



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:29 PM UTC

PDB ID : 1LFH / pdb_00001lfh
Title : MOLECULAR REPLACEMENT SOLUTION OF THE STRUCTURE OF
APOLACTOFERRIN, A PROTEIN DISPLAYING LARGE-SCALE CON-
FORMATIONAL CHANGE
Authors : Anderson, B.F.; Baker, E.N.; Norris, G.E.
Deposited on : 1991-09-04
Resolution : 2.80 Å(reported)

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

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

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
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

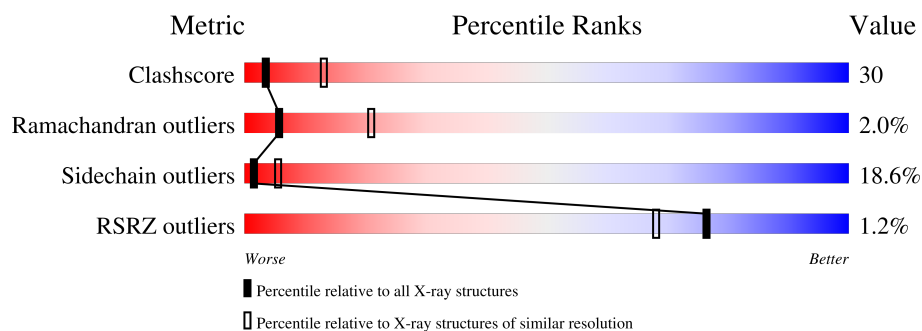
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	691	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5716 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	691	Total	C	N	O	S	0	0	0
			5342	3337	954	1014	37			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	ASN	GLN	conflict	UNP P02788
A	200	LYS	ARG	conflict	UNP P02788
A	512	GLU	GLN	conflict	UNP P02788

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		

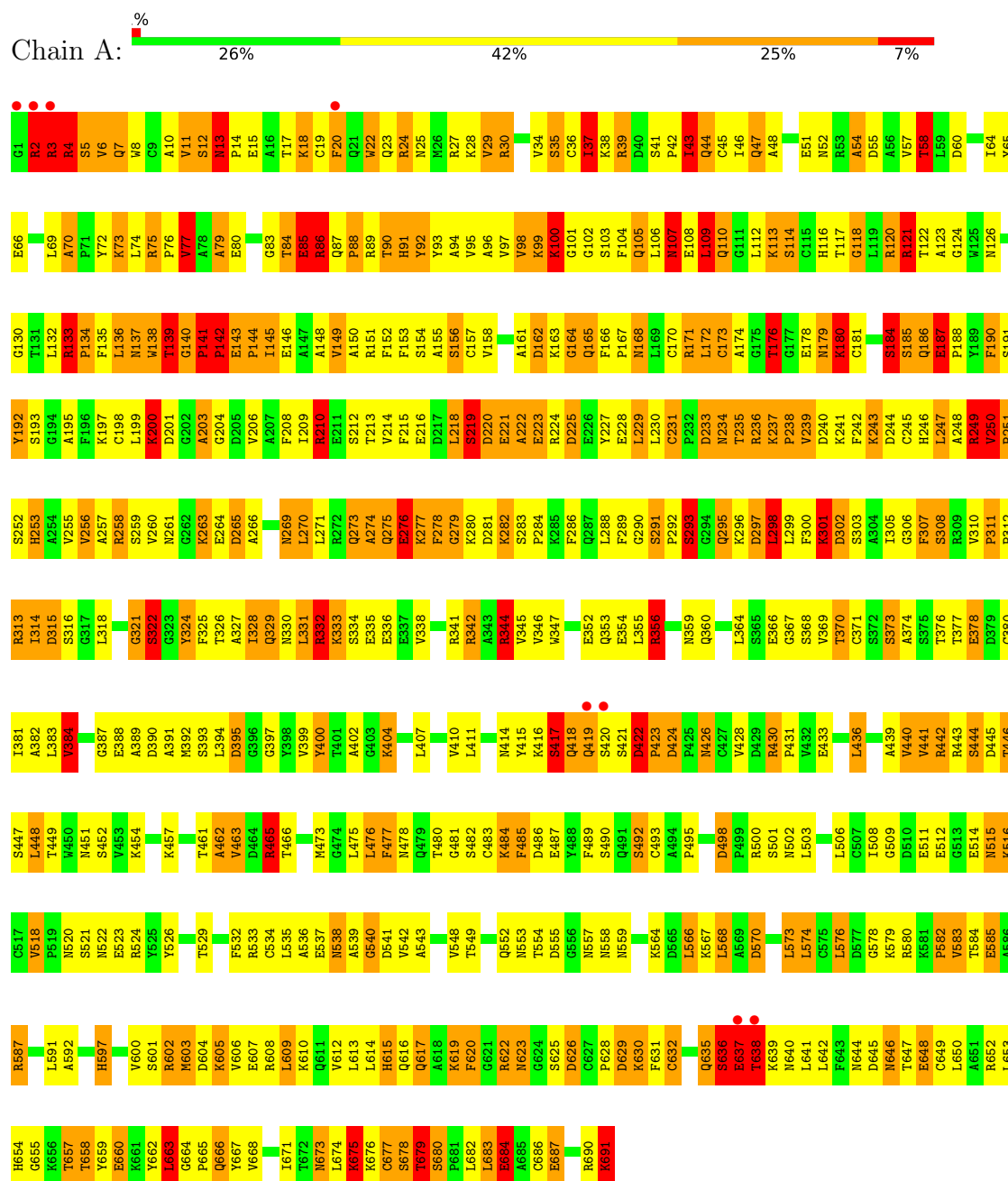
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	373	Total	O	0	0
			373	373		

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: LACTOFERRIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	152.09Å 94.58Å 55.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.80 80.32 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80) 86.4 (80.32-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.80Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.213 , (Not available) 0.190 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 72.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5716	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.19% 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: CL

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	1.17	5/5456 (0.1%)	3.02	679/7378 (9.2%)

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	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	58	THR	N-CA	5.72	1.52	1.46
1	A	321	GLY	N-CA	5.63	1.50	1.45
1	A	293	SER	C-O	5.40	1.30	1.24
1	A	37	ILE	N-CA	5.17	1.51	1.46
1	A	143	GLU	N-CA	-5.13	1.39	1.46

All (679) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	442	ARG	CD-NE-CZ	28.39	164.15	124.40
1	A	210	ARG	CD-NE-CZ	23.32	157.05	124.40
1	A	142	PRO	CA-C-N	22.80	177.43	121.80
1	A	142	PRO	C-N-CA	22.80	177.43	121.80
1	A	225	ASP	CA-CB-CG	21.31	133.91	112.60
1	A	250	VAL	CA-C-O	19.23	131.69	119.19
1	A	258	ARG	NE-CZ-NH2	-16.98	103.91	119.20
1	A	524	ARG	NE-CZ-NH1	-13.96	107.54	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	314	ILE	CA-C-N	13.57	149.35	122.07
1	A	314	ILE	C-N-CA	13.57	149.35	122.07
1	A	293	SER	CA-C-O	-13.06	101.83	120.51
1	A	687	GLU	CB-CG-CD	12.56	133.95	112.60
1	A	609	LEU	CA-C-O	-12.41	108.12	120.90
1	A	249	ARG	N-CA-CB	12.34	129.95	110.57
1	A	250	VAL	CB-CA-C	12.14	123.40	110.53
1	A	11	VAL	N-CA-CB	-12.02	98.99	112.21
1	A	482	SER	CA-C-O	11.57	133.88	120.69
1	A	41	SER	CA-C-O	-11.50	110.24	120.13
1	A	133	ARG	CD-NE-CZ	11.45	140.43	124.40
1	A	248	ALA	CA-C-O	-11.38	108.01	120.75
1	A	25	ASN	OD1-CG-ND2	11.30	133.90	122.60
1	A	557	ASN	CA-CB-CG	-11.18	101.42	112.60
1	A	258	ARG	NH1-CZ-NH2	10.94	133.53	119.30
1	A	41	SER	O-C-N	10.83	133.54	122.17
1	A	179	ASN	OD1-CG-ND2	10.75	133.35	122.60
1	A	249	ARG	CA-C-N	-10.74	113.16	123.04
1	A	249	ARG	C-N-CA	-10.74	113.16	123.04
1	A	393	SER	CA-C-O	-10.69	108.46	120.54
1	A	199	LEU	CA-C-O	10.58	131.87	120.55
1	A	314	ILE	O-C-N	-10.52	111.20	122.67
1	A	644	ASN	OD1-CG-ND2	10.44	133.04	122.60
1	A	356	ARG	CD-NE-CZ	10.42	138.99	124.40
1	A	376	THR	O-C-N	10.40	136.06	122.96
1	A	654	HIS	CA-CB-CG	-10.39	103.41	113.80
1	A	315	ASP	N-CA-CB	-10.29	93.99	110.46
1	A	428	VAL	CA-C-O	-10.27	107.60	120.03
1	A	37	ILE	CB-CA-C	10.22	127.57	110.30
1	A	395	ASP	CA-C-O	-10.15	110.70	121.87
1	A	619	LYS	CA-CB-CG	10.13	134.36	114.10
1	A	315	ASP	O-C-N	-10.06	111.67	122.94
1	A	223	GLU	CA-CB-CG	9.91	133.92	114.10
1	A	39	ARG	NE-CZ-NH1	9.88	131.38	121.50
1	A	52	ASN	OD1-CG-ND2	9.86	132.46	122.60
1	A	648	GLU	CA-C-O	9.80	131.12	120.24
1	A	236	ARG	CA-C-O	-9.79	109.71	121.06
1	A	493	CYS	N-CA-CB	9.74	126.75	110.87
1	A	549	THR	O-C-N	9.63	131.99	122.07
1	A	419	GLN	CA-C-O	-9.61	109.78	121.02
1	A	313	ARG	CG-CD-NE	9.51	132.93	112.00
1	A	606	VAL	N-CA-C	9.45	120.28	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	445	ASP	CA-C-N	9.42	134.63	120.31
1	A	445	ASP	C-N-CA	9.42	134.63	120.31
1	A	298	LEU	CA-C-O	-9.33	109.75	120.58
1	A	684	GLU	CA-C-N	9.33	133.13	120.54
1	A	684	GLU	C-N-CA	9.33	133.13	120.54
1	A	691	LYS	N-CA-CB	9.30	126.31	110.50
1	A	660	GLU	O-C-N	-9.28	112.51	122.07
1	A	58	THR	CB-CA-C	9.23	124.99	109.48
1	A	36	CYS	O-C-N	9.19	134.16	123.41
1	A	660	GLU	CA-C-O	9.15	130.43	120.82
1	A	626	ASP	CA-C-O	-9.13	108.88	119.56
1	A	502	ASN	CA-CB-CG	-9.10	103.50	112.60
1	A	657	THR	N-CA-C	9.02	122.76	112.57
1	A	625	SER	CA-C-O	-9.02	110.82	120.92
1	A	227	TYR	CA-CB-CG	-9.00	97.69	113.90
1	A	677	CYS	O-C-N	9.00	131.66	122.12
1	A	683	LEU	CA-C-O	8.98	130.07	120.55
1	A	88	PRO	CA-C-O	-8.96	111.86	121.27
1	A	157	CYS	N-CA-CB	8.92	125.41	110.69
1	A	673	ASN	OD1-CG-ND2	8.91	131.51	122.60
1	A	39	ARG	CA-C-O	-8.89	111.55	121.51
1	A	187	GLU	CA-CB-CG	8.82	131.75	114.10
1	A	423	PRO	CB-CA-C	-8.81	100.54	111.64
1	A	52	ASN	CA-CB-CG	-8.78	103.82	112.60
1	A	296	LYS	CA-C-N	8.73	138.21	121.54
1	A	296	LYS	C-N-CA	8.73	138.21	121.54
1	A	324	TYR	CA-C-O	-8.72	111.66	120.82
1	A	390	ASP	CA-CB-CG	8.72	121.32	112.60
1	A	57	VAL	CA-C-O	-8.71	113.64	120.96
1	A	210	ARG	NE-CZ-NH1	-8.70	112.80	121.50
1	A	486	ASP	CA-CB-CG	8.68	121.28	112.60
1	A	13	ASN	CA-CB-CG	8.65	121.25	112.60
1	A	190	PHE	CA-C-N	8.56	137.90	121.54
1	A	190	PHE	C-N-CA	8.56	137.90	121.54
1	A	660	GLU	CA-C-N	8.55	132.07	120.44
1	A	660	GLU	C-N-CA	8.55	132.07	120.44
1	A	602	ARG	NE-CZ-NH2	-8.53	111.52	119.20
1	A	626	ASP	O-C-N	8.44	132.47	122.34
1	A	366	GLU	CA-CB-CG	8.42	130.94	114.10
1	A	644	ASN	CA-CB-CG	-8.40	104.20	112.60
1	A	316	SER	CA-C-N	8.39	129.26	119.94
1	A	316	SER	C-N-CA	8.39	129.26	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	ARG	NH1-CZ-NH2	-8.37	108.42	119.30
1	A	660	GLU	CA-CB-CG	8.35	130.81	114.10
1	A	70	ALA	CA-C-O	-8.34	112.05	120.64
1	A	10	ALA	CA-C-O	8.32	129.69	120.70
1	A	154	SER	CA-C-O	8.31	129.07	119.18
1	A	265	ASP	CA-C-N	8.31	132.34	120.79
1	A	265	ASP	C-N-CA	8.31	132.34	120.79
1	A	420	SER	CA-C-O	-8.30	111.19	120.32
1	A	123	ALA	CA-C-O	-8.28	111.65	120.42
1	A	682	LEU	CA-C-O	-8.28	111.69	120.55
1	A	606	VAL	CA-C-O	-8.27	112.67	121.27
1	A	176	THR	CA-C-O	8.26	129.97	120.80
1	A	583	VAL	CA-C-O	-8.25	111.75	120.57
1	A	39	ARG	CD-NE-CZ	8.22	135.91	124.40
1	A	457	LYS	CA-C-O	-8.20	111.50	120.43
1	A	629	ASP	CA-CB-CG	-8.19	104.41	112.60
1	A	374	ALA	CA-C-O	8.15	130.17	121.45
1	A	25	ASN	CA-C-O	-8.14	109.37	119.38
1	A	430	ARG	CD-NE-CZ	-8.14	113.00	124.40
1	A	203	ALA	CA-C-N	-8.14	115.23	122.47
1	A	203	ALA	C-N-CA	-8.14	115.23	122.47
1	A	523	GLU	O-C-N	-8.11	112.28	122.82
1	A	70	ALA	N-CA-C	-8.09	98.43	110.24
1	A	46	ILE	O-C-N	8.07	130.14	121.83
1	A	36	CYS	CA-C-O	-8.06	110.63	120.54
1	A	249	ARG	CA-C-O	-8.04	111.62	120.38
1	A	168	ASN	O-C-N	8.00	131.57	122.22
1	A	482	SER	O-C-N	-7.99	113.69	123.04
1	A	342	ARG	CD-NE-CZ	-7.98	113.23	124.40
1	A	100	LYS	CA-C-O	7.97	129.40	120.80
1	A	158	VAL	O-C-N	7.97	130.18	121.10
1	A	359	ASN	CA-C-N	7.93	130.75	120.44
1	A	359	ASN	C-N-CA	7.93	130.75	120.44
1	A	387	GLY	CA-C-O	7.91	129.38	119.25
1	A	649	CYS	O-C-N	-7.90	115.39	123.29
1	A	580	ARG	CA-C-O	-7.88	111.85	120.36
1	A	79	ALA	CA-C-O	7.87	130.05	121.16
1	A	47	GLN	OE1-CD-NE2	7.87	130.47	122.60
1	A	37	ILE	CA-C-O	-7.86	113.85	121.63
1	A	605	LYS	CG-CD-CE	7.81	129.27	111.30
1	A	625	SER	CA-CB-OG	7.81	126.72	111.10
1	A	635	GLN	CA-C-O	7.81	129.64	120.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	311	PRO	CB-CA-C	7.78	120.41	110.92
1	A	45	CYS	CA-C-O	-7.78	112.18	120.42
1	A	610	LYS	CA-C-O	7.77	129.22	120.90
1	A	439	ALA	O-C-N	7.74	134.72	122.96
1	A	600	VAL	O-C-N	7.72	131.24	122.97
1	A	249	ARG	CA-CB-CG	7.72	129.54	114.10
1	A	251	PRO	CB-CA-C	7.72	121.25	110.60
1	A	650	LEU	CA-C-O	-7.71	112.05	120.92
1	A	559	ASN	N-CA-C	7.69	120.74	111.82
1	A	449	THR	CA-CB-OG1	-7.68	98.08	109.60
1	A	176	THR	CA-CB-CG2	7.66	123.52	110.50
1	A	511	GLU	O-C-N	7.66	130.93	122.20
1	A	104	PHE	N-CA-CB	7.66	123.15	110.52
1	A	19	CYS	O-C-N	7.63	129.93	122.07
1	A	354	GLU	N-CA-CB	7.63	122.10	110.28
1	A	37	ILE	N-CA-CB	-7.61	98.28	112.36
1	A	38	LYS	CA-C-O	-7.59	111.92	120.66
1	A	368	SER	N-CA-C	7.59	122.54	113.28
1	A	306	GLY	O-C-N	7.58	131.46	123.96
1	A	641	LEU	CA-C-O	-7.57	111.95	120.43
1	A	341	ARG	CA-C-O	-7.56	111.27	119.97
1	A	631	PHE	CA-C-O	-7.55	111.26	120.54
1	A	582	PRO	CA-C-O	7.55	131.74	122.08
1	A	151	ARG	CA-C-O	-7.54	110.15	119.28
1	A	580	ARG	CD-NE-CZ	7.54	134.96	124.40
1	A	77	VAL	CB-CA-C	7.54	118.04	110.65
1	A	102	GLY	N-CA-C	-7.53	96.45	110.83
1	A	314	ILE	CA-C-O	7.52	129.62	121.04
1	A	428	VAL	O-C-N	7.51	130.63	122.06
1	A	383	LEU	CA-C-O	-7.51	111.62	120.10
1	A	542	VAL	CA-C-N	7.49	133.56	122.99
1	A	542	VAL	C-N-CA	7.49	133.56	122.99
1	A	382	ALA	CA-C-O	-7.49	112.61	120.55
1	A	249	ARG	O-C-N	7.46	132.09	123.29
1	A	653	LEU	N-CA-CB	-7.46	99.57	110.53
1	A	295	GLN	N-CA-C	7.45	121.59	109.59
1	A	2	ARG	N-CA-C	7.45	121.10	107.99
1	A	411	LEU	O-C-N	7.44	132.17	123.17
1	A	485	PHE	CA-CB-CG	-7.39	106.41	113.80
1	A	622	ARG	CA-C-N	-7.38	111.22	123.33
1	A	622	ARG	C-N-CA	-7.38	111.22	123.33
1	A	206	VAL	CA-C-O	7.38	128.93	120.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	ARG	CA-CB-CG	7.37	128.85	114.10
1	A	404	LYS	N-CA-C	-7.37	103.25	111.28
1	A	162	ASP	CA-CB-CG	7.36	119.96	112.60
1	A	210	ARG	NE-CZ-NH2	7.36	125.82	119.20
1	A	239	VAL	CA-C-O	-7.36	112.70	120.57
1	A	461	THR	CA-CB-OG1	-7.36	98.57	109.60
1	A	637	GLU	CA-C-O	7.34	131.01	120.51
1	A	549	THR	CA-C-O	-7.34	113.11	120.82
1	A	143	GLU	N-CA-CB	7.34	123.43	110.37
1	A	332	ARG	CA-C-N	7.33	131.24	120.90
1	A	332	ARG	C-N-CA	7.33	131.24	120.90
1	A	332	ARG	CD-NE-CZ	7.33	134.66	124.40
1	A	151	ARG	N-CA-CB	7.32	121.65	110.44
1	A	463	VAL	CB-CA-C	7.31	121.72	111.63
1	A	587	ARG	CD-NE-CZ	-7.31	114.17	124.40
1	A	677	CYS	CB-CA-C	-7.29	98.68	110.79
1	A	553	ASN	CA-CB-CG	-7.29	105.31	112.60
1	A	108	GLU	N-CA-C	7.26	122.11	111.87
1	A	7	GLN	O-C-N	7.26	131.50	123.22
1	A	332	ARG	NE-CZ-NH1	7.26	128.76	121.50
1	A	524	ARG	NE-CZ-NH2	7.26	125.74	119.20
1	A	387	GLY	O-C-N	-7.26	112.69	122.35
1	A	640	ASN	CB-CG-ND2	7.25	127.28	116.40
1	A	210	ARG	N-CA-CB	7.24	122.43	110.85
1	A	422	ASP	N-CA-C	7.23	120.05	110.36
1	A	447	SER	CA-C-O	-7.23	109.85	119.11
1	A	250	VAL	N-CA-C	-7.22	99.53	108.05
1	A	424	ASP	N-CA-CB	-7.21	99.47	110.07
1	A	537	GLU	CA-C-N	7.21	132.85	122.40
1	A	537	GLU	C-N-CA	7.21	132.85	122.40
1	A	615	HIS	CA-CB-CG	-7.20	106.60	113.80
1	A	554	THR	CA-CB-OG1	-7.19	98.82	109.60
1	A	636	SER	N-CA-C	-7.18	95.51	110.80
1	A	30	ARG	CA-C-N	7.15	133.09	121.87
1	A	30	ARG	C-N-CA	7.15	133.09	121.87
1	A	679	THR	CA-CB-OG1	-7.14	98.88	109.60
1	A	623	ASN	CB-CA-C	7.14	123.36	111.51
1	A	399	VAL	N-CA-C	-7.11	103.54	110.72
1	A	43	ILE	O-C-N	7.11	129.83	121.80
1	A	549	THR	CA-CB-OG1	-7.10	98.96	109.60
1	A	480	THR	CA-C-O	-7.09	111.34	119.14
1	A	275	GLN	CG-CD-NE2	7.08	127.02	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	512	GLU	CA-C-O	-7.07	110.72	119.28
1	A	414	ASN	CA-CB-CG	-7.06	105.54	112.60
1	A	246	HIS	O-C-N	7.06	131.31	123.33
1	A	6	VAL	CA-C-O	-7.06	112.39	120.65
1	A	493	CYS	N-CA-C	-7.05	92.97	107.70
1	A	221	GLU	N-CA-C	-7.04	101.88	113.50
1	A	489	PHE	CA-C-O	-7.04	113.23	121.46
1	A	378	GLU	CB-CG-CD	7.01	124.53	112.60
1	A	38	LYS	CB-CG-CD	7.01	127.43	111.30
1	A	142	PRO	O-C-N	-7.00	107.80	121.10
1	A	107	ASN	OD1-CG-ND2	-7.00	115.60	122.60
1	A	424	ASP	OD1-CG-OD2	7.00	139.69	122.90
1	A	29	VAL	CA-C-N	-6.99	112.41	122.68
1	A	29	VAL	C-N-CA	-6.99	112.41	122.68
1	A	258	ARG	N-CA-CB	6.97	120.22	109.97
1	A	629	ASP	O-C-N	6.96	129.53	122.08
1	A	18	LYS	CA-C-O	6.95	127.92	120.55
1	A	657	THR	N-CA-CB	-6.95	99.94	110.91
1	A	400	TYR	O-C-N	-6.93	114.82	122.03
1	A	43	ILE	CA-C-O	-6.92	112.99	120.47
1	A	258	ARG	O-C-N	6.91	131.32	122.89
1	A	225	ASP	CB-CA-C	6.89	122.42	110.01
1	A	120	ARG	CA-C-O	-6.87	112.22	120.12
1	A	104	PHE	N-CA-C	-6.87	98.50	109.76
1	A	249	ARG	N-CA-C	-6.86	98.03	109.07
1	A	274	ALA	CA-C-O	6.85	128.03	120.63
1	A	508	ILE	CA-C-O	-6.83	113.75	119.97
1	A	539	ALA	N-CA-C	-6.83	103.77	111.14
1	A	441	VAL	CA-C-N	6.83	131.18	121.42
1	A	441	VAL	C-N-CA	6.83	131.18	121.42
1	A	648	GLU	CB-CG-CD	6.82	124.20	112.60
1	A	112	LEU	CA-C-O	6.80	130.24	121.67
1	A	444	SER	N-CA-C	6.80	119.32	111.02
1	A	487	GLU	CB-CG-CD	6.79	124.15	112.60
1	A	442	ARG	NE-CZ-NH2	6.79	125.31	119.20
1	A	233	ASP	CA-C-N	6.78	132.65	122.68
1	A	233	ASP	C-N-CA	6.78	132.65	122.68
1	A	70	ALA	N-CA-CB	6.78	119.19	110.04
1	A	98	VAL	CA-C-O	-6.78	114.56	121.67
1	A	533	ARG	CD-NE-CZ	-6.77	114.92	124.40
1	A	617	GLN	CG-CD-OE1	-6.76	107.27	120.80
1	A	146	GLU	CB-CG-CD	6.76	124.10	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	583	VAL	O-C-N	6.76	128.70	121.87
1	A	143	GLU	O-C-N	6.75	129.08	121.32
1	A	489	PHE	CA-C-N	6.73	129.53	120.65
1	A	489	PHE	C-N-CA	6.73	129.53	120.65
1	A	620	PHE	CA-C-O	-6.73	111.24	119.18
1	A	632	CYS	CA-C-O	-6.72	113.11	120.30
1	A	370	THR	CA-CB-OG1	-6.72	99.52	109.60
1	A	345	VAL	CA-C-O	-6.72	113.34	120.53
1	A	637	GLU	CB-CG-CD	6.72	124.02	112.60
1	A	675	LYS	N-CA-C	-6.71	104.36	112.54
1	A	484	LYS	CA-C-O	6.70	129.70	122.13
1	A	559	ASN	OD1-CG-ND2	6.70	129.29	122.60
1	A	509	GLY	CA-C-O	-6.69	113.42	122.39
1	A	236	ARG	N-CA-C	-6.69	98.86	109.23
1	A	555	ASP	CA-CB-CG	6.68	119.28	112.60
1	A	184	SER	CB-CA-C	-6.68	95.92	111.09
1	A	665	PRO	CA-C-O	-6.67	109.42	119.55
1	A	297	ASP	CA-CB-CG	6.67	119.27	112.60
1	A	265	ASP	CA-CB-CG	-6.66	105.94	112.60
1	A	515	ASN	O-C-N	6.65	131.35	122.04
1	A	233	ASP	CA-CB-CG	-6.63	105.97	112.60
1	A	149	VAL	CB-CA-C	6.63	123.00	112.26
1	A	660	GLU	CB-CG-CD	6.63	123.86	112.60
1	A	476	LEU	CA-C-N	6.62	129.99	120.79
1	A	476	LEU	C-N-CA	6.62	129.99	120.79
1	A	243	LYS	CA-C-O	-6.61	111.50	119.49
1	A	384	VAL	CA-C-O	-6.60	113.64	120.71
1	A	534	CYS	N-CA-C	-6.60	104.08	111.28
1	A	607	GLU	CB-CG-CD	6.59	123.80	112.60
1	A	283	SER	O-C-N	6.59	126.98	121.84
1	A	298	LEU	O-C-N	6.59	131.26	122.96
1	A	73	LYS	CA-C-O	-6.54	114.00	121.65
1	A	475	LEU	O-C-N	6.54	128.83	122.03
1	A	666	GLN	N-CA-CB	6.54	120.36	110.30
1	A	24	ARG	CD-NE-CZ	-6.53	115.25	124.40
1	A	426	ASN	CA-CB-CG	-6.53	106.07	112.60
1	A	322	SER	O-C-N	6.52	129.58	122.15
1	A	39	ARG	N-CA-C	-6.52	99.43	109.14
1	A	579	LYS	CA-C-O	-6.52	114.44	121.94
1	A	7	GLN	OE1-CD-NE2	6.51	129.11	122.60
1	A	502	ASN	N-CA-C	-6.50	104.28	111.82
1	A	284	PRO	CB-CA-C	6.50	122.28	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	PHE	CA-CB-CG	6.48	120.28	113.80
1	A	680	SER	O-C-N	6.48	126.89	121.83
1	A	377	THR	CA-C-O	-6.48	114.03	120.70
1	A	75	ARG	NE-CZ-NH2	6.47	125.03	119.20
1	A	192	TYR	CA-C-N	6.47	128.95	120.28
1	A	192	TYR	C-N-CA	6.47	128.95	120.28
1	A	148	ALA	CA-C-N	-6.46	109.70	120.30
1	A	148	ALA	C-N-CA	-6.46	109.70	120.30
1	A	641	LEU	O-C-N	6.46	130.56	123.13
1	A	601	SER	O-C-N	6.44	130.13	122.72
1	A	424	ASP	CB-CG-OD2	-6.44	103.59	118.40
1	A	657	THR	CA-CB-OG1	-6.44	99.94	109.60
1	A	237	LYS	N-CA-CB	6.43	119.52	111.35
1	A	193	SER	CA-C-N	-6.42	112.94	120.00
1	A	193	SER	C-N-CA	-6.42	112.94	120.00
1	A	171	ARG	CA-C-O	-6.40	112.06	119.61
1	A	321	GLY	N-CA-C	-6.39	105.13	112.29
1	A	608	ARG	NE-CZ-NH1	-6.37	115.13	121.50
1	A	520	ASN	CB-CG-ND2	6.36	125.95	116.40
1	A	587	ARG	NE-CZ-NH1	-6.36	115.14	121.50
1	A	121	ARG	CA-C-O	-6.35	114.31	121.81
1	A	216	GLU	CA-CB-CG	6.35	126.80	114.10
1	A	457	LYS	CA-CB-CG	-6.34	101.42	114.10
1	A	666	GLN	CA-CB-CG	6.33	126.76	114.10
1	A	136	LEU	N-CA-C	6.32	120.60	113.01
1	A	630	LYS	CB-CA-C	-6.31	100.86	110.83
1	A	245	CYS	N-CA-CB	-6.30	101.37	111.58
1	A	580	ARG	O-C-N	6.29	130.79	123.30
1	A	511	GLU	CA-C-O	-6.28	113.17	120.20
1	A	424	ASP	CA-CB-CG	-6.27	106.33	112.60
1	A	578	GLY	CA-C-O	-6.27	112.27	119.10
1	A	168	ASN	CA-CB-CG	-6.26	106.34	112.60
1	A	566	LEU	CA-C-O	-6.25	114.74	121.56
1	A	625	SER	O-C-N	6.25	129.29	122.11
1	A	342	ARG	NE-CZ-NH1	-6.25	115.25	121.50
1	A	168	ASN	OD1-CG-ND2	6.24	128.84	122.60
1	A	328	ILE	CA-C-O	-6.24	114.56	121.17
1	A	559	ASN	CA-CB-CG	-6.22	106.38	112.60
1	A	597	HIS	CA-CB-CG	-6.21	107.59	113.80
1	A	614	LEU	O-C-N	6.21	128.55	122.09
1	A	231	CYS	CA-C-O	6.21	127.03	120.63
1	A	248	ALA	O-C-N	6.21	130.14	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	580	ARG	N-CA-C	-6.20	98.79	108.90
1	A	630	LYS	O-C-N	6.20	129.99	121.92
1	A	136	LEU	CA-C-O	-6.20	110.99	119.05
1	A	27	ARG	N-CA-C	-6.20	104.45	111.14
1	A	275	GLN	CA-C-O	-6.18	113.37	120.24
1	A	321	GLY	CA-C-O	-6.17	117.97	122.23
1	A	411	LEU	CA-C-O	-6.17	114.42	121.40
1	A	286	PHE	CA-C-O	6.17	127.28	120.31
1	A	415	TYR	CA-C-O	-6.16	114.11	121.56
1	A	313	ARG	CD-NE-CZ	-6.14	115.80	124.40
1	A	604	ASP	CA-C-O	-6.14	111.82	119.38
1	A	452	SER	CA-C-O	-6.14	112.66	119.78
1	A	35	SER	N-CA-C	-6.14	100.90	110.17
1	A	308	SER	CA-C-O	-6.14	113.73	120.30
1	A	173	CYS	CB-CA-C	6.13	120.14	109.65
1	A	533	ARG	NE-CZ-NH1	6.13	127.63	121.50
1	A	574	LEU	O-C-N	-6.13	116.23	123.22
1	A	277	LYS	CA-C-O	-6.10	112.56	120.00
1	A	558	ASN	O-C-N	6.09	130.44	123.31
1	A	153	PHE	N-CA-C	-6.08	101.77	110.59
1	A	457	LYS	O-C-N	6.08	130.14	123.27
1	A	113	LYS	O-C-N	6.08	130.53	123.30
1	A	397	GLY	N-CA-C	-6.08	105.45	112.50
1	A	37	ILE	CB-CG1-CD1	-6.07	101.05	113.80
1	A	675	LYS	CB-CA-C	6.07	122.99	110.31
1	A	584	THR	CA-C-O	6.06	126.93	119.05
1	A	623	ASN	CA-CB-CG	-6.06	106.54	112.60
1	A	118	GLY	O-C-N	6.06	130.57	122.70
1	A	451	ASN	CA-CB-CG	-6.04	106.56	112.60
1	A	345	VAL	N-CA-CB	6.03	119.06	111.46
1	A	490	SER	CB-CA-C	-6.02	101.69	110.96
1	A	529	THR	O-C-N	6.01	129.00	122.15
1	A	234	ASN	CA-CB-CG	-6.00	106.60	112.60
1	A	535	LEU	CA-C-N	6.00	128.91	120.28
1	A	535	LEU	C-N-CA	6.00	128.91	120.28
1	A	674	LEU	N-CA-C	6.00	118.78	111.82
1	A	376	THR	CA-C-O	-5.99	114.80	121.51
1	A	532	PHE	CA-C-N	5.98	128.29	120.28
1	A	532	PHE	C-N-CA	5.98	128.29	120.28
1	A	151	ARG	N-CA-C	-5.98	105.75	113.16
1	A	150	ALA	O-C-N	5.97	129.61	122.27
1	A	289	PHE	CA-CB-CG	5.97	119.77	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	650	LEU	N-CA-C	-5.96	99.94	109.96
1	A	394	LEU	CA-C-O	-5.96	114.38	121.11
1	A	133	ARG	CG-CD-NE	5.95	125.09	112.00
1	A	617	GLN	CG-CD-NE2	5.95	125.32	116.40
1	A	347	TRP	CA-C-N	-5.95	114.72	123.05
1	A	347	TRP	C-N-CA	-5.95	114.72	123.05
1	A	99	LYS	N-CA-CB	5.94	119.96	110.46
1	A	557	ASN	OD1-CG-ND2	5.94	128.54	122.60
1	A	605	LYS	CA-C-O	-5.94	112.52	119.05
1	A	580	ARG	N-CA-CB	5.93	120.64	110.68
1	A	57	VAL	CA-C-N	-5.92	113.83	122.65
1	A	57	VAL	C-N-CA	-5.92	113.83	122.65
1	A	522	ASN	OD1-CG-ND2	-5.92	116.68	122.60
1	A	538	ASN	CA-CB-CG	5.91	118.51	112.60
1	A	603	MET	CA-CB-CG	-5.91	102.28	114.10
1	A	282	LYS	O-C-N	5.91	130.45	122.59
1	A	20	PHE	O-C-N	5.90	128.38	122.12
1	A	476	LEU	CA-C-O	-5.89	114.59	120.90
1	A	498	ASP	O-C-N	5.89	126.66	121.18
1	A	637	GLU	CA-CB-CG	5.89	125.88	114.10
1	A	39	ARG	CG-CD-NE	-5.88	99.06	112.00
1	A	465	ARG	CB-CA-C	5.88	120.12	109.83
1	A	248	ALA	CA-C-N	-5.88	114.89	123.00
1	A	248	ALA	C-N-CA	-5.88	114.89	123.00
1	A	258	ARG	CG-CD-NE	-5.88	99.07	112.00
1	A	336	GLU	N-CA-CB	5.88	118.86	110.16
1	A	145	ILE	O-C-N	5.87	127.64	121.89
1	A	440	VAL	CB-CA-C	5.87	119.25	110.98
1	A	153	PHE	CA-C-N	-5.86	111.16	122.06
1	A	153	PHE	C-N-CA	-5.86	111.16	122.06
1	A	12	SER	CA-C-O	-5.86	115.00	121.33
1	A	109	LEU	CB-CA-C	5.86	122.56	110.31
1	A	57	VAL	CA-CB-CG1	5.85	120.35	110.40
1	A	446	THR	CA-C-O	5.85	126.70	119.97
1	A	652	ARG	NE-CZ-NH2	-5.85	113.93	119.20
1	A	642	LEU	O-C-N	5.84	130.36	122.59
1	A	508	ILE	N-CA-CB	-5.83	104.58	112.16
1	A	99	LYS	O-C-N	5.83	129.46	122.94
1	A	482	SER	N-CA-C	5.82	119.02	109.76
1	A	360	GLN	N-CA-C	-5.82	104.84	111.07
1	A	347	TRP	CA-C-O	-5.81	114.39	121.36
1	A	135	PHE	CA-CB-CG	-5.81	107.99	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	256	VAL	CA-C-O	5.81	128.78	121.40
1	A	652	ARG	CB-CG-CD	5.81	124.66	111.30
1	A	92	TYR	CB-CA-C	5.80	123.60	110.67
1	A	506	LEU	CA-C-O	-5.79	112.55	119.15
1	A	146	GLU	CG-CD-OE1	5.79	131.72	118.40
1	A	462	ALA	O-C-N	5.78	128.70	123.26
1	A	80	GLU	N-CA-CB	5.78	118.46	109.97
1	A	264	GLU	CA-CB-CG	5.78	125.66	114.10
1	A	236	ARG	O-C-N	5.77	129.97	123.27
1	A	466	THR	CA-CB-OG1	-5.77	100.95	109.60
1	A	515	ASN	CB-CG-ND2	5.76	125.03	116.40
1	A	592	ALA	O-C-N	5.75	129.02	123.04
1	A	473	MET	CA-C-O	-5.75	113.36	119.97
1	A	15	GLU	CB-CG-CD	5.74	122.36	112.60
1	A	237	LYS	N-CA-C	-5.74	101.55	108.14
1	A	515	ASN	CA-C-O	-5.74	113.64	119.78
1	A	259	SER	N-CA-C	-5.73	105.00	112.23
1	A	210	ARG	O-C-N	5.73	130.38	123.16
1	A	85	GLU	N-CA-CB	5.72	118.53	109.71
1	A	439	ALA	CA-C-N	-5.72	114.73	122.91
1	A	439	ALA	C-N-CA	-5.72	114.73	122.91
1	A	604	ASP	O-C-N	5.72	130.09	122.43
1	A	448	LEU	CA-C-O	-5.71	113.96	120.58
1	A	653	LEU	CB-CA-C	5.71	119.68	109.29
1	A	255	VAL	N-CA-CB	5.70	117.34	110.95
1	A	278	PHE	O-C-N	5.68	129.25	122.26
1	A	276	GLU	CA-C-O	5.68	126.78	120.82
1	A	666	GLN	N-CA-C	-5.68	105.07	112.23
1	A	179	ASN	O-C-N	5.68	129.26	122.27
1	A	524	ARG	NH1-CZ-NH2	5.67	126.68	119.30
1	A	96	ALA	CA-C-O	-5.67	113.43	120.57
1	A	606	VAL	N-CA-CB	-5.67	104.22	110.51
1	A	140	GLY	N-CA-C	5.67	123.90	112.34
1	A	315	ASP	CA-C-O	-5.66	115.04	121.72
1	A	397	GLY	CA-C-O	-5.66	114.88	121.00
1	A	6	VAL	N-CA-C	-5.65	99.58	108.23
1	A	39	ARG	O-C-N	5.65	130.08	122.96
1	A	44	GLN	CA-C-O	5.65	126.54	120.55
1	A	7	GLN	CB-CG-CD	-5.64	103.01	112.60
1	A	636	SER	N-CA-CB	5.64	120.02	110.49
1	A	332	ARG	NH1-CZ-NH2	-5.64	111.97	119.30
1	A	612	VAL	CA-C-O	-5.64	114.88	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	422	ASP	CA-CB-CG	5.63	118.23	112.60
1	A	215	PHE	CA-CB-CG	-5.63	108.17	113.80
1	A	258	ARG	CB-CG-CD	-5.63	98.36	111.30
1	A	314	ILE	N-CA-C	5.62	116.32	109.30
1	A	480	THR	N-CA-C	5.62	120.41	113.50
1	A	103	SER	CA-C-N	-5.61	114.29	122.65
1	A	103	SER	C-N-CA	-5.61	114.29	122.65
1	A	184	SER	O-C-N	5.61	129.55	123.10
1	A	180	LYS	CA-C-O	-5.61	112.49	120.51
1	A	258	ARG	CD-NE-CZ	-5.61	116.55	124.40
1	A	223	GLU	N-CA-CB	5.60	122.32	110.67
1	A	395	ASP	O-C-N	-5.60	116.20	122.75
1	A	307	PHE	CA-CB-CG	5.60	119.40	113.80
1	A	616	GLN	CA-C-O	5.60	126.40	119.79
1	A	251	PRO	O-C-N	-5.60	116.31	123.14
1	A	570	ASP	OD1-CG-OD2	5.60	136.33	122.90
1	A	30	ARG	CA-C-O	5.59	129.07	122.14
1	A	620	PHE	O-C-N	5.59	128.80	122.20
1	A	108	GLU	N-CA-CB	-5.59	102.67	111.39
1	A	291	SER	CA-CB-OG	-5.59	99.92	111.10
1	A	148	ALA	CA-C-O	-5.58	114.05	120.24
1	A	663	LEU	O-C-N	5.58	129.81	122.33
1	A	5	SER	CA-C-N	5.57	129.33	122.37
1	A	5	SER	C-N-CA	5.57	129.33	122.37
1	A	95	VAL	CA-C-O	-5.57	115.41	121.92
1	A	388	GLU	CA-CB-CG	5.56	125.21	114.10
1	A	45	CYS	O-C-N	5.55	128.48	122.15
1	A	402	ALA	CA-C-O	-5.54	113.84	120.10
1	A	529	THR	CA-C-N	-5.54	113.18	120.22
1	A	529	THR	C-N-CA	-5.54	113.18	120.22
1	A	222	ALA	CA-C-O	-5.54	112.22	120.42
1	A	137	ASN	CA-C-N	5.52	132.09	121.54
1	A	137	ASN	C-N-CA	5.52	132.09	121.54
1	A	333	LYS	N-CA-C	5.51	118.01	110.24
1	A	373	SER	CA-C-O	5.51	127.28	121.33
1	A	281	ASP	CA-C-O	-5.51	115.15	122.03
1	A	43	ILE	CB-CA-C	-5.50	103.34	112.26
1	A	532	PHE	CA-C-O	5.50	126.25	120.42
1	A	673	ASN	CA-CB-CG	-5.50	107.10	112.60
1	A	65	TYR	O-C-N	5.50	127.75	122.03
1	A	243	LYS	N-CA-C	-5.50	105.67	112.38
1	A	511	GLU	N-CA-CB	5.49	118.82	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	465	ARG	NH1-CZ-NH2	-5.49	112.16	119.30
1	A	138	TRP	CB-CA-C	-5.49	99.50	110.42
1	A	327	ALA	N-CA-C	-5.49	105.20	111.07
1	A	492	SER	O-C-N	5.49	129.41	123.10
1	A	275	GLN	OE1-CD-NE2	-5.48	117.12	122.60
1	A	543	ALA	CA-C-O	5.48	126.28	120.36
1	A	658	THR	OG1-CB-CG2	5.48	120.26	109.30
1	A	381	ILE	CA-C-N	5.47	127.61	120.28
1	A	381	ILE	C-N-CA	5.47	127.61	120.28
1	A	516	LYS	N-CA-CB	5.47	117.96	109.48
1	A	518	VAL	CB-CA-C	5.47	116.36	111.00
1	A	585	GLU	CG-CD-OE1	-5.47	105.83	118.40
1	A	293	SER	CA-CB-OG	-5.46	100.18	111.10
1	A	84	THR	CA-CB-OG1	-5.45	101.42	109.60
1	A	684	GLU	CG-CD-OE2	-5.45	105.86	118.40
1	A	617	GLN	CA-C-O	5.45	126.54	120.82
1	A	647	THR	CA-CB-CG2	5.45	119.76	110.50
1	A	223	GLU	N-CA-C	-5.44	105.86	113.37
1	A	139	THR	CA-CB-OG1	-5.44	101.44	109.60
1	A	485	PHE	O-C-N	5.43	127.74	122.09
1	A	164	GLY	O-C-N	5.43	129.76	122.70
1	A	662	TYR	CB-CG-CD2	5.43	128.94	120.80
1	A	395	ASP	CA-C-N	5.42	126.92	120.14
1	A	395	ASP	C-N-CA	5.42	126.92	120.14
1	A	597	HIS	CA-C-O	-5.42	115.66	121.56
1	A	5	SER	CA-C-O	5.41	127.15	120.92
1	A	431	PRO	CA-C-O	-5.41	115.25	121.36
1	A	324	TYR	CA-CB-CG	5.41	123.63	113.90
1	A	301	LYS	CA-C-O	-5.40	114.89	121.05
1	A	391	ALA	N-CA-CB	-5.40	103.03	111.56
1	A	433	GLU	CA-C-O	-5.40	112.81	119.18
1	A	91	HIS	CA-CB-CG	-5.39	108.41	113.80
1	A	388	GLU	CA-C-N	5.39	131.06	122.59
1	A	388	GLU	C-N-CA	5.39	131.06	122.59
1	A	422	ASP	CA-C-O	5.39	126.84	120.96
1	A	452	SER	O-C-N	5.39	129.65	122.26
1	A	58	THR	CA-C-O	5.39	126.79	120.80
1	A	515	ASN	CA-CB-CG	-5.39	107.21	112.60
1	A	509	GLY	O-C-N	5.39	129.53	122.96
1	A	225	ASP	N-CA-C	-5.39	106.48	113.16
1	A	161	ALA	CA-C-N	5.38	131.78	122.32
1	A	161	ALA	C-N-CA	5.38	131.78	122.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	402	ALA	N-CA-C	-5.36	105.55	111.71
1	A	17	THR	CA-CB-OG1	-5.36	101.56	109.60
1	A	253	HIS	CA-C-N	-5.36	113.45	122.29
1	A	253	HIS	C-N-CA	-5.36	113.45	122.29
1	A	193	SER	CA-C-O	-5.35	114.88	120.55
1	A	629	ASP	N-CA-C	5.35	117.55	111.02
1	A	335	GLU	CA-CB-CG	5.35	124.80	114.10
1	A	360	GLN	OE1-CD-NE2	5.34	127.94	122.60
1	A	230	LEU	CA-C-O	-5.33	114.51	120.54
1	A	208	PHE	CB-CA-C	5.33	119.31	110.78
1	A	371	CYS	N-CA-C	5.33	118.25	109.72
1	A	395	ASP	N-CA-CB	-5.33	102.64	110.26
1	A	433	GLU	O-C-N	5.33	128.49	122.20
1	A	481	GLY	N-CA-C	-5.33	108.66	115.42
1	A	540	GLY	CA-C-O	-5.33	115.65	121.77
1	A	153	PHE	CA-C-O	-5.32	115.66	121.89
1	A	662	TYR	CB-CG-CD1	-5.32	112.82	120.80
1	A	442	ARG	N-CA-C	-5.32	101.80	110.20
1	A	635	GLN	OE1-CD-NE2	-5.32	117.28	122.60
1	A	308	SER	O-C-N	5.31	129.43	123.27
1	A	265	ASP	CA-C-O	5.31	126.40	120.82
1	A	446	THR	CA-CB-CG2	5.31	119.52	110.50
1	A	141	PRO	N-CA-C	5.31	117.17	110.70
1	A	201	ASP	CA-CB-CG	5.30	117.90	112.60
1	A	22	TRP	CA-CB-CG	5.30	123.67	113.60
1	A	255	VAL	N-CA-C	-5.30	100.70	108.54
1	A	329	GLN	CA-C-O	-5.29	114.12	120.10
1	A	259	SER	CA-C-N	-5.29	116.07	123.10
1	A	259	SER	C-N-CA	-5.29	116.07	123.10
1	A	266	ALA	N-CA-C	-5.29	104.57	111.02
1	A	273	GLN	OE1-CD-NE2	5.28	127.88	122.60
1	A	526	TYR	CA-C-N	5.27	135.60	120.36
1	A	526	TYR	C-N-CA	5.27	135.60	120.36
1	A	604	ASP	CA-C-N	-5.27	113.88	122.26
1	A	604	ASP	C-N-CA	-5.27	113.88	122.26
1	A	558	ASN	CA-C-N	5.27	128.32	120.31
1	A	558	ASN	C-N-CA	5.27	128.32	120.31
1	A	585	GLU	CB-CG-CD	-5.27	103.65	112.60
1	A	35	SER	CA-C-O	-5.26	115.04	121.88
1	A	490	SER	CA-CB-OG	-5.26	100.58	111.10
1	A	354	GLU	CB-CA-C	-5.24	100.61	110.67
1	A	603	MET	CB-CG-SD	-5.24	96.98	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	PRO	O-C-N	5.23	128.96	123.10
1	A	652	ARG	NH1-CZ-NH2	5.22	126.09	119.30
1	A	143	GLU	N-CA-C	-5.22	98.28	109.81
1	A	647	THR	CA-C-O	-5.22	114.44	120.49
1	A	122	THR	CA-CB-OG1	-5.21	101.78	109.60
1	A	334	SER	O-C-N	-5.21	116.29	122.65
1	A	454	LYS	CA-C-N	-5.21	112.62	122.05
1	A	454	LYS	C-N-CA	-5.21	112.62	122.05
1	A	539	ALA	CA-C-N	-5.21	117.83	122.47
1	A	539	ALA	C-N-CA	-5.21	117.83	122.47
1	A	691	LYS	CB-CA-C	-5.21	100.21	110.10
1	A	568	LEU	CA-C-O	5.20	126.74	120.92
1	A	449	THR	CA-C-O	-5.20	115.63	121.40
1	A	582	PRO	CB-CA-C	5.20	117.76	110.95
1	A	146	GLU	CA-CB-CG	5.20	124.49	114.10
1	A	301	LYS	N-CA-CB	5.20	117.91	110.06
1	A	617	GLN	CA-C-N	5.19	127.55	120.54
1	A	617	GLN	C-N-CA	5.19	127.55	120.54
1	A	369	VAL	CA-CB-CG2	5.19	119.23	110.40
1	A	116	HIS	CA-C-O	-5.19	115.29	121.16
1	A	306	GLY	N-CA-C	-5.19	103.21	110.63
1	A	330	ASN	CB-CG-ND2	5.19	124.19	116.40
1	A	516	LYS	CA-C-O	5.19	126.62	120.96
1	A	252	SER	N-CA-C	-5.19	103.68	110.53
1	A	614	LEU	CA-C-O	5.18	126.45	120.90
1	A	636	SER	O-C-N	5.18	129.47	122.59
1	A	391	ALA	N-CA-C	5.17	116.67	108.96
1	A	98	VAL	CA-CB-CG1	5.17	119.19	110.40
1	A	134	PRO	O-C-N	-5.17	116.30	122.24
1	A	269	ASN	N-CA-C	-5.17	105.29	111.03
1	A	338	VAL	O-C-N	5.17	127.16	121.83
1	A	204	GLY	O-C-N	5.17	127.79	123.29
1	A	305	ILE	CA-C-N	-5.17	114.31	121.23
1	A	305	ILE	C-N-CA	-5.17	114.31	121.23
1	A	69	LEU	N-CA-C	5.16	116.76	110.41
1	A	475	LEU	CA-C-O	-5.16	115.58	121.00
1	A	295	GLN	N-CA-CB	-5.15	102.39	110.69
1	A	344	ARG	NE-CZ-NH2	-5.15	114.56	119.20
1	A	176	THR	CA-C-N	5.15	131.50	121.41
1	A	176	THR	C-N-CA	5.15	131.50	121.41
1	A	77	VAL	N-CA-C	-5.14	108.49	113.53
1	A	341	ARG	CA-C-N	-5.13	112.51	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	ARG	C-N-CA	-5.13	112.51	122.06
1	A	126	ASN	O-C-N	5.13	127.37	122.03
1	A	400	TYR	N-CA-CB	-5.12	102.43	109.91
1	A	84	THR	CA-C-O	-5.12	115.12	121.06
1	A	114	SER	N-CA-C	5.12	117.91	109.72
1	A	387	GLY	N-CA-C	-5.12	107.93	115.30
1	A	23	GLN	CA-C-N	5.11	127.39	120.44
1	A	23	GLN	C-N-CA	5.11	127.39	120.44
1	A	162	ASP	N-CA-CB	-5.11	103.20	110.46
1	A	43	ILE	N-CA-CB	5.10	120.01	110.77
1	A	246	HIS	CA-CB-CG	5.10	118.90	113.80
1	A	369	VAL	O-C-N	5.10	128.71	123.20
1	A	328	ILE	N-CA-CB	5.10	116.51	110.55
1	A	54	ALA	CA-C-N	-5.09	114.14	122.79
1	A	54	ALA	C-N-CA	-5.09	114.14	122.79
1	A	200	LYS	O-C-N	5.09	127.38	122.09
1	A	167	PRO	O-C-N	5.08	128.08	122.24
1	A	382	ALA	N-CA-C	-5.08	105.74	111.28
1	A	477	PHE	CA-CB-CG	5.08	118.88	113.80
1	A	242	PHE	CA-C-O	-5.07	114.52	120.20
1	A	630	LYS	CA-C-O	-5.07	112.60	120.16
1	A	51	GLU	CA-C-O	5.07	125.49	119.56
1	A	574	LEU	CB-CA-C	5.07	118.40	110.19
1	A	679	THR	CA-CB-CG2	5.05	119.09	110.50
1	A	383	LEU	O-C-N	5.05	128.13	122.22
1	A	373	SER	CA-CB-OG	5.05	121.20	111.10
1	A	356	ARG	CA-C-N	5.05	127.00	120.44
1	A	356	ARG	C-N-CA	5.05	127.00	120.44
1	A	443	ARG	O-C-N	-5.04	115.68	122.43
1	A	176	THR	CB-CA-C	5.04	117.94	109.48
1	A	178	GLU	CA-CB-CG	5.04	124.17	114.10
1	A	242	PHE	O-C-N	5.03	127.94	122.20
1	A	448	LEU	O-C-N	5.03	129.30	122.96
1	A	186	GLN	O-C-N	5.02	129.11	122.43
1	A	64	ILE	N-CA-C	-5.02	105.50	110.62
1	A	536	ALA	CA-C-O	-5.02	114.43	120.10
1	A	238	PRO	CA-C-N	5.02	128.40	120.47
1	A	238	PRO	C-N-CA	5.02	128.40	120.47
1	A	541	ASP	CA-CB-CG	-5.01	107.58	112.60
1	A	171	ARG	CA-C-N	-5.00	114.79	122.60
1	A	171	ARG	C-N-CA	-5.00	114.79	122.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	258	ARG	Sidechain
1	A	465	ARG	Sidechain

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	5342	0	5205	312	0
2	A	1	0	0	0	0
3	A	373	0	0	33	0
All	All	5716	0	5205	312	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 30.

All (312) 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:37:ILE:HD11	1:A:39:ARG:NH2	1.50	1.23
1:A:37:ILE:HD11	1:A:39:ARG:HH21	1.02	1.10
1:A:105:GLN:HA	1:A:105:GLN:HE21	1.24	1.02
1:A:679:THR:HG23	1:A:680:SER:H	1.22	1.00
1:A:622:ARG:NH1	1:A:635:GLN:HE21	1.57	0.99
1:A:622:ARG:HH12	1:A:635:GLN:NE2	1.59	0.98
1:A:37:ILE:CD1	1:A:39:ARG:HH21	1.79	0.95
1:A:85:GLU:O	1:A:86:ARG:HB2	1.66	0.95
1:A:87:GLN:N	1:A:88:PRO:HD3	1.82	0.95
1:A:269:ASN:HB3	3:A:783:HOH:O	1.66	0.94
1:A:155:ALA:HB1	1:A:172:LEU:HD21	1.50	0.93
1:A:4:ARG:HH11	1:A:4:ARG:HB2	1.32	0.92
1:A:87:GLN:N	1:A:88:PRO:CD	2.36	0.88
1:A:636:SER:HB2	1:A:639:LYS:CB	2.02	0.88
1:A:679:THR:CG2	1:A:680:SER:H	1.87	0.88
1:A:311:PRO:HD2	1:A:314:ILE:HD12	1.56	0.87
1:A:344:ARG:CD	1:A:370:THR:HG21	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:626:ASP:HB3	1:A:630:LYS:HG3	1.60	0.84
1:A:218:LEU:HD23	1:A:224:ARG:HG2	1.59	0.84
1:A:636:SER:HB2	1:A:639:LYS:HB3	1.59	0.82
1:A:155:ALA:CB	1:A:172:LEU:HD21	2.09	0.82
1:A:8:TRP:O	1:A:37:ILE:HG22	1.81	0.81
1:A:121:ARG:HH12	1:A:191:SER:HB2	1.46	0.80
1:A:100:LYS:C	1:A:100:LYS:HD2	2.05	0.80
1:A:276:GLU:O	1:A:282:LYS:HD2	1.82	0.79
1:A:3:ARG:C	1:A:5:SER:H	1.90	0.79
1:A:344:ARG:HD2	1:A:370:THR:HG21	1.66	0.78
1:A:515:ASN:O	1:A:518:VAL:HG22	1.84	0.78
1:A:346:VAL:HG22	1:A:370:THR:CG2	2.15	0.76
1:A:344:ARG:O	1:A:605:LYS:NZ	2.19	0.76
1:A:4:ARG:HH11	1:A:4:ARG:CB	1.99	0.75
1:A:13:ASN:N	1:A:14:PRO:CD	2.49	0.75
1:A:77:VAL:HG11	1:A:257:ALA:HB3	1.69	0.74
1:A:105:GLN:HA	1:A:105:GLN:NE2	1.99	0.74
1:A:344:ARG:HD3	1:A:370:THR:CG2	2.17	0.74
1:A:86:ARG:H	1:A:88:PRO:HD3	1.53	0.74
1:A:143:GLU:HG3	1:A:144:PRO:CD	2.18	0.74
1:A:293:SER:HB2	3:A:977:HOH:O	1.87	0.74
1:A:646:ASN:HD22	1:A:646:ASN:H	1.31	0.74
1:A:105:GLN:HE22	1:A:236:ARG:HG3	1.53	0.73
1:A:110:GLN:HG2	1:A:152:PHE:CE2	2.22	0.73
1:A:3:ARG:O	1:A:5:SER:N	2.22	0.72
1:A:344:ARG:HD3	1:A:370:THR:HG21	1.72	0.72
1:A:162:ASP:OD1	1:A:165:GLN:HB2	1.89	0.72
1:A:3:ARG:NH1	1:A:3:ARG:HB3	2.05	0.72
1:A:418:GLN:NE2	1:A:587:ARG:NH1	2.37	0.71
1:A:686:CYS:O	1:A:690:ARG:HG3	1.91	0.71
1:A:570:ASP:OD2	3:A:1041:HOH:O	2.08	0.70
1:A:133:ARG:NH1	1:A:333:LYS:O	2.23	0.70
1:A:663:LEU:HG	1:A:667:TYR:HD2	1.54	0.70
1:A:2:ARG:HH11	1:A:2:ARG:HG2	1.56	0.70
1:A:87:GLN:HG3	3:A:706:HOH:O	1.92	0.70
1:A:180:LYS:HG2	3:A:952:HOH:O	1.92	0.70
1:A:636:SER:HB2	1:A:639:LYS:HB2	1.73	0.69
1:A:86:ARG:N	1:A:88:PRO:HD3	2.08	0.69
1:A:14:PRO:HB3	1:A:295:GLN:OE1	1.93	0.68
1:A:613:LEU:O	1:A:617:GLN:HB2	1.93	0.68
1:A:138:TRP:CH2	1:A:141:PRO:HD3	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ASP:HB3	3:A:962:HOH:O	1.94	0.68
1:A:174:ALA:HB3	1:A:188:PRO:HG2	1.76	0.68
1:A:249:ARG:HG3	1:A:249:ARG:NH1	2.07	0.68
1:A:143:GLU:HG3	1:A:144:PRO:HD2	1.75	0.68
1:A:679:THR:CG2	1:A:680:SER:N	2.52	0.68
1:A:70:ALA:HB2	1:A:73:LYS:HE2	1.76	0.68
1:A:315:ASP:HB3	1:A:318:LEU:H	1.57	0.67
1:A:2:ARG:HG2	1:A:2:ARG:NH1	2.09	0.67
1:A:155:ALA:HB1	1:A:172:LEU:CD2	2.23	0.66
1:A:346:VAL:HG22	1:A:370:THR:HG23	1.76	0.66
1:A:171:ARG:HD3	3:A:806:HOH:O	1.96	0.66
1:A:638:THR:N	1:A:645:ASP:OD2	2.28	0.66
1:A:691:LYS:O	1:A:691:LYS:HG2	1.94	0.66
1:A:241:LYS:HA	3:A:963:HOH:O	1.97	0.65
1:A:105:GLN:HB2	1:A:107:ASN:HD21	1.60	0.65
1:A:637:GLU:C	1:A:639:LYS:H	2.03	0.65
1:A:133:ARG:N	1:A:134:PRO:HD2	2.12	0.65
1:A:646:ASN:H	1:A:646:ASN:ND2	1.95	0.65
1:A:42:PRO:HG3	3:A:927:HOH:O	1.97	0.65
1:A:114:SER:O	1:A:156:SER:HA	1.96	0.65
1:A:107:ASN:H	1:A:107:ASN:HD22	1.45	0.64
1:A:22:TRP:CZ2	1:A:270:LEU:HD21	2.32	0.64
1:A:91:HIS:C	1:A:91:HIS:CD2	2.76	0.63
1:A:184:SER:HB2	1:A:186:GLN:H	1.63	0.63
1:A:241:LYS:HE3	1:A:244:ASP:HB2	1.80	0.63
1:A:18:LYS:NZ	1:A:288:LEU:O	2.33	0.62
1:A:344:ARG:CD	1:A:370:THR:CG2	2.75	0.62
1:A:418:GLN:HE22	1:A:587:ARG:HD3	1.64	0.62
1:A:3:ARG:HB3	1:A:3:ARG:HH11	1.63	0.61
1:A:105:GLN:HB2	1:A:107:ASN:ND2	2.15	0.61
1:A:86:ARG:C	1:A:88:PRO:HD3	2.24	0.61
1:A:93:TYR:OH	1:A:243:LYS:HE2	2.00	0.61
1:A:100:LYS:HD2	1:A:101:GLY:N	2.16	0.61
1:A:675:LYS:HE2	3:A:1024:HOH:O	2.01	0.61
1:A:39:ARG:HB3	1:A:44:GLN:HB3	1.83	0.61
1:A:384:VAL:HG22	1:A:407:LEU:HD11	1.81	0.61
1:A:87:GLN:H	1:A:88:PRO:HD3	1.65	0.61
1:A:4:ARG:HB2	1:A:4:ARG:NH1	2.10	0.60
1:A:132:LEU:C	1:A:134:PRO:HD2	2.26	0.60
1:A:573:LEU:HD22	1:A:583:VAL:HA	1.83	0.60
1:A:424:ASP:OD1	1:A:426:ASN:N	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:ASP:HA	3:A:696:HOH:O	2.02	0.59
1:A:324:TYR:CE1	1:A:328:ILE:HD11	2.37	0.59
1:A:106:LEU:HD12	1:A:109:LEU:CD2	2.32	0.59
1:A:4:ARG:HH11	1:A:4:ARG:CG	2.15	0.59
1:A:663:LEU:HG	1:A:667:TYR:CD2	2.37	0.59
1:A:680:SER:O	1:A:684:GLU:HB2	2.03	0.59
1:A:29:VAL:HG11	1:A:277:LYS:HD3	1.85	0.59
1:A:587:ARG:HG2	3:A:881:HOH:O	2.02	0.59
1:A:664:GLY:O	1:A:668:VAL:HG23	2.03	0.58
1:A:192:TYR:CE1	1:A:210:ARG:HG3	2.37	0.58
1:A:442:ARG:NH1	1:A:540:GLY:O	2.36	0.58
1:A:24:ARG:NH1	3:A:919:HOH:O	2.37	0.58
1:A:279:GLY:HA3	1:A:282:LYS:HG3	1.86	0.58
1:A:120:ARG:HB2	3:A:944:HOH:O	2.03	0.58
1:A:424:ASP:OD1	1:A:424:ASP:C	2.41	0.58
1:A:8:TRP:HZ2	1:A:58:THR:HG22	1.68	0.58
1:A:92:TYR:CE2	1:A:250:VAL:HG22	2.40	0.57
1:A:218:LEU:HB3	1:A:224:ARG:HG3	1.85	0.57
1:A:691:LYS:NZ	1:A:691:LYS:HB3	2.20	0.57
1:A:130:GLY:HA2	1:A:331:LEU:HD13	1.87	0.57
1:A:139:THR:HG22	1:A:140:GLY:N	2.19	0.57
1:A:192:TYR:CD1	1:A:210:ARG:HG3	2.40	0.57
1:A:691:LYS:NZ	1:A:691:LYS:CB	2.67	0.57
1:A:210:ARG:HD3	1:A:212:SER:OG	2.05	0.57
1:A:329:GLN:O	1:A:333:LYS:HG3	2.04	0.57
1:A:20:PHE:HB3	1:A:24:ARG:HH21	1.69	0.56
1:A:568:LEU:HD11	1:A:583:VAL:HB	1.86	0.56
1:A:400:TYR:CZ	1:A:404:LYS:HE3	2.40	0.56
1:A:270:LEU:C	1:A:270:LEU:CD2	2.79	0.56
1:A:275:GLN:HE22	1:A:307:PHE:H	1.52	0.56
1:A:197:LYS:HA	1:A:200:LYS:HB2	1.87	0.56
1:A:416:LYS:HE3	1:A:648:GLU:HG3	1.88	0.55
1:A:312:PRO:HG2	3:A:981:HOH:O	2.05	0.55
1:A:462:ALA:HB3	1:A:465:ARG:HD3	1.88	0.55
1:A:378:GLU:HG3	3:A:737:HOH:O	2.06	0.55
1:A:637:GLU:O	1:A:639:LYS:N	2.39	0.55
1:A:2:ARG:O	1:A:3:ARG:O	2.25	0.55
1:A:4:ARG:CG	1:A:4:ARG:O	2.55	0.54
1:A:58:THR:HG23	3:A:693:HOH:O	2.06	0.54
1:A:233:ASP:HB3	1:A:603:MET:HB3	1.88	0.54
1:A:162:ASP:OD1	1:A:165:GLN:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:VAL:HG11	1:A:448:LEU:HD23	1.89	0.54
1:A:18:LYS:NZ	3:A:695:HOH:O	2.39	0.54
1:A:421:SER:OG	1:A:422:ASP:N	2.38	0.54
1:A:79:ALA:O	1:A:307:PHE:HA	2.07	0.54
1:A:655:GLY:C	1:A:657:THR:HG23	2.33	0.54
1:A:222:ALA:C	1:A:224:ARG:H	2.16	0.54
1:A:133:ARG:HD3	1:A:133:ARG:C	2.33	0.53
1:A:191:SER:OG	1:A:192:TYR:N	2.40	0.53
1:A:13:ASN:ND2	3:A:781:HOH:O	2.41	0.53
1:A:77:VAL:CG1	1:A:257:ALA:HB3	2.38	0.53
1:A:118:GLY:O	1:A:121:ARG:HG3	2.09	0.53
1:A:297:ASP:HB3	1:A:301:LYS:HA	1.90	0.53
1:A:133:ARG:HD3	1:A:133:ARG:O	2.09	0.53
1:A:637:GLU:C	1:A:639:LYS:N	2.67	0.53
1:A:498:ASP:O	1:A:501:SER:OG	2.25	0.52
1:A:275:GLN:HG2	3:A:819:HOH:O	2.09	0.52
1:A:516:LYS:CD	3:A:1035:HOH:O	2.57	0.52
1:A:94:ALA:O	1:A:247:LEU:HB2	2.10	0.52
1:A:107:ASN:H	1:A:107:ASN:ND2	2.08	0.52
1:A:136:LEU:O	1:A:137:ASN:HB2	2.09	0.52
1:A:622:ARG:HH12	1:A:635:GLN:HE21	0.75	0.52
1:A:353:GLN:NE2	1:A:521:SER:HB3	2.24	0.52
1:A:180:LYS:O	1:A:181:CYS:CB	2.57	0.51
1:A:2:ARG:HH11	1:A:2:ARG:CG	2.23	0.51
1:A:4:ARG:O	1:A:4:ARG:HG3	2.11	0.51
1:A:233:ASP:OD1	1:A:233:ASP:C	2.50	0.51
1:A:279:GLY:CA	1:A:282:LYS:HG3	2.40	0.51
1:A:291:SER:HB3	1:A:295:GLN:O	2.11	0.51
1:A:288:LEU:HD22	1:A:300:PHE:CE2	2.46	0.51
1:A:3:ARG:C	1:A:5:SER:N	2.60	0.51
1:A:404:LYS:O	1:A:690:ARG:HD2	2.11	0.51
1:A:389:ALA:O	1:A:602:ARG:NH1	2.44	0.51
1:A:7:GLN:O	1:A:55:ASP:N	2.32	0.51
1:A:106:LEU:HD12	1:A:109:LEU:HD21	1.92	0.51
1:A:671:ILE:HG22	1:A:675:LYS:HG3	1.92	0.51
1:A:98:VAL:HG22	1:A:228:GLU:O	2.11	0.50
1:A:675:LYS:HA	1:A:678:SER:O	2.11	0.50
1:A:12:SER:HB2	1:A:14:PRO:HD2	1.93	0.50
1:A:622:ARG:HG2	1:A:648:GLU:O	2.12	0.50
1:A:417:SER:O	1:A:418:GLN:HB2	2.12	0.50
1:A:418:GLN:NE2	1:A:587:ARG:HH11	2.06	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:LEU:HD21	1:A:587:ARG:HD2	1.92	0.50
1:A:55:ASP:OD2	1:A:263:LYS:NZ	2.43	0.50
1:A:270:LEU:C	1:A:270:LEU:HD23	2.37	0.50
1:A:13:ASN:N	1:A:14:PRO:HD3	2.26	0.49
1:A:249:ARG:HG3	1:A:249:ARG:HH11	1.77	0.49
1:A:14:PRO:CB	1:A:295:GLN:OE1	2.61	0.49
1:A:234:ASN:N	1:A:234:ASN:ND2	2.57	0.49
1:A:229:LEU:HD22	1:A:239:VAL:HA	1.93	0.49
1:A:628:PRO:HA	1:A:632:CYS:SG	2.52	0.49
1:A:290:GLY:N	3:A:696:HOH:O	2.45	0.49
1:A:29:VAL:O	1:A:30:ARG:C	2.56	0.49
1:A:218:LEU:HB3	1:A:224:ARG:CG	2.42	0.48
1:A:55:ASP:OD2	1:A:263:LYS:CE	2.61	0.48
1:A:422:ASP:HB3	1:A:423:PRO:HD2	1.94	0.48
1:A:91:HIS:C	1:A:91:HIS:HD2	2.20	0.48
1:A:6:VAL:HG11	1:A:270:LEU:HD12	1.96	0.48
1:A:195:ALA:O	1:A:198:CYS:HB3	2.14	0.48
1:A:142:PRO:HD2	3:A:800:HOH:O	2.12	0.48
1:A:250:VAL:HA	1:A:251:PRO:HD3	1.55	0.48
1:A:138:TRP:CE2	1:A:140:GLY:HA2	2.49	0.48
1:A:214:VAL:O	1:A:218:LEU:HB2	2.13	0.48
1:A:12:SER:CB	1:A:14:PRO:HD2	2.44	0.48
1:A:380:CYS:HB3	1:A:392:MET:SD	2.54	0.48
1:A:133:ARG:N	1:A:134:PRO:CD	2.77	0.47
1:A:222:ALA:C	1:A:224:ARG:N	2.71	0.47
1:A:47:GLN:O	1:A:48:ALA:C	2.54	0.47
1:A:192:TYR:CE1	1:A:210:ARG:CG	2.98	0.47
1:A:241:LYS:HD2	3:A:963:HOH:O	2.14	0.47
1:A:162:ASP:C	1:A:164:GLY:H	2.22	0.47
1:A:176:THR:O	1:A:179:ASN:HB2	2.14	0.47
1:A:170:CYS:O	1:A:173:CYS:HB2	2.15	0.47
1:A:325:PHE:O	1:A:329:GLN:HG3	2.15	0.47
1:A:410:VAL:HG21	1:A:609:LEU:HD23	1.95	0.47
1:A:417:SER:O	1:A:418:GLN:CB	2.62	0.47
1:A:66:GLU:OE2	1:A:332:ARG:NH2	2.48	0.47
1:A:91:HIS:HB2	1:A:250:VAL:O	2.15	0.47
1:A:209:ILE:HD12	1:A:213:THR:CG2	2.45	0.47
1:A:13:ASN:N	1:A:14:PRO:HD2	2.30	0.46
1:A:43:ILE:HG13	3:A:699:HOH:O	2.16	0.46
1:A:83:GLY:N	3:A:937:HOH:O	2.45	0.46
1:A:37:ILE:HG21	1:A:54:ALA:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:LEU:O	1:A:299:LEU:HB2	2.14	0.46
1:A:22:TRP:CZ2	1:A:270:LEU:CD2	2.99	0.46
1:A:86:ARG:C	1:A:88:PRO:CD	2.84	0.46
1:A:691:LYS:O	1:A:691:LYS:CG	2.64	0.46
1:A:100:LYS:CD	1:A:101:GLY:N	2.78	0.45
1:A:105:GLN:NE2	3:A:718:HOH:O	2.48	0.45
1:A:113:LYS:HA	1:A:155:ALA:O	2.15	0.45
1:A:187:GLU:HA	1:A:188:PRO:HD2	1.78	0.45
1:A:613:LEU:O	1:A:617:GLN:N	2.44	0.45
1:A:121:ARG:HE	1:A:121:ARG:HB3	1.63	0.45
1:A:105:GLN:NE2	1:A:236:ARG:HG3	2.26	0.45
1:A:322:SER:O	1:A:326:THR:HG23	2.17	0.45
1:A:548:VAL:O	1:A:552:GLN:HG3	2.16	0.45
1:A:43:ILE:O	1:A:47:GLN:HG3	2.17	0.45
1:A:92:TYR:CZ	1:A:250:VAL:HG22	2.52	0.45
1:A:367:GLY:HA2	3:A:733:HOH:O	2.17	0.45
1:A:515:ASN:HB3	1:A:518:VAL:HG21	1.99	0.45
1:A:4:ARG:NH1	1:A:4:ARG:CG	2.76	0.44
1:A:113:LYS:HE2	1:A:203:ALA:O	2.17	0.44
1:A:171:ARG:HH11	1:A:171:ARG:HD2	1.54	0.44
1:A:400:TYR:OH	1:A:404:LYS:HE3	2.17	0.44
1:A:477:PHE:O	1:A:478:ASN:C	2.59	0.44
1:A:500:ARG:CD	3:A:1033:HOH:O	2.65	0.44
1:A:615:HIS:ND1	1:A:615:HIS:C	2.75	0.44
1:A:187:GLU:O	1:A:190:PHE:HB3	2.17	0.44
1:A:442:ARG:HD3	3:A:870:HOH:O	2.17	0.44
1:A:141:PRO:HG2	1:A:332:ARG:O	2.16	0.44
1:A:185:SER:C	1:A:187:GLU:H	2.25	0.44
1:A:89:ARG:HH21	1:A:92:TYR:HB3	1.81	0.44
1:A:235:THR:HG22	1:A:236:ARG:H	1.83	0.44
1:A:87:GLN:HG3	1:A:87:GLN:O	2.18	0.44
1:A:384:VAL:HG22	1:A:407:LEU:CD1	2.46	0.44
1:A:100:LYS:C	1:A:100:LYS:CD	2.86	0.43
1:A:321:GLY:O	1:A:325:PHE:HB2	2.17	0.43
1:A:619:LYS:HD3	1:A:620:PHE:CZ	2.53	0.43
1:A:117:THR:OG1	1:A:124:GLY:HA3	2.18	0.43
1:A:166:PHE:HD1	3:A:804:HOH:O	2.00	0.43
1:A:573:LEU:HD13	1:A:583:VAL:HG22	2.01	0.43
1:A:238:PRO:O	1:A:241:LYS:HB2	2.17	0.43
1:A:430:ARG:HH11	1:A:430:ARG:HD3	1.49	0.43
1:A:679:THR:HG23	1:A:680:SER:N	2.05	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:ASN:HB3	1:A:518:VAL:CG2	2.48	0.43
1:A:603:MET:HE3	3:A:742:HOH:O	2.19	0.43
1:A:219:SER:O	1:A:220:ASP:O	2.37	0.43
1:A:622:ARG:HH22	1:A:635:GLN:NE2	2.16	0.43
1:A:55:ASP:CG	1:A:263:LYS:CE	2.92	0.42
1:A:622:ARG:HH22	1:A:635:GLN:HE22	1.67	0.42
1:A:483:CYS:HB3	1:A:677:CYS:HB3	1.90	0.42
1:A:162:ASP:C	1:A:164:GLY:N	2.77	0.42
1:A:311:PRO:HD2	1:A:314:ILE:CD1	2.40	0.42
1:A:352:GLU:O	1:A:356:ARG:HD3	2.19	0.42
1:A:185:SER:C	1:A:187:GLU:N	2.75	0.42
1:A:47:GLN:HG2	1:A:72:TYR:CE1	2.54	0.42
1:A:192:TYR:HB3	1:A:213:THR:OG1	2.20	0.42
1:A:355:LEU:HD22	1:A:373:SER:OG	2.19	0.42
1:A:90:THR:O	1:A:91:HIS:HB3	2.19	0.42
1:A:395:ASP:HA	1:A:597:HIS:CD2	2.55	0.42
1:A:233:ASP:OD1	1:A:233:ASP:N	2.53	0.42
1:A:587:ARG:HD3	1:A:587:ARG:HH11	1.43	0.42
1:A:639:LYS:HA	1:A:639:LYS:HD3	1.77	0.41
1:A:291:SER:HA	1:A:292:PRO:HD3	1.78	0.41
1:A:485:PHE:CD2	3:A:1027:HOH:O	2.57	0.41
1:A:582:PRO:HD2	1:A:585:GLU:OE2	2.21	0.41
1:A:34:VAL:HG22	1:A:35:SER:O	2.19	0.41
1:A:168:ASN:OD1	1:A:171:ARG:NE	2.53	0.41
1:A:492:SER:HB2	1:A:503:LEU:HA	2.02	0.41
1:A:655:GLY:O	1:A:657:THR:HG23	2.20	0.41
1:A:132:LEU:O	1:A:133:ARG:C	2.64	0.41
1:A:60:ASP:HA	1:A:253:HIS:CD2	2.56	0.41
1:A:74:LEU:HB3	1:A:257:ALA:O	2.20	0.41
1:A:75:ARG:HA	1:A:76:PRO:HD3	1.80	0.41
1:A:84:THR:OG1	1:A:87:GLN:HB3	2.21	0.41
1:A:155:ALA:HB3	1:A:172:LEU:HD21	1.97	0.41
1:A:273:GLN:O	1:A:274:ALA:C	2.64	0.41
1:A:275:GLN:NE2	1:A:307:PHE:H	2.18	0.41
1:A:278:PHE:O	1:A:279:GLY:O	2.37	0.41
1:A:622:ARG:NH2	1:A:645:ASP:O	2.54	0.41
1:A:229:LEU:CD2	1:A:239:VAL:HA	2.51	0.41
1:A:91:HIS:HD2	1:A:91:HIS:O	2.05	0.40
1:A:43:ILE:HG13	1:A:43:ILE:H	1.68	0.40
1:A:156:SER:C	1:A:172:LEU:HG	2.46	0.40
1:A:270:LEU:HD23	1:A:270:LEU:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:LEU:HA	1:A:566:LEU:HD23	1.75	0.40
1:A:2:ARG:O	1:A:3:ARG:C	2.65	0.40
1:A:6:VAL:CG1	1:A:270:LEU:HD12	2.51	0.40
1:A:136:LEU:C	1:A:138:TRP:H	2.29	0.40
1:A:273:GLN:C	1:A:275:GLN:N	2.76	0.40
1:A:418:GLN:NE2	1:A:587:ARG:HD3	2.33	0.40
1:A:576:LEU:HD13	1:A:591:LEU:HD23	2.03	0.40
1:A:658:THR:O	1:A:659:TYR:C	2.64	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	689/691 (100%)	624 (91%)	51 (7%)	14 (2%)	6 21

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	4	ARG
1	A	220	ASP
1	A	279	GLY
1	A	417	SER
1	A	418	GLN
1	A	86	ARG
1	A	219	SER
1	A	638	THR
1	A	293	SER
1	A	637	GLU
1	A	141	PRO
1	A	180	LYS

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Mol	Chain	Res	Type
1	A	142	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	574/574 (100%)	467 (81%)	107 (19%)	1 5

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	3	ARG
1	A	4	ARG
1	A	11	VAL
1	A	13	ASN
1	A	28	LYS
1	A	37	ILE
1	A	43	ILE
1	A	58	THR
1	A	77	VAL
1	A	85	GLU
1	A	86	ARG
1	A	90	THR
1	A	97	VAL
1	A	99	LYS
1	A	100	LYS
1	A	105	GLN
1	A	107	ASN
1	A	109	LEU
1	A	110	GLN
1	A	121	ARG
1	A	133	ARG
1	A	139	THR
1	A	142	PRO
1	A	145	ILE

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Mol	Chain	Res	Type
1	A	149	VAL
1	A	156	SER
1	A	163	LYS
1	A	165	GLN
1	A	172	LEU
1	A	176	THR
1	A	184	SER
1	A	185	SER
1	A	187	GLU
1	A	200	LYS
1	A	210	ARG
1	A	218	LEU
1	A	219	SER
1	A	221	GLU
1	A	223	GLU
1	A	225	ASP
1	A	229	LEU
1	A	231	CYS
1	A	235	THR
1	A	237	LYS
1	A	247	LEU
1	A	249	ARG
1	A	250	VAL
1	A	256	VAL
1	A	260	VAL
1	A	261	ASN
1	A	263	LYS
1	A	265	ASP
1	A	270	LEU
1	A	271	LEU
1	A	276	GLU
1	A	280	LYS
1	A	298	LEU
1	A	301	LYS
1	A	302	ASP
1	A	303	SER
1	A	308	SER
1	A	310	VAL
1	A	313	ARG
1	A	322	SER
1	A	331	LEU
1	A	332	ARG

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Mol	Chain	Res	Type
1	A	342	ARG
1	A	344	ARG
1	A	356	ARG
1	A	364	LEU
1	A	384	VAL
1	A	417	SER
1	A	419	GLN
1	A	422	ASP
1	A	436	LEU
1	A	440	VAL
1	A	444	SER
1	A	446	THR
1	A	463	VAL
1	A	476	LEU
1	A	484	LYS
1	A	495	PRO
1	A	514	GLU
1	A	538	ASN
1	A	564	LYS
1	A	567	LYS
1	A	573	LEU
1	A	574	LEU
1	A	576	LEU
1	A	623	ASN
1	A	629	ASP
1	A	636	SER
1	A	638	THR
1	A	646	ASN
1	A	660	GLU
1	A	663	LEU
1	A	666	GLN
1	A	673	ASN
1	A	675	LYS
1	A	676	LYS
1	A	678	SER
1	A	679	THR
1	A	683	LEU
1	A	684	GLU
1	A	687	GLU
1	A	691	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	47	GLN
1	A	52	ASN
1	A	91	HIS
1	A	105	GLN
1	A	107	ASN
1	A	110	GLN
1	A	165	GLN
1	A	234	ASN
1	A	275	GLN
1	A	353	GLN
1	A	418	GLN
1	A	419	GLN
1	A	479	GLN
1	A	502	ASN
1	A	522	ASN
1	A	552	GLN
1	A	597	HIS
1	A	635	GLN
1	A	646	ASN
1	A	673	ASN

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 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	691/691 (100%)	-0.02	8 (1%) 76 68	18, 35, 62, 95	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	419	GLN	2.9
1	A	3	ARG	2.9
1	A	637	GLU	2.8
1	A	420	SER	2.7
1	A	1	GLY	2.4
1	A	20	PHE	2.1
1	A	2	ARG	2.1
1	A	638	THR	2.1

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($\text{\AA}^2$)	Q<0.9
2	CL	A	692	1/1	0.98	0.07	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.