90
1	A	259	SER	N-CA-C	5.06	116.60	111.14
1	A	565	LYS	N-CA-C	-5.06	104.00	110.53
1	A	379	ASP	CA-CB-CG	-5.05	107.55	112.60
1	A	440	ARG	CG-CD-NE	5.04	123.10	112.00
1	A	625	CYS	O-C-N	5.04	127.12	121.32
1	A	630	CYS	N-CA-CB	5.04	118.69	110.77
1	A	389	ALA	O-C-N	-5.04	117.83	123.48
1	A	584	ALA	CA-C-O	5.04	125.25	119.35
1	A	573	CYS	CA-C-O	5.03	127.71	120.51
1	A	667	THR	CB-CA-C	-5.03	103.21	110.96
1	A	295	GLN	CA-C-N	-5.03	115.90	122.99
1	A	295	GLN	C-N-CA	-5.03	115.90	122.99
1	A	528	GLY	O-C-N	-5.03	116.16	122.70
1	A	74	LEU	N-CA-CB	5.03	118.06	110.42
1	A	230	LEU	CA-C-O	-5.03	114.98	120.36
1	A	440	ARG	CD-NE-CZ	5.03	131.44	124.40
1	A	632	PHE	N-CA-C	5.03	118.56	112.23
1	A	450	SER	CA-C-O	5.02	125.60	119.78
1	A	657	TYR	CA-CB-CG	5.01	122.92	113.90
1	A	247	LEU	N-CA-C	-5.01	106.86	113.12
1	A	173	CYS	CA-C-N	-5.00	114.67	122.37
1	A	173	CYS	C-N-CA	-5.00	114.67	122.37

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	70	ASP	CA

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	282	LYS	Mainchain
1	A	319	TYR	Sidechain
1	A	379	ASP	Mainchain
1	A	400	TYR	Mainchain
1	A	429	PRO	Mainchain
1	A	430	VAL	Mainchain
1	A	435	ALA	Mainchain
1	A	499	SER	Mainchain
1	A	529	ALA	Mainchain
1	A	569	PHE	Mainchain
1	A	572	LEU	Peptide,Mainchain
1	A	622	GLY	Mainchain
1	A	636	THR	Mainchain
1	A	70	ASP	Sidechain
1	A	94	ALA	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	5284	0	5238	439	0
2	A	2	0	0	0	0
3	A	8	0	0	0	0
4	A	233	0	0	8	0
All	All	5527	0	5238	439	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 42.

All (439) 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:92:TYR:CB	1:A:92:TYR:CA	1.80	1.58
1:A:526:TYR:N	1:A:526:TYR:CA	1.93	1.31
1:A:343:ALA:O	1:A:606:HIS:NE2	1.66	1.29
1:A:423:LEU:HD12	1:A:423:LEU:O	1.25	1.27
1:A:233:ASN:O	1:A:234:ASN:HB2	1.50	1.11
1:A:423:LEU:O	1:A:423:LEU:CD1	1.98	1.11
1:A:23:GLN:HB2	1:A:34:VAL:O	1.51	1.07
1:A:18:LYS:NZ	1:A:288:LEU:O	1.90	1.03
1:A:463:ARG:HG2	1:A:463:ARG:HH11	1.22	1.03
1:A:168:ASN:HA	1:A:171:GLN:HB2	1.36	1.03
1:A:423:LEU:HD12	1:A:423:LEU:C	1.84	1.02
1:A:129:MET:HE2	1:A:149:VAL:HG22	1.45	0.96
1:A:334:THR:O	1:A:336:ALA:N	1.98	0.96
1:A:440:ARG:HD2	1:A:536:ASN:HD21	1.29	0.96
1:A:364:GLN:HG3	1:A:629:PHE:HB2	1.47	0.95
1:A:679:PRO:HA	1:A:682:GLU:HG3	1.50	0.94
1:A:543:VAL:HG11	1:A:547:THR:HG21	1.50	0.94
1:A:352:SER:O	1:A:355:GLN:HB3	1.68	0.93
1:A:44:GLU:HA	1:A:47:GLN:HE21	1.31	0.93
1:A:518:ASN:HD22	1:A:519:SER:H	1.13	0.93
1:A:430:VAL:CG1	1:A:594:ASN:HD22	1.83	0.92
1:A:178:GLU:O	1:A:178:GLU:HG2	1.70	0.91
1:A:410:VAL:HG11	1:A:607:LEU:HD23	1.53	0.90
1:A:469:ILE:HD13	1:A:590:PRO:HG2	1.53	0.89
1:A:16:SER:HB3	1:A:38:LYS:HG2	1.56	0.87
1:A:548:VAL:HG11	1:A:581:VAL:HG21	1.56	0.87
1:A:638:ASN:HD22	1:A:643:ASP:H	1.21	0.87
1:A:219:PRO:O	1:A:220:ALA:O	1.93	0.85
1:A:334:THR:OG1	1:A:337:GLU:OE2	1.93	0.85
1:A:160:CYS:HG	1:A:183:CYS:HG	1.22	0.84
1:A:97:ILE:O	1:A:206:VAL:HG12	1.78	0.83
1:A:145:LEU:HD23	1:A:145:LEU:O	1.78	0.83
1:A:484:ASP:HB2	1:A:500:LYS:HD3	1.59	0.83
1:A:160:CYS:SG	4:A:724:HOH:O	2.36	0.82
1:A:14:ALA:HA	1:A:17:LYS:HD3	1.59	0.82
1:A:430:VAL:HG12	1:A:594:ASN:HD22	1.43	0.81
1:A:395:ASP:O	1:A:399:ILE:HG13	1.80	0.81
1:A:638:ASN:ND2	1:A:643:ASP:H	1.77	0.80
1:A:382:ALA:HA	1:A:385:LEU:HD12	1.63	0.80
1:A:589:LEU:HB3	1:A:590:PRO:HD2	1.64	0.79
1:A:44:GLU:HA	1:A:47:GLN:NE2	1.99	0.78
1:A:559:GLN:H	1:A:562:LYS:HG3	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:GLY:O	4:A:820:HOH:O	2.02	0.77
1:A:434:LEU:HG	1:A:591:VAL:CG2	2.14	0.77
1:A:472:GLY:HA3	1:A:668:ALA:HA	1.65	0.77
1:A:364:GLN:HG3	1:A:629:PHE:CB	2.16	0.76
1:A:380:CYS:HB3	1:A:392:LEU:HD22	1.66	0.76
1:A:571:LEU:HD12	1:A:581:VAL:HA	1.67	0.76
1:A:507:GLY:HA3	1:A:514:LYS:HG2	1.67	0.76
1:A:615:GLN:HE22	1:A:648:LEU:H	1.35	0.74
1:A:593:PRO:HG2	1:A:661:LEU:HD12	1.68	0.74
1:A:660:TYR:HD2	1:A:661:LEU:HD13	1.53	0.74
1:A:469:ILE:O	1:A:473:PRO:HD2	1.87	0.74
1:A:143:GLU:HG3	1:A:147:LYS:HE2	1.69	0.73
1:A:342:ARG:HH11	1:A:342:ARG:HA	1.52	0.73
1:A:430:VAL:HG12	1:A:594:ASN:ND2	2.03	0.73
1:A:32:PRO:HB2	1:A:270:LEU:HB2	1.69	0.73
1:A:229:LEU:HB2	1:A:237:LYS:O	1.89	0.73
1:A:429:PRO:HA	1:A:652:GLN:HE22	1.53	0.73
1:A:429:PRO:HA	1:A:652:GLN:NE2	2.04	0.72
1:A:145:LEU:HD23	1:A:145:LEU:C	2.14	0.72
1:A:133:ARG:HB3	1:A:134:PRO:HD3	1.72	0.72
1:A:293:ALA:O	1:A:294:GLY:C	2.27	0.71
1:A:119:LEU:HD23	1:A:120:GLY:N	2.05	0.71
1:A:383:LEU:HD22	1:A:388:GLU:HB3	1.70	0.71
1:A:460:ALA:HA	1:A:493:PRO:HD2	1.73	0.71
1:A:376:THR:OG1	1:A:377:THR:N	2.18	0.70
1:A:343:ALA:O	1:A:606:HIS:CE1	2.43	0.70
1:A:518:ASN:HD22	1:A:519:SER:N	1.88	0.70
1:A:334:THR:C	1:A:336:ALA:H	1.99	0.70
1:A:133:ARG:HB3	1:A:134:PRO:CD	2.22	0.70
1:A:530:PHE:HB2	1:A:547:THR:HG22	1.74	0.70
1:A:447:THR:HG23	1:A:450:SER:HB3	1.73	0.70
1:A:352:SER:O	1:A:356:LEU:HG	1.92	0.70
1:A:582:THR:HG22	1:A:583:GLU:HG3	1.73	0.69
1:A:67:ALA:HB1	1:A:74:LEU:HD12	1.75	0.69
1:A:560:TRP:CZ3	1:A:561:ALA:HB2	2.27	0.69
1:A:16:SER:CB	1:A:38:LYS:HG2	2.21	0.69
1:A:530:PHE:HB2	1:A:547:THR:CG2	2.23	0.69
1:A:107:ASN:OD1	1:A:234:ASN:ND2	2.26	0.68
1:A:233:ASN:O	1:A:234:ASN:CB	2.31	0.68
1:A:242:PHE:O	1:A:246:HIS:HB3	1.92	0.68
1:A:160:CYS:HA	1:A:183:CYS:HB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:ALA:CB	1:A:543:VAL:HG13	2.23	0.68
1:A:219:PRO:C	1:A:220:ALA:O	2.34	0.68
1:A:476:LYS:HD2	1:A:667:THR:HG21	1.75	0.68
1:A:119:LEU:HD23	1:A:120:GLY:H	1.55	0.68
1:A:518:ASN:ND2	1:A:519:SER:H	1.90	0.67
1:A:334:THR:C	1:A:336:ALA:N	2.50	0.67
1:A:434:LEU:HG	1:A:591:VAL:HG22	1.76	0.67
1:A:445:LYS:O	1:A:446:ILE:HB	1.91	0.67
1:A:295:GLN:OE1	1:A:295:GLN:HA	1.94	0.67
1:A:23:GLN:OE1	1:A:35:THR:HG22	1.95	0.67
1:A:499:SER:HB2	1:A:500:LYS:HE2	1.77	0.67
1:A:136:LEU:O	1:A:137:ASP:HB2	1.94	0.66
1:A:346:VAL:HA	1:A:370:VAL:HG23	1.76	0.66
1:A:433:TYR:CD2	1:A:544:LYS:HB3	2.30	0.66
1:A:358:CYS:HB3	1:A:371:CYS:SG	2.36	0.66
1:A:469:ILE:HG21	1:A:590:PRO:HD2	1.76	0.66
1:A:159:PRO:O	1:A:161:VAL:N	2.29	0.66
1:A:559:GLN:N	1:A:562:LYS:HG3	2.11	0.66
1:A:311:PRO:HB2	1:A:314:ILE:HD12	1.78	0.65
1:A:334:THR:O	1:A:335:ALA:C	2.36	0.65
1:A:122:SER:O	1:A:127:ILE:N	2.23	0.65
1:A:101:GLY:O	1:A:102:THR:C	2.39	0.65
1:A:660:TYR:CD2	1:A:661:LEU:HD13	2.32	0.65
1:A:156:SER:HA	1:A:172:LEU:HD12	1.78	0.64
1:A:523:LEU:HG	1:A:532:CYS:HB3	1.80	0.64
1:A:436:VAL:HG11	1:A:545:ASP:HB3	1.78	0.64
1:A:522:ARG:HD3	1:A:531:ARG:NH1	2.13	0.64
1:A:637:LYS:NZ	1:A:639:LEU:HD21	2.12	0.64
1:A:168:ASN:CA	1:A:171:GLN:HB2	2.20	0.64
1:A:526:TYR:HD2	1:A:543:VAL:HG12	1.61	0.64
1:A:359:GLN:O	1:A:363:ARG:HG3	1.97	0.63
1:A:448:TRP:O	1:A:449:ASN:HB2	1.97	0.63
1:A:84:THR:HG23	1:A:87:GLN:H	1.64	0.63
1:A:145:LEU:C	1:A:145:LEU:CD2	2.71	0.63
1:A:484:ASP:HB2	1:A:500:LYS:CD	2.29	0.63
1:A:27:LYS:HD3	4:A:834:HOH:O	1.99	0.62
1:A:275:GLN:NE2	1:A:307:LEU:HB2	2.15	0.62
1:A:119:LEU:HD12	1:A:161:VAL:HA	1.82	0.62
1:A:467:TRP:HD1	1:A:468:ASN:HD22	1.48	0.62
1:A:77:ILE:HD12	1:A:257:ALA:HB3	1.82	0.61
1:A:507:GLY:CA	1:A:514:LYS:HG2	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:ALA:HB3	1:A:543:VAL:HG13	1.83	0.61
1:A:317:GLY:HA2	1:A:325:ILE:HD11	1.81	0.61
1:A:473:PRO:HD3	1:A:668:ALA:CA	2.31	0.61
1:A:471:MET:O	1:A:475:PHE:HB2	2.01	0.61
1:A:162:ASP:C	1:A:164:LYS:H	2.08	0.61
1:A:418:PRO:HD3	1:A:644:ASN:HB2	1.82	0.61
1:A:92:TYR:CB	1:A:92:TYR:C	2.71	0.60
1:A:500:LYS:HE2	1:A:500:LYS:H	1.67	0.60
1:A:157:CYS:SG	1:A:159:PRO:HD3	2.41	0.60
1:A:413:GLU:HB2	1:A:595:HIS:O	2.01	0.60
1:A:30:ARG:NH2	1:A:31:GLY:O	2.34	0.60
1:A:282:LYS:HE3	1:A:282:LYS:HA	1.83	0.60
1:A:339:GLU:HA	1:A:342:ARG:HB2	1.82	0.60
1:A:400:TYR:O	1:A:401:ILE:C	2.44	0.60
1:A:600:ARG:HB3	1:A:602:ASP:OD2	2.01	0.60
1:A:125:TRP:O	1:A:129:MET:HB2	2.02	0.59
1:A:562:LYS:O	1:A:563:ASP:C	2.45	0.59
1:A:573:CYS:HB3	1:A:577:THR:O	2.02	0.59
1:A:593:PRO:HG3	1:A:661:LEU:HA	1.84	0.59
1:A:358:CYS:CB	1:A:371:CYS:SG	2.90	0.59
1:A:144:PRO:HG2	1:A:147:LYS:HD2	1.84	0.59
1:A:332:ARG:CG	1:A:332:ARG:O	2.47	0.59
1:A:513:LEU:HD13	1:A:516:VAL:HG11	1.85	0.59
1:A:548:VAL:HG21	1:A:581:VAL:HG11	1.85	0.59
1:A:92:TYR:CB	1:A:92:TYR:N	2.64	0.58
1:A:657:TYR:O	1:A:661:LEU:HD22	2.03	0.58
1:A:113:LYS:HB3	1:A:172:LEU:HD11	1.86	0.58
1:A:119:LEU:CD2	1:A:120:GLY:N	2.66	0.58
1:A:344:GLN:NE2	4:A:726:HOH:O	2.35	0.58
1:A:529:ALA:HB3	1:A:543:VAL:CG1	2.34	0.58
1:A:129:MET:HE2	1:A:149:VAL:CG2	2.28	0.58
1:A:588:HIS:ND1	1:A:589:LEU:O	2.37	0.58
1:A:99:LYS:HE3	1:A:226:GLN:O	2.04	0.57
1:A:384:VAL:HA	1:A:389:ALA:O	2.04	0.57
1:A:434:LEU:O	1:A:436:VAL:HG13	2.05	0.57
1:A:544:LYS:HD2	1:A:546:VAL:HG23	1.85	0.57
1:A:42:ARG:NH2	4:A:709:HOH:O	2.32	0.57
1:A:159:PRO:O	1:A:160:CYS:C	2.45	0.57
1:A:473:PRO:HD3	1:A:668:ALA:HA	1.86	0.57
1:A:385:LEU:HD21	1:A:405:CYS:HB3	1.86	0.57
1:A:513:LEU:HD22	1:A:516:VAL:HG21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LEU:HD12	1:A:236:ARG:HD2	1.87	0.56
1:A:15:GLU:HG3	1:A:299:LEU:HD23	1.86	0.56
1:A:408:VAL:O	1:A:598:VAL:HA	2.04	0.56
1:A:499:SER:CB	1:A:500:LYS:HE2	2.36	0.56
1:A:637:LYS:HG3	1:A:639:LEU:HG	1.86	0.56
1:A:433:TYR:CE2	1:A:544:LYS:HB3	2.40	0.56
1:A:219:PRO:O	1:A:220:ALA:C	2.48	0.56
1:A:526:TYR:N	1:A:526:TYR:CB	2.68	0.56
1:A:529:ALA:HB1	1:A:543:VAL:HG13	1.88	0.56
1:A:45:CYS:O	1:A:49:ILE:HG13	2.06	0.56
1:A:619:GLY:O	1:A:622:GLY:N	2.35	0.56
1:A:144:PRO:HG2	1:A:147:LYS:CD	2.36	0.56
1:A:615:GLN:O	1:A:619:GLY:N	2.38	0.55
1:A:229:LEU:HD22	1:A:238:PRO:O	2.06	0.55
1:A:448:TRP:O	1:A:449:ASN:CB	2.52	0.55
1:A:665:TYR:CE2	1:A:669:ILE:HD11	2.41	0.55
1:A:113:LYS:HA	1:A:155:ALA:O	2.07	0.55
1:A:133:ARG:CB	1:A:134:PRO:CD	2.84	0.55
1:A:656:THR:HB	1:A:659:GLU:HB3	1.88	0.55
1:A:65:TYR:HB2	1:A:320:LEU:HD11	1.87	0.55
1:A:158:VAL:O	1:A:159:PRO:O	2.25	0.55
1:A:678:SER:O	1:A:681:LEU:HB3	2.07	0.54
1:A:452:ARG:HA	1:A:486:PHE:O	2.08	0.54
1:A:463:ARG:HG2	1:A:463:ARG:NH1	2.00	0.54
1:A:469:ILE:HG21	1:A:590:PRO:CD	2.36	0.54
1:A:133:ARG:HD2	1:A:133:ARG:O	2.08	0.54
1:A:556:GLY:HA3	1:A:561:ALA:HB3	1.90	0.54
1:A:17:LYS:HE3	1:A:292:PRO:HG2	1.90	0.53
1:A:147:LYS:O	1:A:151:LYS:HD3	2.08	0.53
1:A:410:VAL:HG11	1:A:607:LEU:CD2	2.33	0.53
1:A:665:TYR:O	1:A:669:ILE:HG12	2.09	0.53
1:A:395:ASP:O	1:A:399:ILE:CG1	2.55	0.53
1:A:456:SER:OG	1:A:490:SER:HB3	2.09	0.53
1:A:476:LYS:NZ	4:A:898:HOH:O	2.41	0.53
1:A:160:CYS:CB	1:A:183:CYS:HG	2.21	0.53
1:A:324:TYR:CE2	1:A:328:ILE:HD11	2.43	0.53
1:A:429:PRO:CA	1:A:652:GLN:HE22	2.19	0.53
1:A:197:LYS:O	1:A:198:CYS:C	2.48	0.53
1:A:460:ALA:HA	1:A:493:PRO:HG2	1.89	0.53
1:A:448:TRP:CH2	1:A:474:LEU:HD13	2.44	0.53
1:A:358:CYS:CB	1:A:371:CYS:HG	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:LEU:CD1	1:A:423:LEU:C	2.58	0.52
1:A:97:ILE:HG22	1:A:98:ALA:H	1.75	0.52
1:A:353:ASP:HB2	1:A:639:LEU:CD1	2.40	0.52
1:A:434:LEU:HD23	1:A:588:HIS:CG	2.44	0.52
1:A:549:LEU:HB3	1:A:566:LEU:HD13	1.90	0.52
1:A:344:GLN:HG3	1:A:370:VAL:HG22	1.92	0.52
1:A:144:PRO:O	1:A:145:LEU:C	2.53	0.52
1:A:358:CYS:O	1:A:362:SER:HB2	2.09	0.52
1:A:298:LEU:O	1:A:299:LEU:HB2	2.10	0.52
1:A:399:ILE:HG22	1:A:661:LEU:HD21	1.92	0.52
1:A:544:LYS:HD2	1:A:546:VAL:CG2	2.40	0.52
1:A:455:LYS:HB2	1:A:539:ASP:H	1.74	0.51
1:A:430:VAL:CG1	1:A:594:ASN:ND2	2.62	0.51
1:A:552:THR:HA	1:A:564:LEU:HD12	1.91	0.51
1:A:329:ARG:O	1:A:333:GLU:HG3	2.10	0.51
1:A:14:ALA:CA	1:A:17:LYS:HD3	2.38	0.51
1:A:241:ALA:O	1:A:245:CYS:HB3	2.11	0.51
1:A:525:GLY:C	1:A:526:TYR:CA	2.80	0.51
1:A:556:GLY:HA3	1:A:561:ALA:CB	2.41	0.51
1:A:625:CYS:HB3	1:A:626:PRO:CD	2.40	0.51
1:A:457:CYS:SG	1:A:538:GLY:HA3	2.51	0.51
1:A:560:TRP:CE3	1:A:561:ALA:HB2	2.46	0.51
1:A:460:ALA:HA	1:A:493:PRO:CD	2.40	0.50
1:A:182:ALA:H	1:A:187:GLU:HB2	1.75	0.50
1:A:332:ARG:O	1:A:332:ARG:HG2	2.10	0.50
1:A:133:ARG:CB	1:A:134:PRO:HD3	2.41	0.50
1:A:473:PRO:HA	1:A:476:LYS:HD3	1.92	0.50
1:A:636:THR:O	1:A:637:LYS:CB	2.59	0.50
1:A:635:LYS:O	1:A:637:LYS:HG2	2.11	0.50
1:A:5:SER:HB3	1:A:33:SER:OG	2.12	0.50
1:A:68:GLY:HA3	1:A:316:SER:HB2	1.94	0.50
1:A:356:LEU:HA	1:A:359:GLN:HG3	1.94	0.50
1:A:59:LEU:HD11	1:A:256:VAL:HG21	1.94	0.50
1:A:489:GLN:HG2	1:A:503:ALA:HB3	1.94	0.49
1:A:506:ALA:HB3	1:A:521:GLU:OE1	2.12	0.49
1:A:509:GLU:OE2	1:A:522:ARG:NH2	2.45	0.49
1:A:625:CYS:HB3	1:A:626:PRO:HD3	1.94	0.49
1:A:440:ARG:NH1	1:A:534:ALA:O	2.43	0.49
1:A:5:SER:O	1:A:263:LYS:NZ	2.38	0.49
1:A:411:LEU:HD23	1:A:650:LYS:HA	1.92	0.49
1:A:688:MET:SD	1:A:688:MET:N	2.86	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:PRO:HB2	1:A:319:TYR:CE2	2.48	0.49
1:A:475:PHE:HB3	1:A:671:LYS:HE2	1.95	0.49
1:A:353:ASP:HB2	1:A:639:LEU:HD11	1.95	0.49
1:A:476:LYS:CD	1:A:667:THR:HG21	2.42	0.49
1:A:607:LEU:O	1:A:608:ARG:C	2.54	0.49
1:A:499:SER:OG	1:A:501:LEU:HB2	2.13	0.49
1:A:416:GLN:O	1:A:417:SER:HB2	2.12	0.48
1:A:352:SER:HA	1:A:355:GLN:HB2	1.95	0.48
1:A:469:ILE:HD13	1:A:590:PRO:CG	2.37	0.48
1:A:92:TYR:CA	1:A:92:TYR:CG	2.85	0.48
1:A:357:LYS:NZ	1:A:639:LEU:O	2.37	0.48
1:A:78:ALA:HA	1:A:308:LEU:O	2.13	0.48
1:A:365:SER:O	1:A:366:ASN:HB2	2.12	0.48
1:A:402:ALA:O	1:A:407:LEU:HB2	2.14	0.48
1:A:429:PRO:CA	1:A:652:GLN:NE2	2.76	0.48
1:A:77:ILE:CD1	1:A:257:ALA:HB3	2.42	0.48
1:A:433:TYR:CE2	1:A:544:LYS:HG2	2.49	0.48
1:A:470:PRO:O	1:A:474:LEU:HB2	2.13	0.48
1:A:445:LYS:HE2	1:A:454:LYS:CE	2.44	0.48
1:A:102:THR:HG1	1:A:236:ARG:HH22	1.61	0.48
1:A:138:TRP:HH2	1:A:331:LEU:O	1.96	0.48
1:A:611:LEU:O	1:A:615:GLN:HB3	2.14	0.48
1:A:374:ALA:HB3	1:A:380:CYS:SG	2.54	0.47
1:A:615:GLN:NE2	1:A:648:LEU:H	2.07	0.47
1:A:160:CYS:CB	1:A:183:CYS:SG	3.03	0.47
1:A:516:VAL:O	1:A:521:GLU:HB3	2.14	0.47
1:A:100:LYS:HE2	1:A:225:ASP:O	2.14	0.47
1:A:452:ARG:HG2	4:A:862:HOH:O	2.14	0.47
1:A:17:LYS:HG2	1:A:18:LYS:N	2.28	0.47
1:A:258:ARG:O	1:A:262:GLY:HA3	2.14	0.47
1:A:526:TYR:HB3	1:A:547:THR:OG1	2.13	0.47
1:A:93:TYR:HB3	1:A:246:HIS:HB2	1.97	0.47
1:A:455:LYS:HB2	1:A:538:GLY:HA2	1.97	0.47
1:A:459:THR:HB	1:A:466:GLY:HA3	1.96	0.47
1:A:608:ARG:HE	1:A:650:LYS:NZ	2.13	0.47
1:A:634:SER:CB	1:A:639:LEU:H	2.28	0.47
1:A:93:TYR:CD2	1:A:93:TYR:N	2.81	0.47
1:A:133:ARG:HG2	1:A:133:ARG:HH11	1.80	0.47
1:A:463:ARG:NH1	1:A:463:ARG:CG	2.75	0.47
1:A:552:THR:HG21	1:A:566:LEU:HA	1.97	0.47
1:A:54:ALA:O	1:A:258:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ASN:CG	1:A:234:ASN:HD21	2.22	0.47
1:A:473:PRO:HD3	1:A:668:ALA:HB2	1.97	0.47
1:A:526:TYR:O	1:A:543:VAL:HG11	2.15	0.47
1:A:129:MET:HG3	1:A:149:VAL:HG21	1.97	0.46
1:A:260:VAL:O	1:A:261:ASN:C	2.57	0.46
1:A:665:TYR:CZ	1:A:669:ILE:HD11	2.51	0.46
1:A:122:SER:O	1:A:127:ILE:HG12	2.15	0.46
1:A:634:SER:HB2	1:A:639:LEU:H	1.79	0.46
1:A:496:ASP:OD2	1:A:498:ARG:HG3	2.15	0.46
1:A:258:ARG:HG3	1:A:260:VAL:O	2.16	0.46
1:A:271:LEU:O	1:A:275:GLN:HB2	2.14	0.46
1:A:434:LEU:HD23	1:A:588:HIS:ND1	2.30	0.46
1:A:10:THR:HA	1:A:15:GLU:HG2	1.98	0.46
1:A:49:ILE:HD11	1:A:57:VAL:HG12	1.97	0.46
1:A:268:TRP:O	1:A:272:VAL:HG23	2.16	0.46
1:A:505:CYS:HB3	1:A:521:GLU:OE2	2.15	0.46
1:A:162:ASP:OD1	1:A:164:LYS:HB2	2.15	0.46
1:A:417:SER:O	1:A:419:GLU:N	2.48	0.46
1:A:526:TYR:N	1:A:526:TYR:CG	2.84	0.46
1:A:433:TYR:HD2	1:A:544:LYS:HB3	1.77	0.46
1:A:293:ALA:O	1:A:295:GLN:N	2.48	0.46
1:A:296:LYS:HA	1:A:296:LYS:HD3	1.53	0.46
1:A:412:ALA:HB2	1:A:651:LEU:CD1	2.46	0.46
1:A:424:ASP:O	1:A:428:ARG:NE	2.48	0.46
1:A:127:ILE:HG21	1:A:248:ALA:HB3	1.97	0.45
1:A:147:LYS:HA	1:A:150:ALA:HB3	1.97	0.45
1:A:157:CYS:C	1:A:159:PRO:HD3	2.41	0.45
1:A:17:LYS:CE	1:A:292:PRO:HG2	2.45	0.45
1:A:348:CYS:N	1:A:391:ALA:O	2.46	0.45
1:A:279:GLY:O	1:A:282:LYS:HB2	2.16	0.45
1:A:75:ARG:O	1:A:256:VAL:HA	2.16	0.45
1:A:603:LYS:HE3	1:A:606:HIS:HD2	1.80	0.45
1:A:418:PRO:HD3	1:A:644:ASN:CB	2.45	0.45
1:A:43:PHE:O	1:A:47:GLN:HG3	2.17	0.45
1:A:424:ASP:O	1:A:428:ARG:NH2	2.46	0.45
1:A:471:MET:HE3	1:A:483:PHE:HB3	1.98	0.45
1:A:228:GLU:HB3	1:A:236:ARG:HB3	1.99	0.45
1:A:489:GLN:NE2	1:A:503:ALA:CB	2.80	0.45
1:A:75:ARG:NH1	1:A:314:ILE:O	2.49	0.45
1:A:356:LEU:HG	1:A:356:LEU:H	1.53	0.45
1:A:478:THR:OG1	1:A:479:ASP:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:VAL:CG2	1:A:581:VAL:HG11	2.46	0.45
1:A:128:PRO:O	1:A:132:LEU:HD12	2.17	0.44
1:A:528:GLY:HA2	1:A:531:ARG:HB3	1.99	0.44
1:A:637:LYS:HG3	1:A:639:LEU:CG	2.46	0.44
1:A:473:PRO:HD3	1:A:668:ALA:CB	2.48	0.44
1:A:196:PHE:CZ	1:A:214:VAL:HG13	2.52	0.44
1:A:385:LEU:HD21	1:A:405:CYS:CB	2.46	0.44
1:A:625:CYS:CB	1:A:626:PRO:CD	2.95	0.44
1:A:658:ASP:HB3	1:A:666:VAL:HG21	1.98	0.44
1:A:15:GLU:HG3	1:A:299:LEU:CD2	2.47	0.44
1:A:160:CYS:HB3	1:A:183:CYS:SG	2.58	0.44
1:A:31:GLY:HA2	1:A:273:LYS:HD2	2.00	0.44
1:A:67:ALA:HB1	1:A:74:LEU:CD1	2.44	0.44
1:A:589:LEU:HB3	1:A:590:PRO:CD	2.42	0.44
1:A:637:LYS:HB2	1:A:637:LYS:HE2	1.81	0.44
1:A:310:ILE:O	1:A:311:PRO:C	2.61	0.44
1:A:374:ALA:HB1	1:A:379:ASP:HB2	1.99	0.44
1:A:471:MET:HB3	1:A:483:PHE:CE2	2.52	0.44
1:A:325:ILE:O	1:A:329:ARG:HG3	2.18	0.43
1:A:438:VAL:CG2	1:A:439:VAL:N	2.81	0.43
1:A:15:GLU:OE1	1:A:299:LEU:N	2.38	0.43
1:A:103:ASN:OD1	1:A:103:ASN:N	2.52	0.43
1:A:344:GLN:O	1:A:344:GLN:HG2	2.16	0.43
1:A:364:GLN:CG	1:A:629:PHE:HB2	2.34	0.43
1:A:448:TRP:CZ2	1:A:474:LEU:HD13	2.54	0.43
1:A:380:CYS:CB	1:A:392:LEU:HD22	2.42	0.43
1:A:125:TRP:CZ3	1:A:149:VAL:HG11	2.53	0.43
1:A:361:TRP:HZ2	1:A:614:GLN:HG3	1.83	0.43
1:A:555:LYS:HE3	1:A:555:LYS:HB2	1.78	0.43
1:A:129:MET:CE	1:A:149:VAL:HG22	2.32	0.43
1:A:353:ASP:HA	1:A:356:LEU:HG	2.00	0.43
1:A:435:ALA:O	1:A:588:HIS:HB2	2.19	0.43
1:A:599:SER:OG	1:A:600:ARG:N	2.48	0.43
1:A:556:GLY:CA	1:A:561:ALA:HB3	2.48	0.43
1:A:157:CYS:O	1:A:159:PRO:HD3	2.18	0.43
1:A:453:GLY:O	1:A:488:SER:HB2	2.18	0.43
1:A:101:GLY:O	1:A:102:THR:O	2.37	0.43
1:A:168:ASN:C	1:A:171:GLN:H	2.26	0.43
1:A:278:PHE:HA	1:A:282:LYS:HG2	2.01	0.43
1:A:136:LEU:HA	1:A:136:LEU:HD23	1.74	0.43
1:A:400:TYR:HD1	1:A:657:TYR:HE2	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:TRP:O	1:A:26:MET:HB2	2.19	0.43
1:A:179:ASN:HA	1:A:182:ALA:HB2	2.00	0.43
1:A:441:LYS:O	1:A:441:LYS:HG2	2.18	0.43
1:A:469:ILE:HA	1:A:668:ALA:HB1	2.00	0.43
1:A:543:VAL:HG21	1:A:547:THR:CG2	2.49	0.43
1:A:601:ILE:HD12	1:A:604:VAL:HG11	2.01	0.43
1:A:618:PHE:O	1:A:631:LEU:HB2	2.18	0.43
1:A:117:THR:OG1	1:A:124:GLY:HA3	2.19	0.42
1:A:489:GLN:NE2	1:A:503:ALA:HB1	2.34	0.42
1:A:621:ASN:O	1:A:622:GLY:C	2.61	0.42
1:A:32:PRO:HG2	1:A:270:LEU:HA	2.01	0.42
1:A:113:LYS:HD2	1:A:203:ALA:O	2.18	0.42
1:A:473:PRO:HA	1:A:476:LYS:HB3	2.01	0.42
1:A:662:GLY:O	1:A:665:TYR:HB3	2.19	0.42
1:A:24:ARG:HD3	1:A:24:ARG:HA	1.80	0.42
1:A:118:GLY:HA2	1:A:159:PRO:HB2	2.01	0.42
1:A:143:GLU:HA	1:A:144:PRO:HD2	1.80	0.42
1:A:173:CYS:HB3	1:A:187:GLU:CD	2.44	0.42
1:A:614:GLN:NE2	1:A:614:GLN:HA	2.34	0.42
1:A:182:ALA:N	1:A:187:GLU:HB2	2.34	0.42
1:A:229:LEU:O	1:A:236:ARG:HA	2.19	0.42
1:A:508:ASN:HD22	1:A:512:GLN:HB2	1.83	0.42
1:A:562:LYS:H	1:A:562:LYS:HG2	1.57	0.42
1:A:402:ALA:HB1	1:A:598:VAL:HG11	2.00	0.42
1:A:472:GLY:CA	1:A:668:ALA:HA	2.43	0.42
1:A:582:THR:HG22	1:A:583:GLU:H	1.84	0.42
1:A:84:THR:OG1	1:A:85:GLU:N	2.53	0.42
1:A:97:ILE:O	1:A:206:VAL:CG1	2.58	0.42
1:A:506:ALA:HB2	1:A:523:LEU:HD13	2.01	0.42
1:A:26:MET:HG3	1:A:32:PRO:O	2.19	0.42
1:A:526:TYR:HA	1:A:543:VAL:HG12	2.01	0.42
1:A:23:GLN:OE1	1:A:35:THR:HA	2.20	0.42
1:A:352:SER:O	1:A:355:GLN:CB	2.52	0.42
1:A:291:SER:HB3	1:A:295:GLN:O	2.20	0.42
1:A:399:ILE:O	1:A:403:GLY:N	2.46	0.42
1:A:455:LYS:HG2	1:A:539:ASP:OD2	2.19	0.42
1:A:651:LEU:O	1:A:654:LYS:HB2	2.19	0.42
1:A:13:PRO:O	1:A:17:LYS:N	2.49	0.42
1:A:121:ARG:HD3	1:A:121:ARG:HA	1.72	0.42
1:A:416:GLN:OE1	1:A:620:ARG:NH2	2.52	0.42
1:A:469:ILE:HG21	1:A:590:PRO:CG	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:LEU:O	1:A:70:ASP:C	2.62	0.41
1:A:165:GLU:HB2	1:A:166:TYR:CD1	2.54	0.41
1:A:453:GLY:O	1:A:488:SER:CB	2.68	0.41
1:A:49:ILE:CD1	1:A:57:VAL:HG12	2.50	0.41
1:A:123:ALA:HB3	1:A:192:TYR:OH	2.20	0.41
1:A:447:THR:CG2	1:A:450:SER:HB3	2.47	0.41
1:A:260:VAL:HG12	1:A:261:ASN:HB2	2.03	0.41
1:A:460:ALA:HA	1:A:493:PRO:CG	2.50	0.41
1:A:522:ARG:HD3	1:A:531:ARG:HH12	1.81	0.41
1:A:104:PHE:HZ	1:A:205:ASP:O	2.04	0.41
1:A:214:VAL:CG1	1:A:218:LEU:HD12	2.51	0.41
1:A:412:ALA:O	1:A:648:LEU:HA	2.21	0.41
1:A:418:PRO:HG3	1:A:644:ASN:ND2	2.35	0.41
1:A:99:LYS:O	1:A:236:ARG:NH2	2.55	0.41
1:A:543:VAL:HG21	1:A:547:THR:HG21	2.03	0.41
1:A:104:PHE:CD1	1:A:112:LEU:HD11	2.56	0.40
1:A:11:THR:H	1:A:15:GLU:HG2	1.86	0.40
1:A:360:GLU:O	1:A:364:GLN:HB2	2.20	0.40
1:A:667:THR:O	1:A:668:ALA:C	2.64	0.40
1:A:6:VAL:HG23	1:A:266:LEU:HG	2.03	0.40
1:A:358:CYS:HB2	1:A:640:LEU:HD11	2.02	0.40
1:A:110:GLN:HB3	4:A:838:HOH:O	2.22	0.40
1:A:143:GLU:CG	1:A:147:LYS:HE2	2.44	0.40
1:A:353:ASP:HA	1:A:356:LEU:CD1	2.51	0.40
1:A:467:TRP:HD1	1:A:468:ASN:ND2	2.18	0.40
1:A:636:THR:O	1:A:637:LYS:HB3	2.21	0.40
1:A:102:THR:HB	1:A:104:PHE:CE1	2.56	0.40
1:A:113:LYS:HD3	1:A:172:LEU:HD21	2.03	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	687/689 (100%)	562 (82%)	89 (13%)	36 (5%)	1 3

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	ARG
1	A	159	PRO
1	A	160	CYS
1	A	220	ALA
1	A	335	ALA
1	A	418	PRO
1	A	429	PRO
1	A	446	ILE
1	A	513	LEU
1	A	604	VAL
1	A	154	SER
1	A	234	ASN
1	A	454	LYS
1	A	547	THR
1	A	571	LEU
1	A	624	ASP
1	A	637	LYS
1	A	650	LYS
1	A	102	THR
1	A	137	ASP
1	A	292	PRO
1	A	311	PRO
1	A	472	GLY
1	A	563	ASP
1	A	133	ARG
1	A	417	SER
1	A	511	GLY
1	A	620	ARG
1	A	625	CYS
1	A	122	SER
1	A	551	ASN
1	A	559	GLN
1	A	589	LEU
1	A	209	VAL
1	A	161	VAL
1	A	32	PRO

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	570/570 (100%)	382 (67%)	188 (33%)	0 1

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	4	LYS
1	A	6	VAL
1	A	12	SER
1	A	15	GLU
1	A	16	SER
1	A	17	LYS
1	A	23	GLN
1	A	25	ARG
1	A	28	LYS
1	A	29	VAL
1	A	34	VAL
1	A	38	LYS
1	A	42	ARG
1	A	44	GLU
1	A	47	GLN
1	A	49	ILE
1	A	52	GLU
1	A	58	THR
1	A	59	LEU
1	A	69	LEU
1	A	70	ASP
1	A	74	LEU
1	A	75	ARG
1	A	97	ILE
1	A	99	LYS
1	A	110	GLN
1	A	112	LEU
1	A	121	ARG
1	A	122	SER

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Mol	Chain	Res	Type
1	A	126	ASN
1	A	129	MET
1	A	141	PRO
1	A	145	LEU
1	A	147	LYS
1	A	151	LYS
1	A	154	SER
1	A	158	VAL
1	A	160	CYS
1	A	161	VAL
1	A	164	LYS
1	A	165	GLU
1	A	166	TYR
1	A	185	SER
1	A	197	LYS
1	A	206	VAL
1	A	214	VAL
1	A	219	PRO
1	A	226	GLN
1	A	229	LEU
1	A	230	LEU
1	A	236	ARG
1	A	244	GLU
1	A	247	LEU
1	A	249	ARG
1	A	250	VAL
1	A	258	ARG
1	A	264	GLU
1	A	266	LEU
1	A	270	LEU
1	A	271	LEU
1	A	275	GLN
1	A	276	GLU
1	A	282	LYS
1	A	283	PRO
1	A	284	SER
1	A	291	SER
1	A	296	LYS
1	A	298	LEU
1	A	299	LEU
1	A	303	SER
1	A	305	LEU

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Mol	Chain	Res	Type
1	A	308	LEU
1	A	309	ARG
1	A	311	PRO
1	A	312	LYS
1	A	316	SER
1	A	318	LEU
1	A	329	ARG
1	A	332	ARG
1	A	334	THR
1	A	340	LEU
1	A	342	ARG
1	A	344	GLN
1	A	346	VAL
1	A	353	ASP
1	A	354	GLU
1	A	356	LEU
1	A	359	GLN
1	A	362	SER
1	A	364	GLN
1	A	368	SER
1	A	370	VAL
1	A	371	CYS
1	A	373	THR
1	A	376	THR
1	A	384	VAL
1	A	386	LYS
1	A	388	GLU
1	A	399	ILE
1	A	407	LEU
1	A	408	VAL
1	A	415	GLN
1	A	421	SER
1	A	423	LEU
1	A	424	ASP
1	A	425	CYS
1	A	430	VAL
1	A	433	TYR
1	A	438	VAL
1	A	439	VAL
1	A	444	ASP
1	A	445	LYS
1	A	446	ILE

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Mol	Chain	Res	Type
1	A	447	THR
1	A	452	ARG
1	A	459	THR
1	A	463	ARG
1	A	474	LEU
1	A	477	ASP
1	A	478	THR
1	A	480	SER
1	A	485	GLU
1	A	488	SER
1	A	490	SER
1	A	498	ARG
1	A	499	SER
1	A	500	LYS
1	A	504	LEU
1	A	505	CYS
1	A	510	GLU
1	A	514	LYS
1	A	516	VAL
1	A	518	ASN
1	A	520	SER
1	A	521	GLU
1	A	522	ARG
1	A	523	LEU
1	A	527	THR
1	A	543	VAL
1	A	544	LYS
1	A	546	VAL
1	A	550	ASP
1	A	555	LYS
1	A	557	THR
1	A	558	GLU
1	A	559	GLN
1	A	563	ASP
1	A	565	LYS
1	A	566	LEU
1	A	568	ASP
1	A	573	CYS
1	A	578	ARG
1	A	581	VAL
1	A	582	THR
1	A	583	GLU

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Mol	Chain	Res	Type
1	A	589	LEU
1	A	591	VAL
1	A	598	VAL
1	A	600	ARG
1	A	604	VAL
1	A	608	ARG
1	A	609	GLN
1	A	610	VAL
1	A	612	LEU
1	A	613	ARG
1	A	615	GLN
1	A	621	ASN
1	A	628	LYS
1	A	633	GLN
1	A	635	LYS
1	A	637	LYS
1	A	644	ASN
1	A	646	GLU
1	A	648	LEU
1	A	651	LEU
1	A	652	GLN
1	A	654	LYS
1	A	655	THR
1	A	658	ASP
1	A	661	LEU
1	A	669	ILE
1	A	673	ARG
1	A	674	ARG
1	A	677	THR
1	A	678	SER
1	A	682	GLU
1	A	689	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	47	GLN
1	A	108	GLN
1	A	126	ASN
1	A	226	GLN
1	A	234	ASN

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Mol	Chain	Res	Type
1	A	253	HIS
1	A	261	ASN
1	A	275	GLN
1	A	355	GLN
1	A	366	ASN
1	A	449	ASN
1	A	468	ASN
1	A	508	ASN
1	A	518	ASN
1	A	536	ASN
1	A	575	ASN
1	A	594	ASN
1	A	615	GLN
1	A	638	ASN
1	A	644	ASN
1	A	652	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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
3	CO3	A	693	2	3,3,3	0.86	0	2,3,3	2.96	2 (100%)
3	CO3	A	692	-	3,3,3	0.87	0	2,3,3	1.80	1 (50%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	693	CO3	O3-C-O1	-3.53	110.64	119.68
3	A	693	CO3	O2-C-O1	2.23	125.39	119.68
3	A	692	CO3	O3-C-O1	-2.02	114.50	119.68

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	569:PHE	C	570:GLU	N	0.94
1	A	572:LEU	C	573:CYS	N	0.93
1	A	430:VAL	C	431:LYS	N	0.55

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

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.