



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:45 AM UTC

PDB ID : 1LCF / pdb_00001lcf
Title : CRYSTAL STRUCTURE OF COPPER-AND OXALATE-SUBSTITUTED
HUMAN LACTOFERRIN AT 2.0 ANGSTROMS RESOLUTION
Authors : Smith, C.A.; Anderson, B.F.; Baker, H.M.; Baker, E.N.
Deposited on : 1994-01-11
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

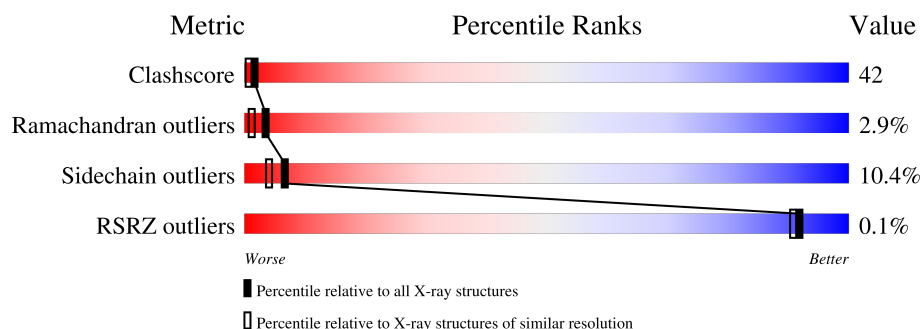
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	691	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	OXL	A	696	-	X	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5664 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.

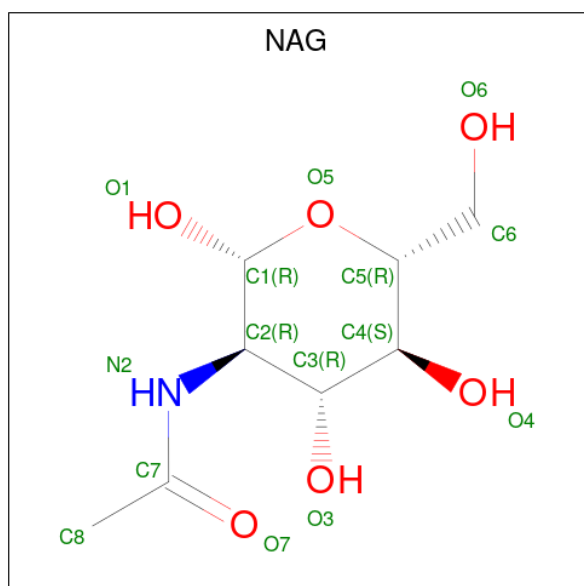
- Molecule 1 is a protein called LACTOFERRIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	691	5313	3321	946	1009	37	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	ASN	GLN	conflict	UNP P02788
A	37	LEU	ILE	conflict	UNP P02788
A	200	LYS	ARG	conflict	UNP P02788

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

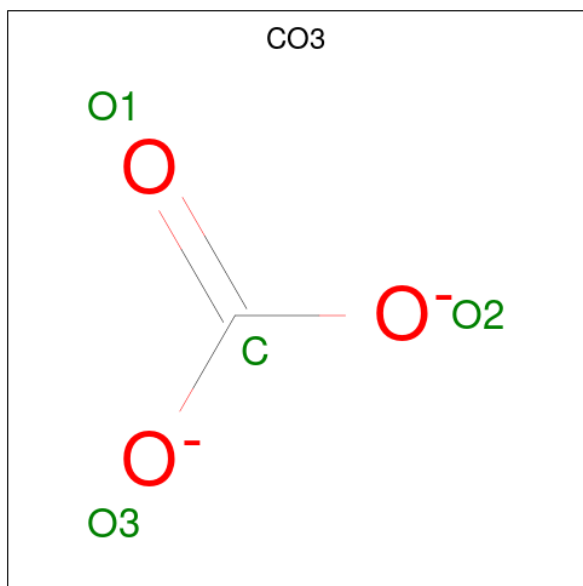


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	14	8	1	5	0	0

- Molecule 3 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

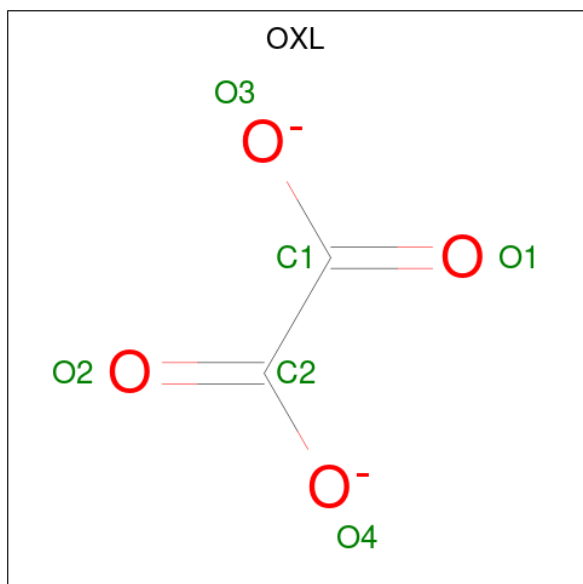
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cu	0	0
			2	2		

- Molecule 4 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).



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

- Molecule 5 is OXALATE ION (CCD ID: OXL) (formula: C₂O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	2	4		

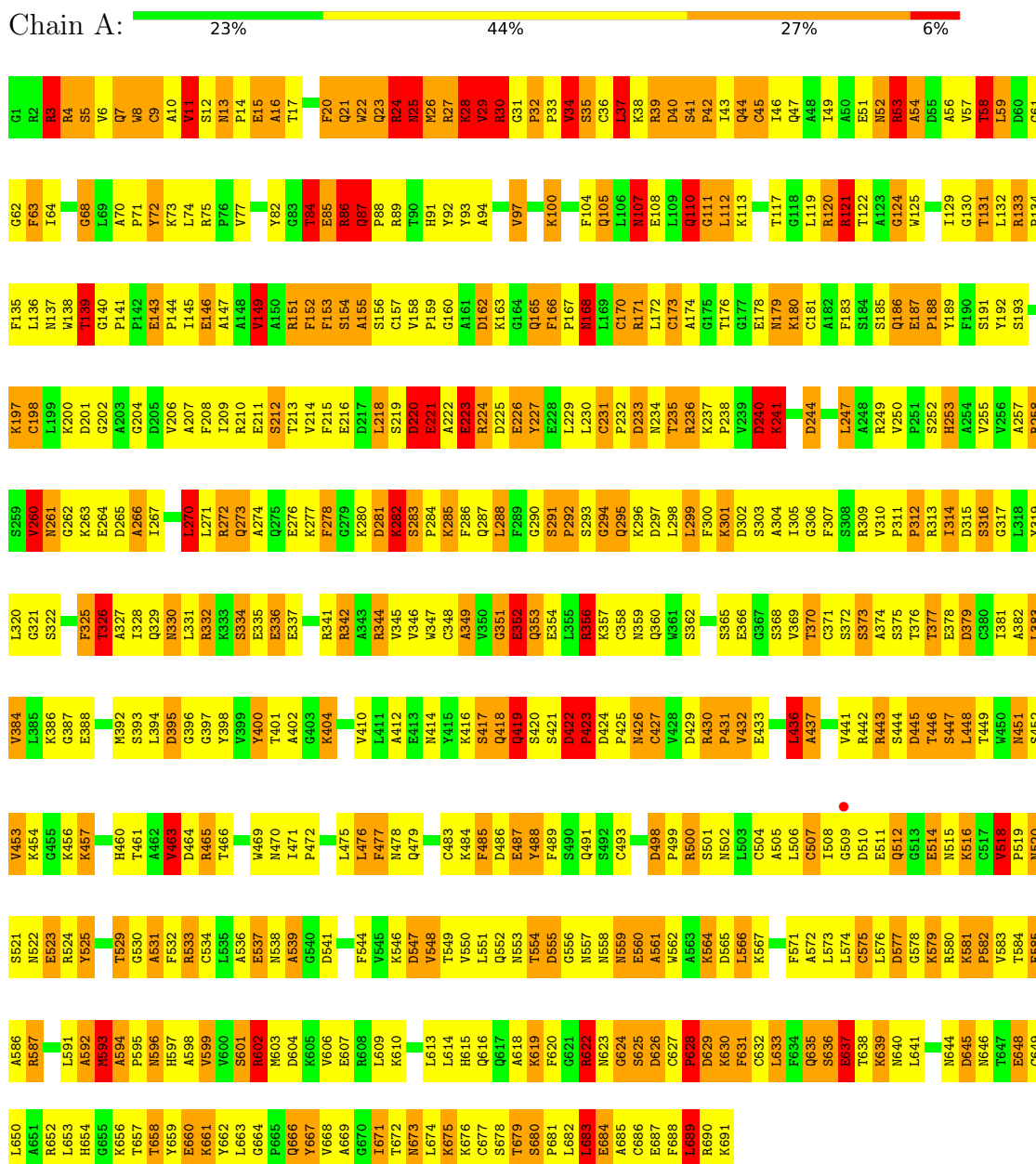
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	325	Total	O	0	0
			325	325		

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	155.80Å 97.10Å 56.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00 8.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.00) 85.2 (8.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.00Å)	Xtriage
Refinement program	PROFFT	Depositor
R, R_{free}	0.193 , (Not available) 0.210 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , 86.1	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	0.96	EDS
Total number of atoms	5664	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.27	4/5427 (0.1%)	3.15	786/7343 (10.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	623	ASN	N-CA	5.60	1.53	1.46
1	A	549	THR	CA-CB	5.55	1.61	1.53
1	A	437	ALA	C-O	5.15	1.30	1.24
1	A	529	THR	CA-CB	5.04	1.61	1.53

All (786) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	ARG	CD-NE-CZ	23.26	156.96	124.40
1	A	30	ARG	CD-NE-CZ	17.94	149.51	124.40
1	A	426	ASN	CA-CB-CG	-16.91	95.69	112.60
1	A	518	VAL	N-CA-CB	-16.45	93.05	109.99
1	A	264	GLU	CB-CG-CD	14.91	137.95	112.60
1	A	87	GLN	CB-CG-CD	14.80	137.76	112.60
1	A	264	GLU	CA-CB-CG	14.71	143.51	114.10
1	A	141	PRO	O-C-N	-14.40	114.69	121.31
1	A	276	GLU	CA-CB-CG	14.31	142.71	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	262	GLY	N-CA-C	14.28	131.95	113.24
1	A	13	ASN	O-C-N	13.98	129.91	120.27
1	A	478	ASN	CA-CB-CG	13.92	126.52	112.60
1	A	430	ARG	NE-CZ-NH2	13.34	131.20	119.20
1	A	443	ARG	CD-NE-CZ	-13.23	105.88	124.40
1	A	587	ARG	CD-NE-CZ	13.23	142.92	124.40
1	A	141	PRO	CA-C-O	13.16	130.38	120.90
1	A	250	VAL	N-CA-CB	-12.94	100.67	111.67
1	A	626	ASP	CA-CB-CG	12.93	125.53	112.60
1	A	602	ARG	NE-CZ-NH2	-12.66	107.81	119.20
1	A	52	ASN	CA-C-O	-12.11	106.99	121.40
1	A	221	GLU	CB-CG-CD	11.52	132.18	112.60
1	A	430	ARG	CD-NE-CZ	-11.12	108.83	124.40
1	A	97	VAL	O-C-N	11.02	134.38	123.14
1	A	418	GLN	CA-C-N	11.01	142.57	121.54
1	A	418	GLN	C-N-CA	11.01	142.57	121.54
1	A	137	ASN	OD1-CG-ND2	10.94	133.54	122.60
1	A	11	VAL	N-CA-CB	-10.88	98.01	112.16
1	A	226	GLU	CB-CG-CD	10.87	131.08	112.60
1	A	560	GLU	N-CA-C	-10.85	96.21	110.53
1	A	141	PRO	CB-CA-C	10.82	121.56	111.39
1	A	75	ARG	CD-NE-CZ	10.80	139.52	124.40
1	A	187	GLU	CA-C-O	10.77	126.29	119.29
1	A	351	GLY	CA-C-O	10.77	131.01	122.29
1	A	378	GLU	CA-C-N	10.69	134.60	120.28
1	A	378	GLU	C-N-CA	10.69	134.60	120.28
1	A	261	ASN	CA-C-N	10.64	133.44	120.14
1	A	261	ASN	C-N-CA	10.64	133.44	120.14
1	A	152	PHE	CA-CB-CG	-10.61	103.19	113.80
1	A	635	GLN	CA-C-N	10.57	138.25	121.44
1	A	635	GLN	C-N-CA	10.57	138.25	121.44
1	A	558	ASN	CA-CB-CG	10.54	123.14	112.60
1	A	485	PHE	CA-CB-CG	10.51	124.31	113.80
1	A	143	GLU	N-CA-CB	10.42	123.88	110.23
1	A	198	CYS	O-C-N	-10.35	110.20	122.11
1	A	4	ARG	CA-C-O	10.25	135.17	120.51
1	A	120	ARG	CD-NE-CZ	-10.25	110.05	124.40
1	A	558	ASN	OD1-CG-ND2	-10.23	112.37	122.60
1	A	370	THR	CA-CB-OG1	-10.19	94.32	109.60
1	A	581	LYS	O-C-N	10.10	129.43	121.55
1	A	426	ASN	OD1-CG-ND2	10.06	132.66	122.60
1	A	193	SER	CA-C-O	-9.98	110.42	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	GLU	N-CA-C	-9.95	100.39	111.14
1	A	41	SER	N-CA-C	9.92	116.90	108.07
1	A	623	ASN	CB-CA-C	9.85	130.01	110.42
1	A	466	THR	CA-C-O	-9.80	110.71	121.00
1	A	687	GLU	N-CA-C	-9.80	100.59	111.07
1	A	212	SER	CA-CB-OG	9.79	130.69	111.10
1	A	466	THR	CA-CB-OG1	-9.73	95.01	109.60
1	A	309	ARG	CD-NE-CZ	9.67	137.94	124.40
1	A	168	ASN	CA-CB-CG	-9.67	102.93	112.60
1	A	537	GLU	CA-C-O	9.62	131.59	119.95
1	A	107	ASN	CA-CB-CG	-9.61	102.99	112.60
1	A	657	THR	CA-C-N	9.60	138.29	122.73
1	A	657	THR	C-N-CA	9.60	138.29	122.73
1	A	20	PHE	O-C-N	9.60	131.96	122.07
1	A	445	ASP	CA-C-O	-9.59	110.26	122.63
1	A	445	ASP	O-C-N	9.52	134.60	122.71
1	A	625	SER	CA-CB-OG	9.51	130.11	111.10
1	A	560	GLU	CA-CB-CG	9.47	133.03	114.10
1	A	447	SER	N-CA-C	9.43	124.04	112.54
1	A	640	ASN	CA-C-N	9.41	135.01	122.30
1	A	640	ASN	C-N-CA	9.41	135.01	122.30
1	A	395	ASP	CA-C-O	-9.41	111.31	121.56
1	A	631	PHE	CA-CB-CG	9.36	123.16	113.80
1	A	133	ARG	NE-CZ-NH1	9.31	130.81	121.50
1	A	37	LEU	CA-C-O	-9.30	110.60	121.11
1	A	677	CYS	O-C-N	9.28	134.45	122.39
1	A	682	LEU	CA-C-O	-9.26	110.61	120.42
1	A	85	GLU	O-C-N	9.25	132.75	122.11
1	A	501	SER	CA-C-N	9.21	133.55	120.28
1	A	501	SER	C-N-CA	9.21	133.55	120.28
1	A	635	GLN	OE1-CD-NE2	9.20	131.80	122.60
1	A	469	TRP	CA-C-O	-9.18	107.39	120.51
1	A	133	ARG	NE-CZ-NH2	-9.16	110.95	119.20
1	A	646	ASN	OD1-CG-ND2	9.15	131.75	122.60
1	A	236	ARG	NE-CZ-NH2	9.14	127.43	119.20
1	A	325	PHE	CA-C-O	9.10	130.20	120.55
1	A	170	CYS	CA-C-O	9.10	129.52	119.15
1	A	637	GLU	CB-CG-CD	9.02	127.93	112.60
1	A	381	ILE	CA-C-O	-9.01	111.30	120.85
1	A	30	ARG	NE-CZ-NH1	8.99	130.50	121.50
1	A	186	GLN	N-CA-C	-8.97	101.51	111.28
1	A	119	LEU	CA-C-O	-8.96	111.12	121.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	648	GLU	CA-CB-CG	8.95	132.01	114.10
1	A	110	GLN	N-CA-CB	8.88	123.24	109.83
1	A	258	ARG	NE-CZ-NH2	8.87	127.18	119.20
1	A	105	GLN	OE1-CD-NE2	8.86	131.46	122.60
1	A	157	CYS	CA-C-O	-8.85	110.59	120.32
1	A	666	GLN	O-C-N	8.83	131.17	122.07
1	A	86	ARG	NE-CZ-NH1	8.80	130.30	121.50
1	A	430	ARG	NE-CZ-NH1	-8.79	112.71	121.50
1	A	356	ARG	N-CA-CB	8.78	123.02	109.94
1	A	11	VAL	CB-CA-C	8.72	122.29	111.65
1	A	351	GLY	CA-C-N	8.71	131.76	120.44
1	A	351	GLY	C-N-CA	8.71	131.76	120.44
1	A	224	ARG	CD-NE-CZ	-8.69	112.23	124.40
1	A	640	ASN	CA-CB-CG	8.69	121.29	112.60
1	A	294	GLY	CA-C-N	8.68	138.12	121.54
1	A	294	GLY	C-N-CA	8.68	138.12	121.54
1	A	502	ASN	O-C-N	8.68	132.38	122.22
1	A	484	LYS	O-C-N	8.66	132.34	122.55
1	A	376	THR	CA-C-N	8.66	132.59	120.29
1	A	376	THR	C-N-CA	8.66	132.59	120.29
1	A	673	ASN	OD1-CG-ND2	8.65	131.25	122.60
1	A	120	ARG	CA-CB-CG	-8.64	96.82	114.10
1	A	87	GLN	CB-CA-C	8.60	127.12	110.17
1	A	442	ARG	NE-CZ-NH2	8.59	126.93	119.20
1	A	278	PHE	CA-CB-CG	-8.59	105.21	113.80
1	A	618	ALA	O-C-N	8.58	132.82	122.27
1	A	417	SER	CA-CB-OG	8.56	128.22	111.10
1	A	514	GLU	CA-CB-CG	8.56	131.21	114.10
1	A	304	ALA	N-CA-C	-8.54	99.26	110.53
1	A	92	TYR	CA-C-O	-8.54	111.95	121.51
1	A	64	ILE	N-CA-C	-8.49	102.55	110.53
1	A	657	THR	CA-CB-OG1	-8.46	96.91	109.60
1	A	559	ASN	CA-CB-CG	-8.39	104.21	112.60
1	A	75	ARG	O-C-N	8.38	129.94	121.72
1	A	309	ARG	NE-CZ-NH2	-8.37	111.67	119.20
1	A	200	LYS	CA-CB-CG	8.37	130.84	114.10
1	A	332	ARG	CA-CB-CG	8.36	130.82	114.10
1	A	420	SER	N-CA-C	-8.34	102.04	112.72
1	A	255	VAL	CA-C-O	-8.34	111.35	120.85
1	A	40	ASP	O-C-N	8.30	132.56	122.35
1	A	548	VAL	N-CA-CB	-8.30	97.54	111.23
1	A	448	LEU	CA-C-O	-8.24	110.93	120.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	ASP	CA-C-O	-8.23	112.55	121.44
1	A	453	VAL	CA-C-O	-8.19	111.95	120.71
1	A	8	TRP	O-C-N	8.17	132.66	123.01
1	A	299	LEU	O-C-N	8.17	133.45	122.59
1	A	629	ASP	O-C-N	8.16	130.81	122.08
1	A	518	VAL	CB-CA-C	8.16	119.00	111.00
1	A	211	GLU	CG-CD-OE1	8.14	137.12	118.40
1	A	15	GLU	N-CA-CB	8.13	122.38	110.26
1	A	153	PHE	CA-CB-CG	8.11	121.91	113.80
1	A	213	THR	CA-CB-OG1	-8.06	97.50	109.60
1	A	432	VAL	CB-CA-C	8.06	122.41	111.28
1	A	530	GLY	CA-C-O	-8.06	112.12	120.66
1	A	553	ASN	CA-CB-CG	8.04	120.64	112.60
1	A	684	GLU	CB-CG-CD	-8.03	98.94	112.60
1	A	39	ARG	NE-CZ-NH1	-8.01	113.49	121.50
1	A	70	ALA	N-CA-C	-8.00	98.68	110.20
1	A	371	CYS	N-CA-C	7.97	122.62	109.95
1	A	197	LYS	N-CA-C	-7.95	102.56	111.14
1	A	493	CYS	N-CA-CB	7.94	123.81	110.87
1	A	233	ASP	CA-CB-CG	-7.93	104.67	112.60
1	A	656	LYS	CB-CA-C	-7.92	99.67	112.03
1	A	442	ARG	NE-CZ-NH1	-7.91	113.59	121.50
1	A	683	LEU	N-CA-CB	7.90	122.53	110.28
1	A	165	GLN	CA-C-O	-7.89	110.48	119.79
1	A	348	CYS	CA-C-N	7.87	133.57	122.72
1	A	348	CYS	C-N-CA	7.87	133.57	122.72
1	A	75	ARG	CA-C-O	-7.86	110.72	120.23
1	A	554	THR	CA-CB-OG1	-7.85	97.82	109.60
1	A	143	GLU	CG-CD-OE2	7.84	136.44	118.40
1	A	470	ASN	OD1-CG-ND2	-7.83	114.77	122.60
1	A	94	ALA	CB-CA-C	7.82	123.72	110.81
1	A	372	SER	CA-C-O	-7.82	112.57	121.40
1	A	131	THR	CA-CB-CG2	7.80	123.76	110.50
1	A	319	TYR	CA-C-O	7.79	128.81	120.55
1	A	258	ARG	CA-C-O	7.79	130.05	121.56
1	A	137	ASN	CA-CB-CG	7.79	120.39	112.60
1	A	52	ASN	O-C-N	7.79	131.47	122.67
1	A	356	ARG	CB-CG-CD	7.78	129.19	111.30
1	A	235	THR	CA-C-O	-7.74	112.38	121.44
1	A	572	ALA	CA-C-O	-7.73	113.18	121.45
1	A	22	TRP	CB-CA-C	7.72	123.00	110.88
1	A	34	VAL	CB-CA-C	-7.69	99.37	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	ILE	O-C-N	7.64	129.28	121.87
1	A	8	TRP	CA-C-O	-7.62	112.36	121.05
1	A	281	ASP	CA-CB-CG	-7.61	104.99	112.60
1	A	575	CYS	O-C-N	7.59	131.60	123.03
1	A	633	LEU	N-CA-CB	-7.59	98.93	110.16
1	A	623	ASN	CA-C-O	7.58	131.35	120.51
1	A	163	LYS	N-CA-CB	7.58	122.02	110.28
1	A	372	SER	CA-CB-OG	-7.57	95.96	111.10
1	A	573	LEU	CA-C-O	-7.57	112.35	121.28
1	A	446	THR	CA-C-N	7.57	133.35	120.72
1	A	446	THR	C-N-CA	7.57	133.35	120.72
1	A	593	MET	CA-CB-CG	7.55	129.20	114.10
1	A	287	GLN	OE1-CD-NE2	7.55	130.15	122.60
1	A	618	ALA	N-CA-C	-7.53	103.09	111.82
1	A	666	GLN	N-CA-C	-7.52	103.02	111.07
1	A	3	ARG	CD-NE-CZ	7.51	134.91	124.40
1	A	648	GLU	CG-CD-OE2	7.50	135.64	118.40
1	A	640	ASN	O-C-N	-7.49	113.87	122.86
1	A	104	PHE	O-C-N	7.49	132.17	123.41
1	A	557	ASN	OD1-CG-ND2	-7.48	115.12	122.60
1	A	313	ARG	NE-CZ-NH1	7.48	128.98	121.50
1	A	34	VAL	CA-C-O	-7.45	112.58	120.48
1	A	657	THR	N-CA-CB	-7.44	99.02	110.92
1	A	168	ASN	CA-C-O	7.41	128.48	120.10
1	A	673	ASN	CA-CB-CG	-7.41	105.19	112.60
1	A	132	LEU	CA-C-O	-7.39	110.70	119.35
1	A	422	ASP	CA-CB-CG	7.38	119.98	112.60
1	A	478	ASN	CA-C-O	-7.37	110.57	119.49
1	A	85	GLU	CB-CG-CD	7.37	125.13	112.60
1	A	70	ALA	CB-CA-C	7.35	123.11	109.51
1	A	550	VAL	CA-C-O	-7.34	112.90	121.05
1	A	105	GLN	CA-CB-CG	-7.33	99.44	114.10
1	A	564	LYS	CG-CD-CE	7.32	128.14	111.30
1	A	337	GLU	N-CA-C	-7.32	103.23	111.14
1	A	32	PRO	CB-CA-C	7.30	119.83	110.92
1	A	444	SER	CA-CB-OG	7.30	125.69	111.10
1	A	168	ASN	N-CA-CB	-7.27	99.02	110.22
1	A	165	GLN	O-C-N	7.25	132.05	122.33
1	A	532	PHE	CA-CB-CG	-7.24	106.56	113.80
1	A	644	ASN	OD1-CG-ND2	-7.24	115.36	122.60
1	A	234	ASN	CA-C-O	-7.22	113.46	121.84
1	A	44	GLN	N-CA-C	-7.22	103.34	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	HIS	CA-CB-CG	-7.22	106.58	113.80
1	A	644	ASN	CB-CG-ND2	7.21	127.22	116.40
1	A	396	GLY	CA-C-N	7.21	129.38	120.22
1	A	396	GLY	C-N-CA	7.21	129.38	120.22
1	A	544	PHE	CA-C-O	-7.20	113.05	120.54
1	A	625	SER	CA-C-O	-7.20	110.22	120.51
1	A	284	PRO	CB-CA-C	7.19	122.12	111.62
1	A	53	ARG	CA-C-N	7.17	136.46	121.91
1	A	53	ARG	C-N-CA	7.17	136.46	121.91
1	A	558	ASN	N-CA-CB	7.16	122.84	110.81
1	A	388	GLU	CB-CG-CD	-7.15	100.45	112.60
1	A	171	ARG	NE-CZ-NH1	7.13	128.63	121.50
1	A	74	LEU	N-CA-C	-7.12	100.94	110.55
1	A	685	ALA	O-C-N	-7.12	114.74	122.07
1	A	144	PRO	O-C-N	7.11	132.02	122.99
1	A	42	PRO	O-C-N	-7.11	114.07	122.24
1	A	597	HIS	CB-CG-CD2	-7.10	121.97	131.20
1	A	54	ALA	N-CA-CB	7.10	122.35	111.56
1	A	273	GLN	OE1-CD-NE2	7.08	129.68	122.60
1	A	157	CYS	CA-C-N	7.08	135.23	122.13
1	A	157	CYS	C-N-CA	7.08	135.23	122.13
1	A	178	GLU	CB-CG-CD	7.08	124.64	112.60
1	A	619	LYS	CA-CB-CG	7.08	128.25	114.10
1	A	520	ASN	CB-CG-ND2	-7.07	105.80	116.40
1	A	270	LEU	O-C-N	-7.06	114.75	122.09
1	A	160	GLY	CA-C-O	-7.05	111.93	119.27
1	A	586	ALA	O-C-N	7.05	130.47	122.22
1	A	637	GLU	CA-C-N	7.05	135.01	121.54
1	A	637	GLU	C-N-CA	7.05	135.01	121.54
1	A	58	THR	CB-CA-C	7.05	121.99	110.22
1	A	326	THR	CB-CA-C	7.04	122.83	110.85
1	A	26	MET	N-CA-C	-7.04	95.80	110.80
1	A	151	ARG	NE-CZ-NH2	-7.03	112.87	119.20
1	A	377	THR	CA-CB-OG1	-7.02	99.07	109.60
1	A	312	PRO	CB-CA-C	7.02	121.86	111.62
1	A	604	ASP	CA-CB-CG	7.00	119.60	112.60
1	A	110	GLN	CA-CB-CG	7.00	128.09	114.10
1	A	386	LYS	O-C-N	6.99	132.10	122.46
1	A	7	GLN	CB-CG-CD	-6.98	100.74	112.60
1	A	326	THR	CA-CB-OG1	-6.97	99.14	109.60
1	A	360	GLN	N-CA-CB	6.97	120.33	109.94
1	A	160	GLY	N-CA-C	-6.97	106.78	115.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	423	PRO	N-CA-C	-6.97	98.11	112.47
1	A	249	ARG	CB-CA-C	6.97	121.73	110.16
1	A	445	ASP	CB-CA-C	-6.96	101.68	112.12
1	A	144	PRO	CA-C-O	-6.96	113.64	121.43
1	A	518	VAL	CA-CB-CG1	6.96	122.22	110.40
1	A	384	VAL	CA-CB-CG1	6.95	122.22	110.40
1	A	603	MET	CB-CG-SD	-6.94	91.88	112.70
1	A	247	LEU	N-CA-C	-6.92	104.65	113.23
1	A	436	LEU	CA-C-O	-6.90	112.91	120.43
1	A	236	ARG	NE-CZ-NH1	-6.89	114.61	121.50
1	A	422	ASP	CB-CA-C	6.89	123.74	110.17
1	A	75	ARG	CG-CD-NE	6.88	127.13	112.00
1	A	75	ARG	NE-CZ-NH2	6.87	125.38	119.20
1	A	337	GLU	O-C-N	-6.87	114.67	122.09
1	A	586	ALA	CA-C-O	-6.87	112.34	120.10
1	A	151	ARG	NH1-CZ-NH2	6.85	128.20	119.30
1	A	331	LEU	O-C-N	6.82	131.57	122.43
1	A	379	ASP	CA-CB-CG	-6.82	105.78	112.60
1	A	37	LEU	O-C-N	6.81	132.04	123.19
1	A	198	CYS	CA-C-O	6.80	128.54	120.92
1	A	384	VAL	N-CA-CB	6.80	123.81	110.95
1	A	168	ASN	OD1-CG-ND2	6.80	129.40	122.60
1	A	16	ALA	CA-C-O	6.79	127.62	120.42
1	A	502	ASN	CA-CB-CG	-6.79	105.81	112.60
1	A	536	ALA	O-C-N	6.79	131.46	122.43
1	A	304	ALA	CA-C-O	-6.77	114.01	121.87
1	A	650	LEU	CA-C-O	-6.77	113.11	120.36
1	A	602	ARG	N-CA-C	-6.76	100.51	110.52
1	A	86	ARG	N-CA-CB	6.75	121.90	110.49
1	A	53	ARG	CB-CG-CD	6.74	126.81	111.30
1	A	489	PHE	CA-CB-CG	-6.72	107.08	113.80
1	A	639	LYS	N-CA-CB	6.72	120.54	110.53
1	A	619	LYS	N-CA-CB	-6.71	100.15	110.42
1	A	278	PHE	N-CA-C	6.71	121.48	113.16
1	A	487	GLU	O-C-N	6.71	130.12	122.20
1	A	56	ALA	N-CA-CB	-6.71	101.16	111.56
1	A	418	GLN	CA-C-O	6.71	130.10	120.51
1	A	640	ASN	N-CA-CB	-6.70	101.52	111.71
1	A	220	ASP	O-C-N	6.70	131.39	122.82
1	A	531	ALA	N-CA-C	-6.69	104.06	111.36
1	A	143	GLU	CG-CD-OE1	-6.68	103.03	118.40
1	A	237	LYS	CA-C-O	-6.68	114.90	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	673	ASN	CB-CG-OD1	-6.68	107.45	120.80
1	A	636	SER	O-C-N	6.67	129.37	122.09
1	A	648	GLU	N-CA-C	-6.67	103.48	111.69
1	A	378	GLU	O-C-N	-6.67	115.05	122.12
1	A	639	LYS	CA-C-O	-6.67	111.55	119.15
1	A	624	GLY	CA-C-O	6.67	126.16	120.76
1	A	592	ALA	CA-C-N	6.65	131.28	122.30
1	A	592	ALA	C-N-CA	6.65	131.28	122.30
1	A	327	ALA	CA-C-N	6.64	129.85	120.42
1	A	327	ALA	C-N-CA	6.64	129.85	120.42
1	A	325	PHE	O-C-N	-6.64	115.08	122.12
1	A	541	ASP	O-C-N	6.63	129.63	122.34
1	A	215	PHE	CA-CB-CG	6.62	120.42	113.80
1	A	546	LYS	CA-C-N	-6.62	111.84	120.44
1	A	546	LYS	C-N-CA	-6.62	111.84	120.44
1	A	582	PRO	O-C-N	-6.61	115.08	123.14
1	A	524	ARG	CD-NE-CZ	6.60	133.63	124.40
1	A	616	GLN	CA-C-O	-6.60	112.81	120.20
1	A	491	GLN	CA-CB-CG	-6.59	100.92	114.10
1	A	53	ARG	CD-NE-CZ	-6.58	115.19	124.40
1	A	598	ALA	CA-C-N	-6.57	113.90	122.37
1	A	598	ALA	C-N-CA	-6.57	113.90	122.37
1	A	22	TRP	N-CA-C	-6.56	104.05	111.07
1	A	223	GLU	CA-C-O	6.55	127.45	120.70
1	A	27	ARG	CA-CB-CG	6.55	127.20	114.10
1	A	178	GLU	CB-CA-C	6.54	122.96	110.27
1	A	171	ARG	NH1-CZ-NH2	-6.54	110.80	119.30
1	A	663	LEU	CA-C-O	-6.53	113.50	120.42
1	A	297	ASP	CA-CB-CG	-6.52	106.08	112.60
1	A	401	THR	CA-CB-OG1	-6.52	99.82	109.60
1	A	260	VAL	CB-CA-C	-6.51	100.61	111.29
1	A	453	VAL	O-C-N	6.51	130.43	121.84
1	A	35	SER	N-CA-C	-6.50	100.84	110.46
1	A	660	GLU	OE1-CD-OE2	6.50	138.49	122.90
1	A	460	HIS	CA-C-O	-6.50	113.77	121.11
1	A	39	ARG	NE-CZ-NH2	6.49	125.04	119.20
1	A	295	GLN	N-CA-C	6.49	124.62	110.80
1	A	602	ARG	NE-CZ-NH1	6.49	127.99	121.50
1	A	489	PHE	CA-C-O	-6.47	113.79	121.11
1	A	309	ARG	NH1-CZ-NH2	6.47	127.71	119.30
1	A	10	ALA	O-C-N	-6.47	115.82	123.06
1	A	61	GLY	CA-C-O	-6.47	114.46	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	538	ASN	O-C-N	6.46	130.86	122.40
1	A	120	ARG	NH1-CZ-NH2	6.45	127.69	119.30
1	A	547	ASP	CA-C-O	6.45	127.59	120.82
1	A	307	PHE	CA-CB-CG	-6.44	107.36	113.80
1	A	404	LYS	N-CA-C	-6.44	105.28	113.01
1	A	629	ASP	CA-CB-CG	-6.43	106.17	112.60
1	A	441	VAL	CA-C-O	-6.42	115.27	121.63
1	A	645	ASP	CA-CB-CG	-6.42	106.18	112.60
1	A	313	ARG	NE-CZ-NH2	-6.42	113.42	119.20
1	A	466	THR	CA-CB-CG2	6.42	121.41	110.50
1	A	12	SER	CA-C-O	6.41	128.18	121.38
1	A	359	ASN	CB-CA-C	6.41	121.06	110.81
1	A	132	LEU	O-C-N	6.41	130.35	122.34
1	A	255	VAL	CB-CA-C	6.40	119.47	111.15
1	A	163	LYS	CA-CB-CG	6.39	126.88	114.10
1	A	400	TYR	O-C-N	-6.38	115.39	122.03
1	A	466	THR	O-C-N	6.38	128.66	122.03
1	A	547	ASP	CA-CB-CG	-6.38	106.22	112.60
1	A	58	THR	O-C-N	-6.38	115.80	123.13
1	A	192	TYR	N-CA-C	6.37	117.89	111.07
1	A	512	GLN	CA-C-O	-6.37	111.66	119.18
1	A	466	THR	N-CA-C	6.37	117.91	110.97
1	A	10	ALA	CB-CA-C	6.36	120.39	109.51
1	A	249	ARG	N-CA-C	-6.36	98.05	108.41
1	A	444	SER	N-CA-C	6.35	120.13	112.38
1	A	326	THR	N-CA-CB	-6.35	100.77	110.16
1	A	441	VAL	O-C-N	6.34	130.19	123.02
1	A	620	PHE	CA-C-O	-6.34	111.70	119.18
1	A	105	GLN	N-CA-CB	-6.34	100.97	110.60
1	A	488	TYR	CB-CG-CD1	6.34	130.31	120.80
1	A	491	GLN	N-CA-CB	6.33	121.23	110.71
1	A	29	VAL	CB-CA-C	6.33	121.68	111.29
1	A	369	VAL	O-C-N	6.33	129.91	123.07
1	A	603	MET	N-CA-CB	-6.33	100.47	110.22
1	A	30	ARG	NE-CZ-NH2	-6.33	113.50	119.20
1	A	220	ASP	CA-CB-CG	-6.33	106.27	112.60
1	A	386	LYS	CB-CA-C	-6.32	97.28	110.17
1	A	414	ASN	CB-CG-ND2	6.32	125.87	116.40
1	A	493	CYS	O-C-N	6.32	132.59	122.99
1	A	460	HIS	O-C-N	6.31	131.40	123.19
1	A	105	GLN	CA-C-O	-6.31	113.21	121.73
1	A	618	ALA	N-CA-CB	6.31	120.06	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	20	PHE	CA-CB-CG	-6.31	107.49	113.80
1	A	224	ARG	NH1-CZ-NH2	6.31	127.50	119.30
1	A	512	GLN	O-C-N	6.29	129.63	122.20
1	A	671	ILE	O-C-N	6.28	128.90	121.80
1	A	548	VAL	CB-CA-C	6.28	121.59	111.29
1	A	572	ALA	O-C-N	6.28	130.32	123.10
1	A	465	ARG	CG-CD-NE	-6.27	98.20	112.00
1	A	54	ALA	N-CA-C	-6.27	98.77	108.42
1	A	129	ILE	CB-CA-C	6.27	120.87	112.22
1	A	393	SER	CA-C-N	-6.27	112.75	122.59
1	A	393	SER	C-N-CA	-6.27	112.75	122.59
1	A	28	LYS	N-CA-CB	-6.24	99.94	110.49
1	A	573	LEU	CA-C-N	6.24	130.72	122.30
1	A	573	LEU	C-N-CA	6.24	130.72	122.30
1	A	146	GLU	O-C-N	6.23	128.57	122.09
1	A	523	GLU	CB-CA-C	6.23	120.00	109.84
1	A	316	SER	CA-C-N	-6.23	113.15	120.00
1	A	316	SER	C-N-CA	-6.23	113.15	120.00
1	A	168	ASN	CA-C-N	6.23	131.26	120.68
1	A	168	ASN	C-N-CA	6.23	131.26	120.68
1	A	533	ARG	CA-C-N	6.22	128.90	120.38
1	A	533	ARG	C-N-CA	6.22	128.90	120.38
1	A	476	LEU	CA-C-O	6.21	127.09	120.70
1	A	15	GLU	CA-C-O	-6.20	112.44	120.00
1	A	461	THR	N-CA-C	-6.20	104.21	110.97
1	A	206	VAL	CA-C-O	-6.18	113.96	120.76
1	A	342	ARG	CA-CB-CG	6.17	126.45	114.10
1	A	104	PHE	N-CA-C	-6.17	98.19	108.75
1	A	470	ASN	CB-CG-ND2	6.15	125.63	116.40
1	A	620	PHE	O-C-N	6.15	129.46	122.20
1	A	635	GLN	CG-CD-NE2	-6.15	107.18	116.40
1	A	676	LYS	CB-CA-C	-6.15	99.26	110.63
1	A	470	ASN	CA-C-N	6.15	133.50	122.13
1	A	470	ASN	C-N-CA	6.15	133.50	122.13
1	A	273	GLN	CA-C-O	6.14	127.27	120.82
1	A	337	GLU	CA-C-N	6.14	128.88	120.46
1	A	337	GLU	C-N-CA	6.14	128.88	120.46
1	A	162	ASP	CA-C-O	-6.14	113.66	120.60
1	A	594	ALA	CB-CA-C	6.14	117.21	108.68
1	A	23	GLN	OE1-CD-NE2	6.13	128.74	122.60
1	A	447	SER	CA-C-O	6.13	126.92	119.38
1	A	21	GLN	CA-CB-CG	6.12	126.35	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	666	GLN	CG-CD-NE2	6.12	125.59	116.40
1	A	660	GLU	CB-CG-CD	-6.12	102.20	112.60
1	A	189	TYR	CA-C-N	6.12	130.17	121.42
1	A	189	TYR	C-N-CA	6.12	130.17	121.42
1	A	604	ASP	CB-CG-OD1	6.12	132.47	118.40
1	A	135	PHE	CA-CB-CG	6.11	119.91	113.80
1	A	577	ASP	CA-CB-CG	6.11	118.71	112.60
1	A	156	SER	CB-CA-C	-6.11	99.20	111.17
1	A	334	SER	N-CA-C	-6.11	102.47	110.53
1	A	108	GLU	CG-CD-OE2	6.11	132.44	118.40
1	A	131	THR	CA-CB-OG1	-6.10	100.45	109.60
1	A	231	CYS	O-C-N	6.10	128.59	121.21
1	A	136	LEU	CA-C-O	-6.09	111.76	119.31
1	A	585	GLU	CB-CG-CD	6.09	122.95	112.60
1	A	84	THR	CA-C-O	6.08	128.64	121.58
1	A	344	ARG	CB-CG-CD	-6.08	97.31	111.30
1	A	584	THR	CB-CA-C	6.06	122.54	110.17
1	A	63	PHE	CA-CB-CG	-6.06	107.74	113.80
1	A	121	ARG	O-C-N	6.04	129.83	123.06
1	A	221	GLU	CA-C-N	6.04	130.26	120.60
1	A	221	GLU	C-N-CA	6.04	130.26	120.60
1	A	273	GLN	CB-CA-C	-6.04	101.40	110.88
1	A	230	LEU	N-CA-C	-6.03	98.90	108.73
1	A	561	ALA	O-C-N	6.03	129.49	122.20
1	A	285	LYS	CA-C-N	6.03	132.52	121.85
1	A	285	LYS	C-N-CA	6.03	132.52	121.85
1	A	29	VAL	CA-CB-CG1	6.02	120.64	110.40
1	A	475	LEU	CA-C-N	6.02	128.63	120.44
1	A	475	LEU	C-N-CA	6.02	128.63	120.44
1	A	610	LYS	CA-C-O	6.01	127.14	120.82
1	A	155	ALA	O-C-N	6.01	130.12	123.33
1	A	332	ARG	N-CA-CB	6.01	120.76	111.39
1	A	287	GLN	CB-CG-CD	-6.00	102.39	112.60
1	A	236	ARG	CD-NE-CZ	-5.99	116.01	124.40
1	A	680	SER	O-C-N	5.99	128.46	121.21
1	A	249	ARG	NE-CZ-NH2	-5.99	113.81	119.20
1	A	288	LEU	CA-C-O	-5.99	113.33	120.10
1	A	597	HIS	N-CA-C	-5.97	101.57	110.23
1	A	188	PRO	CB-CA-C	-5.97	103.37	111.85
1	A	75	ARG	CB-CA-C	-5.96	99.61	109.15
1	A	100	LYS	CA-C-O	-5.96	114.25	121.05
1	A	599	VAL	CB-CA-C	5.96	118.30	110.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	GLU	O-C-N	5.96	126.83	121.35
1	A	486	ASP	CB-CG-OD1	5.95	132.08	118.40
1	A	592	ALA	O-C-N	-5.95	117.67	123.26
1	A	536	ALA	CA-C-O	-5.95	111.61	119.10
1	A	173	CYS	CA-C-O	5.94	127.72	121.19
1	A	237	LYS	CA-C-N	5.94	125.91	120.03
1	A	237	LYS	C-N-CA	5.94	125.91	120.03
1	A	276	GLU	CA-C-N	5.94	132.88	121.54
1	A	276	GLU	C-N-CA	5.94	132.88	121.54
1	A	337	GLU	CB-CG-CD	5.93	122.67	112.60
1	A	619	LYS	CB-CG-CD	-5.92	97.67	111.30
1	A	186	GLN	O-C-N	5.91	128.38	122.12
1	A	186	GLN	OE1-CD-NE2	-5.90	116.70	122.60
1	A	287	GLN	O-C-N	5.90	130.91	123.12
1	A	352	GLU	CA-C-O	-5.90	114.62	120.82
1	A	505	ALA	N-CA-C	5.90	118.47	111.33
1	A	628	PRO	O-C-N	5.90	132.31	121.10
1	A	491	GLN	CB-CA-C	-5.89	99.78	109.80
1	A	381	ILE	N-CA-C	-5.89	104.77	110.72
1	A	171	ARG	N-CA-CB	5.87	120.41	110.49
1	A	130	GLY	CA-C-N	5.87	128.15	120.28
1	A	130	GLY	C-N-CA	5.87	128.15	120.28
1	A	370	THR	CA-C-O	-5.87	114.77	121.58
1	A	156	SER	CA-CB-OG	5.87	122.83	111.10
1	A	550	VAL	O-C-N	5.87	128.00	121.90
1	A	431	PRO	N-CA-CB	5.86	108.45	103.35
1	A	5	SER	N-CA-CB	-5.85	101.54	110.49
1	A	68	GLY	O-C-N	5.85	129.07	122.34
1	A	656	LYS	O-C-N	5.85	129.42	122.46
1	A	180	LYS	CA-CB-CG	-5.85	102.41	114.10
1	A	582	PRO	CB-CA-C	5.83	118.65	110.60
1	A	368	SER	N-CA-CB	5.83	119.22	110.53
1	A	110	GLN	O-C-N	5.83	130.04	122.87
1	A	445	ASP	N-CA-C	-5.83	100.88	109.62
1	A	290	GLY	CA-C-O	-5.82	116.23	121.47
1	A	249	ARG	N-CA-CB	-5.81	101.58	110.65
1	A	392	MET	CA-CB-CG	-5.81	102.48	114.10
1	A	579	LYS	CB-CA-C	-5.81	100.79	112.99
1	A	679	THR	N-CA-CB	5.81	119.62	110.56
1	A	40	ASP	CA-C-N	-5.80	113.65	122.06
1	A	40	ASP	C-N-CA	-5.80	113.65	122.06
1	A	156	SER	CA-C-N	-5.80	114.94	123.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	SER	C-N-CA	-5.80	114.94	123.05
1	A	352	GLU	CG-CD-OE1	5.79	131.72	118.40
1	A	173	CYS	CB-CA-C	5.78	119.31	109.72
1	A	426	ASN	O-C-N	5.78	129.94	122.20
1	A	516	LYS	CA-C-O	5.78	127.50	120.92
1	A	555	ASP	O-C-N	5.78	130.09	122.47
1	A	210	ARG	NE-CZ-NH1	-5.77	115.73	121.50
1	A	139	THR	OG1-CB-CG2	5.76	120.82	109.30
1	A	402	ALA	O-C-N	5.76	128.96	122.22
1	A	326	THR	O-C-N	5.76	128.72	122.15
1	A	6	VAL	N-CA-C	-5.76	99.42	108.23
1	A	487	GLU	OE1-CD-OE2	5.75	136.70	122.90
1	A	427	CYS	CA-C-O	-5.75	111.86	119.10
1	A	165	GLN	CB-CG-CD	-5.74	102.84	112.60
1	A	231	CYS	N-CA-CB	5.74	118.04	109.88
1	A	26	MET	CA-C-N	5.74	132.51	121.54
1	A	26	MET	C-N-CA	5.74	132.51	121.54
1	A	291	SER	CA-C-N	5.74	125.75	119.90
1	A	291	SER	C-N-CA	5.74	125.75	119.90
1	A	383	LEU	CA-C-O	-5.74	113.37	119.97
1	A	557	ASN	N-CA-C	-5.74	105.54	112.54
1	A	507	CYS	N-CA-CB	5.73	118.56	110.36
1	A	556	GLY	O-C-N	5.73	130.15	122.70
1	A	20	PHE	CA-C-O	-5.72	114.81	120.82
1	A	483	CYS	O-C-N	5.71	129.75	122.39
1	A	17	THR	CA-CB-OG1	-5.70	101.05	109.60
1	A	209	ILE	N-CA-CB	-5.70	101.83	111.23
1	A	24	ARG	CA-C-N	5.70	130.23	120.72
1	A	24	ARG	C-N-CA	5.70	130.23	120.72
1	A	72	TYR	N-CA-C	5.70	117.35	111.03
1	A	574	LEU	CA-C-O	-5.69	114.06	120.43
1	A	332	ARG	NH1-CZ-NH2	5.69	126.70	119.30
1	A	285	LYS	CG-CD-CE	5.69	124.38	111.30
1	A	400	TYR	CA-C-N	5.68	128.21	120.54
1	A	400	TYR	C-N-CA	5.68	128.21	120.54
1	A	375	SER	CB-CA-C	5.68	119.57	110.09
1	A	201	ASP	CB-CA-C	-5.67	99.14	110.42
1	A	575	CYS	N-CA-C	-5.67	101.64	110.42
1	A	486	ASP	CA-CB-CG	5.67	118.27	112.60
1	A	46	ILE	CB-CG1-CD1	5.66	125.69	113.80
1	A	273	GLN	CG-CD-NE2	-5.66	107.91	116.40
1	A	500	ARG	N-CA-CB	-5.66	102.09	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	421	SER	N-CA-CB	5.66	123.44	110.88
1	A	353	GLN	OE1-CD-NE2	-5.66	116.94	122.60
1	A	565	ASP	N-CA-C	5.66	120.30	113.17
1	A	234	ASN	O-C-N	5.65	129.56	122.55
1	A	89	ARG	CD-NE-CZ	-5.65	116.50	124.40
1	A	265	ASP	CA-C-O	5.64	127.28	121.07
1	A	607	GLU	N-CA-C	5.64	117.11	111.07
1	A	373	SER	N-CA-CB	-5.64	102.24	111.66
1	A	13	ASN	N-CA-CB	5.64	115.75	110.39
1	A	347	TRP	CA-C-N	-5.63	115.17	123.05
1	A	347	TRP	C-N-CA	-5.63	115.17	123.05
1	A	684	GLU	CG-CD-OE2	-5.62	105.47	118.40
1	A	539	ALA	CA-C-N	5.62	129.57	122.77
1	A	539	ALA	C-N-CA	5.62	129.57	122.77
1	A	26	MET	CA-C-O	-5.62	112.47	120.51
1	A	579	LYS	CA-C-O	5.62	128.33	121.98
1	A	41	SER	N-CA-CB	-5.61	105.51	111.29
1	A	140	GLY	O-C-N	5.61	127.38	121.77
1	A	533	ARG	CD-NE-CZ	5.60	132.25	124.40
1	A	419	GLN	CB-CA-C	5.60	121.57	110.42
1	A	457	LYS	CB-CG-CD	-5.60	98.43	111.30
1	A	514	GLU	N-CA-C	-5.59	101.90	109.95
1	A	541	ASP	CA-CB-CG	-5.59	107.01	112.60
1	A	673	ASN	O-C-N	-5.59	116.28	122.09
1	A	34	VAL	CG1-CB-CG2	5.59	123.09	110.80
1	A	292	PRO	N-CA-CB	5.58	108.17	103.25
1	A	648	GLU	O-C-N	-5.58	114.98	122.23
1	A	165	GLN	N-CA-C	5.58	119.25	112.23
1	A	336	GLU	CB-CA-C	-5.57	99.58	110.11
1	A	601	SER	CA-CB-OG	-5.57	99.96	111.10
1	A	272	ARG	CA-C-N	5.56	127.67	120.44
1	A	272	ARG	C-N-CA	5.56	127.67	120.44
1	A	230	LEU	N-CA-CB	5.56	119.48	110.42
1	A	97	VAL	CA-C-N	5.56	131.46	122.68
1	A	97	VAL	C-N-CA	5.56	131.46	122.68
1	A	104	PHE	CA-C-O	-5.56	113.71	120.54
1	A	84	THR	OG1-CB-CG2	5.55	120.41	109.30
1	A	327	ALA	O-C-N	-5.55	116.23	122.12
1	A	615	HIS	O-C-N	-5.55	116.26	122.03
1	A	288	LEU	CB-CA-C	5.54	120.89	110.63
1	A	660	GLU	O-C-N	5.54	129.44	122.23
1	A	498	ASP	CA-CB-CG	-5.54	107.06	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	523	GLU	N-CA-CB	-5.54	101.36	109.95
1	A	368	SER	CA-C-O	-5.54	112.84	119.15
1	A	11	VAL	CG1-CB-CG2	5.53	122.97	110.80
1	A	358	CYS	N-CA-C	-5.52	105.16	111.07
1	A	525	TYR	CA-CB-CG	-5.51	103.97	113.90
1	A	519	PRO	CB-CA-C	-5.51	104.76	112.64
1	A	388	GLU	N-CA-CB	-5.50	101.44	110.40
1	A	656	LYS	CA-C-O	-5.50	116.05	122.37
1	A	163	LYS	O-C-N	5.49	129.02	122.27
1	A	360	GLN	O-C-N	-5.49	116.38	122.09
1	A	314	ILE	CA-CB-CG1	-5.49	101.07	110.40
1	A	335	GLU	N-CA-CB	-5.49	101.19	110.41
1	A	449	THR	CA-C-N	5.48	127.94	120.54
1	A	449	THR	C-N-CA	5.48	127.94	120.54
1	A	299	LEU	CA-C-O	-5.48	112.68	120.51
1	A	628	PRO	CA-CB-CG	-5.48	93.59	104.00
1	A	352	GLU	CB-CG-CD	5.47	121.91	112.60
1	A	26	MET	N-CA-CB	5.46	119.72	110.49
1	A	112	LEU	N-CA-C	-5.46	102.38	110.46
1	A	315	ASP	CB-CG-OD1	5.46	130.97	118.40
1	A	315	ASP	N-CA-C	-5.46	101.82	109.69
1	A	52	ASN	CB-CA-C	-5.46	104.83	111.82
1	A	240	ASP	CA-C-O	-5.46	112.68	119.18
1	A	249	ARG	CA-CB-CG	5.46	125.02	114.10
1	A	56	ALA	CA-C-O	-5.46	115.39	121.23
1	A	93	TYR	CA-CB-CG	-5.45	104.08	113.90
1	A	442	ARG	CB-CG-CD	5.44	123.82	111.30
1	A	133	ARG	CD-NE-CZ	-5.43	116.79	124.40
1	A	420	SER	CB-CA-C	5.43	119.28	110.37
1	A	330	ASN	N-CA-C	5.43	118.70	111.75
1	A	664	GLY	CA-C-N	5.43	125.51	119.32
1	A	664	GLY	C-N-CA	5.43	125.51	119.32
1	A	28	LYS	CA-CB-CG	5.42	124.95	114.10
1	A	216	GLU	CG-CD-OE2	5.42	130.87	118.40
1	A	272	ARG	N-CA-CB	-5.42	102.00	109.91
1	A	159	PRO	CA-C-O	5.42	127.48	121.36
1	A	493	CYS	N-CA-C	-5.42	96.38	107.70
1	A	227	TYR	N-CA-CB	-5.41	102.64	110.70
1	A	571	PHE	CA-C-O	-5.41	115.13	121.46
1	A	479	GLN	OE1-CD-NE2	5.41	128.01	122.60
1	A	689	LEU	N-CA-CB	-5.40	100.94	110.39
1	A	488	TYR	N-CA-C	-5.39	105.32	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	ARG	NE-CZ-NH2	-5.39	114.35	119.20
1	A	465	ARG	NE-CZ-NH2	-5.39	114.35	119.20
1	A	596	ASN	CB-CG-ND2	5.39	124.48	116.40
1	A	198	CYS	CA-CB-SG	5.38	126.78	114.40
1	A	262	GLY	O-C-N	5.38	127.95	122.24
1	A	351	GLY	N-CA-C	-5.38	105.90	112.68
1	A	334	SER	O-C-N	5.38	128.92	122.79
1	A	149	VAL	CA-C-N	5.37	128.01	120.28
1	A	149	VAL	C-N-CA	5.37	128.01	120.28
1	A	578	GLY	N-CA-C	-5.37	107.12	114.64
1	A	222	ALA	CA-C-N	5.37	127.74	120.44
1	A	222	ALA	C-N-CA	5.37	127.74	120.44
1	A	329	GLN	OE1-CD-NE2	5.36	127.96	122.60
1	A	477	PHE	CA-CB-CG	-5.36	108.44	113.80
1	A	124	GLY	CA-C-O	-5.36	114.36	120.09
1	A	152	PHE	N-CA-CB	-5.36	102.31	110.07
1	A	204	GLY	CA-C-N	5.36	131.09	121.66
1	A	204	GLY	C-N-CA	5.36	131.09	121.66
1	A	111	GLY	CA-C-O	-5.35	112.62	119.58
1	A	629	ASP	OD1-CG-OD2	5.35	135.74	122.90
1	A	241	LYS	N-CA-CB	5.34	118.31	110.57
1	A	185	SER	O-C-N	5.33	129.58	122.43
1	A	599	VAL	N-CA-CB	5.33	116.53	110.72
1	A	671	ILE	CA-CB-CG1	-5.33	101.34	110.40
1	A	421	SER	CA-C-N	5.33	134.80	121.80
1	A	421	SER	C-N-CA	5.33	134.80	121.80
1	A	155	ALA	CA-C-O	-5.32	115.03	120.99
1	A	274	ALA	CA-C-N	-5.32	111.20	121.58
1	A	274	ALA	C-N-CA	-5.32	111.20	121.58
1	A	5	SER	CA-C-O	5.32	128.25	121.82
1	A	539	ALA	O-C-N	-5.31	115.74	122.17
1	A	64	ILE	CB-CG1-CD1	5.31	124.95	113.80
1	A	447	SER	CB-CA-C	-5.31	99.21	110.31
1	A	284	PRO	N-CA-C	-5.31	107.14	113.98
1	A	597	HIS	CB-CG-ND1	5.31	130.66	122.70
1	A	356	ARG	CB-CA-C	-5.30	102.32	110.81
1	A	276	GLU	N-CA-C	-5.30	104.41	111.24
1	A	596	ASN	O-C-N	5.30	129.32	122.81
1	A	669	ALA	O-C-N	5.30	127.73	122.12
1	A	504	CYS	CA-C-O	5.29	124.72	118.90
1	A	45	CYS	CB-CA-C	5.29	119.19	110.88
1	A	149	VAL	CA-CB-CG1	5.29	119.39	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	349	ALA	CA-C-N	5.29	129.51	122.95
1	A	349	ALA	C-N-CA	5.29	129.51	122.95
1	A	224	ARG	CA-C-O	5.29	126.07	120.10
1	A	206	VAL	CA-C-N	-5.29	115.01	122.94
1	A	206	VAL	C-N-CA	-5.29	115.01	122.94
1	A	622	ARG	CA-C-N	-5.28	111.45	121.54
1	A	622	ARG	C-N-CA	-5.28	111.45	121.54
1	A	122	THR	O-C-N	5.27	129.60	122.59
1	A	183	PHE	N-CA-CB	5.27	116.25	110.35
1	A	401	THR	CA-CB-CG2	5.27	119.45	110.50
1	A	684	GLU	CB-CA-C	-5.26	102.61	110.88
1	A	653	LEU	N-CA-C	5.26	119.70	113.28
1	A	317	GLY	CA-C-O	-5.26	115.09	120.66
1	A	15	GLU	O-C-N	5.25	130.00	122.28
1	A	581	LYS	CA-CB-CG	-5.25	103.60	114.10
1	A	637	GLU	CG-CD-OE1	5.25	130.47	118.40
1	A	267	ILE	CA-C-O	-5.25	115.49	120.95
1	A	356	ARG	CA-CB-CG	5.25	124.59	114.10
1	A	25	ASN	CB-CG-ND2	-5.24	108.53	116.40
1	A	202	GLY	CA-C-O	-5.24	112.73	119.13
1	A	557	ASN	O-C-N	5.24	129.46	122.43
1	A	9	CYS	CB-CA-C	5.24	118.68	110.19
1	A	633	LEU	CA-C-O	5.24	125.97	120.42
1	A	154	SER	CA-C-N	5.24	131.12	121.85
1	A	154	SER	C-N-CA	5.24	131.12	121.85
1	A	436	LEU	N-CA-CB	-5.24	101.89	110.43
1	A	345	VAL	CA-C-O	-5.23	114.89	120.59
1	A	306	GLY	CA-C-N	5.23	131.02	122.81
1	A	306	GLY	C-N-CA	5.23	131.02	122.81
1	A	224	ARG	NE-CZ-NH1	-5.23	116.27	121.50
1	A	121	ARG	CA-CB-CG	-5.22	103.66	114.10
1	A	533	ARG	NE-CZ-NH1	5.21	126.71	121.50
1	A	255	VAL	N-CA-CB	-5.21	104.86	110.53
1	A	354	GLU	CA-CB-CG	5.20	124.50	114.10
1	A	310	VAL	N-CA-CB	-5.20	104.84	111.23
1	A	378	GLU	CG-CD-OE2	-5.20	106.44	118.40
1	A	423	PRO	CB-CA-C	5.20	120.14	111.56
1	A	530	GLY	O-C-N	5.20	127.23	122.19
1	A	610	LYS	N-CA-CB	-5.20	102.48	110.01
1	A	179	ASN	O-C-N	5.19	129.78	122.41
1	A	32	PRO	CA-C-O	5.19	128.09	120.56
1	A	454	LYS	CB-CA-C	-5.18	102.06	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	ARG	N-CA-C	-5.18	101.44	109.72
1	A	310	VAL	CA-C-N	5.18	125.71	120.38
1	A	310	VAL	C-N-CA	5.18	125.71	120.38
1	A	11	VAL	CA-C-N	5.17	130.65	121.80
1	A	11	VAL	C-N-CA	5.17	130.65	121.80
1	A	326	THR	OG1-CB-CG2	5.17	119.64	109.30
1	A	636	SER	CA-C-O	5.17	124.63	118.79
1	A	5	SER	CA-C-N	5.16	128.82	122.37
1	A	5	SER	C-N-CA	5.16	128.82	122.37
1	A	87	GLN	N-CA-C	-5.16	98.41	109.81
1	A	4	ARG	CA-CB-CG	5.16	124.41	114.10
1	A	215	PHE	N-CA-CB	5.15	118.79	110.40
1	A	266	ALA	N-CA-CB	-5.15	102.00	109.82
1	A	537	GLU	CB-CG-CD	-5.14	103.87	112.60
1	A	30	ARG	CA-CB-CG	5.13	124.37	114.10
1	A	629	ASP	CB-CG-OD2	-5.13	106.59	118.40
1	A	311	PRO	N-CA-CB	5.12	108.05	103.08
1	A	498	ASP	CB-CG-OD1	5.12	130.17	118.40
1	A	613	LEU	CA-C-O	-5.12	115.00	120.42
1	A	166	PHE	O-C-N	5.11	125.89	121.34
1	A	616	GLN	CG-CD-NE2	-5.11	108.74	116.40
1	A	623	ASN	N-CA-C	-5.11	99.93	110.80
1	A	31	GLY	O-C-N	5.09	126.86	121.77
1	A	210	ARG	O-C-N	-5.09	117.24	122.94
1	A	216	GLU	CA-CB-CG	5.09	124.28	114.10
1	A	301	LYS	O-C-N	5.09	129.19	122.93
1	A	326	THR	CA-CB-CG2	5.09	119.15	110.50
1	A	223	GLU	CA-C-N	5.09	127.61	120.28
1	A	223	GLU	C-N-CA	5.09	127.61	120.28
1	A	463	VAL	N-CA-CB	-5.09	102.19	110.13
1	A	366	GLU	CB-CA-C	-5.08	105.05	111.86
1	A	675	LYS	CA-C-N	5.08	127.59	120.28
1	A	675	LYS	C-N-CA	5.08	127.59	120.28
1	A	86	ARG	NE-CZ-NH2	-5.07	114.63	119.20
1	A	566	LEU	O-C-N	5.07	129.08	122.89
1	A	369	VAL	CA-C-N	-5.07	114.30	122.82
1	A	369	VAL	C-N-CA	-5.07	114.30	122.82
1	A	412	ALA	CA-C-O	-5.07	115.43	121.16
1	A	158	VAL	N-CA-CB	5.06	118.29	111.21
1	A	290	GLY	N-CA-C	-5.05	103.17	110.90
1	A	233	ASP	N-CA-C	-5.05	106.43	112.59
1	A	211	GLU	CB-CG-CD	5.05	121.18	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	CYS	O-C-N	-5.04	116.67	122.87
1	A	483	CYS	CA-C-N	-5.04	115.30	122.41
1	A	483	CYS	C-N-CA	-5.04	115.30	122.41
1	A	630	LYS	N-CA-CB	-5.04	101.25	110.27
1	A	623	ASN	CA-C-N	5.04	126.45	121.62
1	A	623	ASN	C-N-CA	5.04	126.45	121.62
1	A	585	GLU	CA-C-O	-5.04	114.46	120.55
1	A	237	LYS	CB-CG-CD	5.03	122.88	111.30
1	A	330	ASN	OD1-CG-ND2	5.03	127.63	122.60
1	A	667	TYR	CB-CG-CD2	5.03	128.34	120.80
1	A	8	TRP	CB-CG-CD2	-5.02	119.77	126.80
1	A	110	GLN	CA-C-O	-5.02	115.67	121.19
1	A	382	ALA	CA-C-O	-5.01	115.24	120.55
1	A	599	VAL	CA-CB-CG1	5.01	118.92	110.40
1	A	661	LYS	CA-CB-CG	-5.01	104.08	114.10
1	A	244	ASP	CB-CA-C	-5.01	102.26	110.72
1	A	77	VAL	CA-CB-CG1	5.00	118.91	110.40
1	A	430	ARG	CA-C-N	5.00	124.93	119.78
1	A	430	ARG	C-N-CA	5.00	124.93	119.78
1	A	397	GLY	CA-C-N	5.00	130.72	121.52
1	A	397	GLY	C-N-CA	5.00	130.72	121.52

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	272	ARG	Sidechain
1	A	602	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	5313	0	5156	434	0
2	A	14	0	12	0	0
3	A	2	0	0	0	0
4	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	6	0	0	2	0
6	A	325	0	0	57	0
All	All	5664	0	5168	436	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 (436) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:LEU:CD1	1:A:593:MET:HE3	1.19	1.57
1:A:260:VAL:CG1	1:A:261:ASN:H	1.11	1.48
1:A:436:LEU:CD1	1:A:593:MET:CE	1.99	1.39
1:A:296:LYS:HE3	6:A:1153:HOH:O	1.37	1.24
1:A:176:THR:HA	6:A:1148:HOH:O	1.10	1.22
1:A:220:ASP:OD2	1:A:223:GLU:N	1.75	1.20
1:A:36:CYS:C	1:A:37:LEU:HD22	1.67	1.17
1:A:107:ASN:HD22	1:A:107:ASN:N	1.37	1.16
1:A:296:LYS:CE	6:A:1153:HOH:O	1.88	1.16
1:A:432:VAL:HG13	6:A:1087:HOH:O	1.44	1.16
1:A:37:LEU:HD22	1:A:37:LEU:N	1.50	1.16
1:A:260:VAL:HG13	1:A:261:ASN:N	1.06	1.15
1:A:680:SER:HB2	6:A:1170:HOH:O	1.49	1.11
1:A:436:LEU:HD13	1:A:593:MET:CE	1.73	1.09
1:A:87:GLN:H	1:A:88:PRO:HD3	1.04	1.08
1:A:107:ASN:H	1:A:107:ASN:ND2	1.35	1.07
1:A:25:ASN:N	1:A:25:ASN:HD22	1.48	1.05
1:A:87:GLN:H	1:A:88:PRO:CD	1.57	1.05
1:A:87:GLN:N	1:A:88:PRO:CD	2.18	1.04
1:A:220:ASP:OD2	1:A:223:GLU:HB2	1.57	1.04
1:A:577:ASP:OD1	1:A:579:LYS:HG2	1.58	1.03
1:A:87:GLN:N	1:A:88:PRO:HD3	1.75	1.02
1:A:37:LEU:N	1:A:37:LEU:CD2	2.21	1.02
1:A:86:ARG:O	1:A:87:GLN:HB2	1.56	1.02
1:A:680:SER:CB	6:A:1170:HOH:O	2.07	1.00
1:A:356:ARG:HG2	1:A:356:ARG:HH11	1.26	0.99
1:A:622:ARG:HD3	1:A:622:ARG:C	1.85	0.99
1:A:8:TRP:O	1:A:37:LEU:HD23	1.62	0.98
1:A:430:ARG:HH21	1:A:648:GLU:CD	1.72	0.96
1:A:436:LEU:HD12	1:A:593:MET:CE	1.75	0.96
1:A:24:ARG:O	1:A:27:ARG:HG2	1.67	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:PRO:C	1:A:426:ASN:HD22	1.73	0.94
1:A:30:ARG:HH11	1:A:30:ARG:HA	1.31	0.94
1:A:436:LEU:HD11	1:A:593:MET:HE3	1.49	0.93
1:A:436:LEU:HD13	1:A:593:MET:HE1	1.47	0.93
1:A:173:CYS:O	1:A:180:LYS:HD2	1.69	0.93
1:A:672:THR:OG1	6:A:1226:HOH:O	1.85	0.92
1:A:417:SER:C	1:A:419:GLN:H	1.64	0.91
1:A:105:GLN:HB2	1:A:107:ASN:HD21	1.35	0.91
1:A:43:ILE:CG2	6:A:1130:HOH:O	2.19	0.91
1:A:260:VAL:HG12	1:A:261:ASN:H	1.32	0.90
1:A:430:ARG:NH2	1:A:648:GLU:CD	2.31	0.89
1:A:138:TRP:HE1	1:A:143:GLU:HG3	1.36	0.88
1:A:3:ARG:HB3	1:A:3:ARG:HH11	1.37	0.88
1:A:3:ARG:HE	1:A:7:GLN:CG	1.85	0.88
1:A:113:LYS:HE3	1:A:172:LEU:HD21	1.56	0.88
1:A:686:CYS:O	1:A:690:ARG:HG2	1.73	0.88
1:A:425:PRO:C	1:A:426:ASN:ND2	2.32	0.87
1:A:25:ASN:HD22	1:A:25:ASN:H	1.20	0.87
1:A:241:LYS:HD2	1:A:241:LYS:N	1.87	0.86
1:A:138:TRP:NE1	1:A:143:GLU:O	2.09	0.86
1:A:260:VAL:CG1	1:A:261:ASN:N	1.81	0.86
1:A:283:SER:OG	1:A:285:LYS:HG2	1.75	0.86
1:A:667:TYR:CE2	1:A:671:ILE:HD11	2.11	0.85
1:A:658:THR:HG22	1:A:660:GLU:H	1.39	0.85
1:A:436:LEU:HD12	1:A:593:MET:HE3	0.87	0.85
1:A:638:THR:HA	6:A:1188:HOH:O	1.76	0.84
1:A:3:ARG:HE	1:A:7:GLN:HG2	1.43	0.84
1:A:425:PRO:O	1:A:426:ASN:ND2	2.10	0.83
1:A:357:LYS:NZ	1:A:633:LEU:O	2.10	0.83
1:A:654:HIS:HD2	6:A:1264:HOH:O	1.60	0.83
1:A:559:ASN:HB2	1:A:564:LYS:NZ	1.94	0.82
1:A:139:THR:HG22	6:A:1302:HOH:O	1.79	0.82
1:A:295:GLN:HG3	1:A:298:LEU:HD11	1.59	0.82
1:A:422:ASP:HB2	1:A:423:PRO:CD	2.10	0.82
1:A:43:ILE:HG23	6:A:1130:HOH:O	1.75	0.81
1:A:238:PRO:HD2	1:A:241:LYS:HD3	1.60	0.81
1:A:658:THR:HG22	1:A:660:GLU:N	1.96	0.80
1:A:626:ASP:O	1:A:630:LYS:N	2.13	0.80
5:A:696:OXL:O4	6:A:1205:HOH:O	1.98	0.80
1:A:220:ASP:OD2	1:A:223:GLU:CB	2.29	0.79
1:A:658:THR:CG2	1:A:660:GLU:H	1.94	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:TRP:NE1	1:A:143:GLU:HG3	1.96	0.79
1:A:22:TRP:HB2	1:A:286:PHE:CZ	2.17	0.78
1:A:451:ASN:OD1	6:A:1289:HOH:O	2.00	0.78
1:A:422:ASP:O	1:A:424:ASP:N	2.16	0.78
1:A:422:ASP:HB2	1:A:423:PRO:HD3	1.65	0.77
1:A:485:PHE:CZ	1:A:674:LEU:HD22	2.20	0.77
1:A:7:GLN:HB3	1:A:37:LEU:HD21	1.66	0.76
1:A:509:GLY:HA3	1:A:514:GLU:O	1.86	0.76
1:A:430:ARG:NH2	1:A:648:GLU:OE2	2.15	0.75
1:A:577:ASP:CG	1:A:579:LYS:HG2	2.12	0.75
1:A:86:ARG:C	1:A:86:ARG:HD3	2.11	0.75
1:A:658:THR:HG22	1:A:661:LYS:H	1.51	0.75
1:A:465:ARG:NH2	6:A:1204:HOH:O	2.21	0.74
1:A:452:SER:O	1:A:456:LYS:CE	2.36	0.74
1:A:105:GLN:HA	1:A:105:GLN:NE2	2.03	0.74
1:A:100:LYS:NZ	1:A:225:ASP:O	2.17	0.73
1:A:238:PRO:HB2	1:A:240:ASP:OD1	1.89	0.73
1:A:356:ARG:HG2	1:A:356:ARG:NH1	2.00	0.73
1:A:430:ARG:NH2	1:A:648:GLU:OE1	2.21	0.73
1:A:113:LYS:CE	1:A:172:LEU:HD21	2.18	0.73
1:A:231:CYS:HB3	1:A:232:PRO:HD2	1.71	0.73
1:A:25:ASN:N	1:A:25:ASN:ND2	2.28	0.72
1:A:296:LYS:HE2	6:A:1153:HOH:O	1.72	0.72
1:A:260:VAL:HG13	1:A:261:ASN:CA	2.16	0.71
1:A:11:VAL:HG23	1:A:45:CYS:SG	2.31	0.71
1:A:686:CYS:O	1:A:690:ARG:CG	2.37	0.71
1:A:667:TYR:HB2	6:A:1202:HOH:O	1.91	0.71
1:A:424:ASP:OD1	1:A:424:ASP:C	2.34	0.71
1:A:165:GLN:C	1:A:167:PRO:HD3	2.16	0.71
1:A:146:GLU:OE1	1:A:146:GLU:N	2.24	0.70
1:A:452:SER:O	1:A:456:LYS:NZ	2.24	0.70
1:A:688:PHE:HD1	1:A:689:LEU:HD13	1.57	0.70
1:A:233:ASP:OD2	1:A:235:THR:HB	1.93	0.69
1:A:121:ARG:NH1	6:A:1128:HOH:O	2.12	0.69
1:A:658:THR:HB	1:A:661:LYS:HG3	1.73	0.69
1:A:7:GLN:HG2	1:A:35:SER:OG	1.93	0.68
1:A:9:CYS:HB2	1:A:54:ALA:CB	2.24	0.68
1:A:622:ARG:C	1:A:622:ARG:CD	2.65	0.68
1:A:24:ARG:HE	1:A:24:ARG:CA	2.05	0.67
1:A:342:ARG:HH11	1:A:342:ARG:HG2	1.58	0.67
1:A:457:LYS:HB3	1:A:506:LEU:HD11	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:LYS:O	1:A:283:SER:HB2	1.93	0.67
1:A:36:CYS:CA	1:A:37:LEU:HD22	2.24	0.67
1:A:147:ALA:O	1:A:151:ARG:HG3	1.93	0.67
1:A:352:GLU:H	1:A:352:GLU:CD	2.01	0.67
1:A:24:ARG:HE	1:A:24:ARG:HA	1.59	0.67
1:A:533:ARG:O	1:A:537:GLU:HG3	1.95	0.67
1:A:322:SER:O	1:A:326:THR:HB	1.95	0.66
1:A:223:GLU:OE1	1:A:223:GLU:HA	1.94	0.66
1:A:221:GLU:O	1:A:224:ARG:HB2	1.95	0.66
1:A:679:THR:CG2	1:A:683:LEU:HB2	2.25	0.66
1:A:622:ARG:HD3	1:A:622:ARG:O	1.96	0.66
1:A:577:ASP:OD1	1:A:579:LYS:CG	2.42	0.66
1:A:105:GLN:CA	1:A:105:GLN:HE21	2.09	0.65
1:A:559:ASN:CB	1:A:564:LYS:NZ	2.59	0.65
1:A:86:ARG:O	1:A:87:GLN:CB	2.38	0.65
1:A:445:ASP:O	1:A:580:ARG:NH1	2.30	0.65
1:A:627:CYS:HB2	1:A:631:PHE:O	1.97	0.65
1:A:344:ARG:HD3	1:A:370:THR:HG22	1.78	0.65
1:A:91:HIS:ND1	6:A:1252:HOH:O	2.29	0.64
1:A:220:ASP:OD2	1:A:223:GLU:CA	2.45	0.64
1:A:684:GLU:OE1	6:A:1254:HOH:O	2.15	0.64
1:A:14:PRO:O	1:A:298:LEU:HD13	1.98	0.63
1:A:283:SER:OG	1:A:285:LYS:CG	2.46	0.63
1:A:13:ASN:HB3	1:A:14:PRO:HD3	1.80	0.63
1:A:561:ALA:HB3	6:A:1177:HOH:O	1.97	0.63
1:A:30:ARG:HA	1:A:30:ARG:NH1	2.09	0.63
1:A:430:ARG:HD2	6:A:1174:HOH:O	1.99	0.63
1:A:652:ARG:HB3	6:A:1266:HOH:O	1.99	0.63
1:A:362:SER:O	1:A:365:SER:OG	2.16	0.63
1:A:666:GLN:H	1:A:666:GLN:NE2	1.96	0.63
1:A:353:GLN:HE22	1:A:639:LYS:CD	2.12	0.62
1:A:424:ASP:HB3	1:A:648:GLU:OE2	1.99	0.62
1:A:559:ASN:HB2	1:A:564:LYS:CE	2.30	0.62
1:A:559:ASN:HB2	1:A:564:LYS:HZ3	1.63	0.62
1:A:84:THR:O	1:A:88:PRO:N	2.33	0.62
1:A:374:ALA:HB1	1:A:379:ASP:HB3	1.80	0.62
1:A:394:LEU:HD22	1:A:398:TYR:HB3	1.81	0.62
1:A:7:GLN:CG	1:A:35:SER:OG	2.48	0.62
1:A:437:ALA:CB	1:A:471:ILE:HD13	2.30	0.62
1:A:465:ARG:NH2	6:A:1205:HOH:O	2.32	0.62
1:A:485:PHE:CZ	1:A:674:LEU:CD2	2.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:CYS:HB2	1:A:235:THR:HG22	1.81	0.61
1:A:509:GLY:CA	1:A:514:GLU:O	2.48	0.61
1:A:105:GLN:NE2	1:A:105:GLN:CA	2.59	0.61
1:A:559:ASN:HB2	1:A:564:LYS:HD3	1.82	0.61
1:A:174:ALA:HB3	1:A:188:PRO:HG2	1.82	0.61
1:A:652:ARG:HH11	1:A:652:ARG:HG2	1.65	0.61
1:A:510:ASP:OD2	1:A:515:ASN:ND2	2.33	0.61
1:A:635:GLN:NE2	6:A:1273:HOH:O	2.34	0.61
1:A:24:ARG:NH2	1:A:28:LYS:HE3	2.16	0.61
1:A:639:LYS:HD3	6:A:1080:HOH:O	1.99	0.60
1:A:341:ARG:O	1:A:341:ARG:HG3	2.01	0.60
1:A:8:TRP:O	1:A:37:LEU:CD2	2.46	0.60
1:A:82:TYR:CE2	1:A:252:SER:HB2	2.35	0.60
1:A:291:SER:HB3	1:A:295:GLN:HB2	1.82	0.60
1:A:395:ASP:OD2	1:A:465:ARG:HA	2.02	0.60
1:A:25:ASN:H	1:A:25:ASN:ND2	1.94	0.60
1:A:107:ASN:N	1:A:107:ASN:ND2	2.10	0.60
1:A:477:PHE:HA	1:A:488:TYR:OH	2.00	0.60
1:A:431:PRO:HA	6:A:1264:HOH:O	2.00	0.60
1:A:25:ASN:HB3	1:A:278:PHE:CZ	2.37	0.60
1:A:117:THR:OG1	1:A:124:GLY:HA3	2.01	0.60
1:A:212:SER:OG	6:A:1151:HOH:O	2.13	0.59
1:A:437:ALA:CB	1:A:471:ILE:CD1	2.79	0.59
1:A:38:LYS:O	1:A:39:ARG:HG2	2.01	0.59
1:A:559:ASN:HB2	1:A:564:LYS:CD	2.33	0.59
1:A:3:ARG:HB3	1:A:3:ARG:NH1	2.15	0.59
1:A:105:GLN:HA	1:A:105:GLN:HE21	1.65	0.59
1:A:162:ASP:CG	1:A:165:GLN:HG2	2.27	0.59
1:A:25:ASN:OD1	1:A:286:PHE:HB2	2.03	0.59
1:A:33:PRO:HD2	6:A:1124:HOH:O	2.02	0.58
1:A:38:LYS:C	1:A:39:ARG:HG2	2.27	0.58
1:A:100:LYS:HG3	1:A:226:GLU:O	2.03	0.58
1:A:121:ARG:HD3	6:A:1128:HOH:O	2.03	0.58
1:A:258:ARG:NH1	1:A:261:ASN:O	2.36	0.58
1:A:688:PHE:CD1	1:A:689:LEU:HD13	2.38	0.58
1:A:292:PRO:C	1:A:294:GLY:N	2.62	0.58
1:A:582:PRO:HG2	1:A:585:GLU:HG3	1.86	0.58
1:A:11:VAL:HG22	1:A:41:SER:C	2.29	0.57
1:A:667:TYR:O	1:A:671:ILE:HG13	2.03	0.57
1:A:560:GLU:CD	1:A:562:TRP:HE1	2.12	0.57
1:A:342:ARG:HG2	1:A:342:ARG:NH1	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:ILE:O	1:A:675:LYS:HG2	2.04	0.57
1:A:295:GLN:O	6:A:1154:HOH:O	2.18	0.57
1:A:143:GLU:HG3	1:A:143:GLU:O	2.04	0.56
1:A:145:ILE:O	1:A:149:VAL:HG12	2.05	0.56
1:A:138:TRP:CD1	1:A:143:GLU:HG3	2.39	0.56
1:A:485:PHE:HZ	1:A:674:LEU:HD22	1.69	0.56
1:A:485:PHE:HZ	1:A:674:LEU:CD2	2.18	0.56
1:A:666:GLN:H	1:A:666:GLN:CD	2.12	0.56
1:A:162:ASP:HB3	1:A:165:GLN:HG3	1.86	0.56
1:A:282:LYS:O	1:A:283:SER:CB	2.52	0.56
1:A:283:SER:OG	1:A:285:LYS:HD3	2.05	0.56
1:A:667:TYR:CZ	1:A:671:ILE:HD11	2.41	0.56
1:A:47:GLN:HG2	1:A:72:TYR:CE1	2.41	0.56
1:A:374:ALA:HB1	1:A:379:ASP:CB	2.35	0.56
1:A:3:ARG:HD2	1:A:7:GLN:OE1	2.06	0.56
1:A:166:PHE:N	1:A:167:PRO:HD3	2.19	0.56
1:A:170:CYS:O	1:A:171:ARG:C	2.48	0.56
1:A:353:GLN:HE22	1:A:639:LYS:NZ	2.04	0.56
1:A:146:GLU:HA	1:A:149:VAL:HG13	1.88	0.56
1:A:559:ASN:CB	1:A:564:LYS:HZ3	2.16	0.55
1:A:452:SER:O	1:A:456:LYS:HE2	2.06	0.55
1:A:547:ASP:OD1	1:A:547:ASP:N	2.37	0.55
1:A:24:ARG:HG2	1:A:27:ARG:HH21	1.71	0.55
1:A:529:THR:OG1	6:A:1069:HOH:O	2.18	0.55
1:A:32:PRO:CD	1:A:273:GLN:HG3	2.37	0.54
1:A:328:ILE:O	1:A:332:ARG:NH1	2.40	0.54
1:A:278:PHE:CE1	1:A:285:LYS:NZ	2.76	0.54
1:A:100:LYS:HG3	1:A:226:GLU:C	2.32	0.54
1:A:520:ASN:OD1	1:A:522:ASN:HB2	2.08	0.54
1:A:7:GLN:HB3	1:A:37:LEU:CD2	2.36	0.54
1:A:353:GLN:HE22	1:A:639:LYS:HD3	1.71	0.54
1:A:24:ARG:NH2	1:A:28:LYS:HB2	2.23	0.53
1:A:487:GLU:O	6:A:1045:HOH:O	2.18	0.53
1:A:637:GLU:HA	6:A:1190:HOH:O	2.08	0.53
1:A:231:CYS:HB3	1:A:232:PRO:CD	2.39	0.53
1:A:38:LYS:O	1:A:39:ARG:NH1	2.36	0.53
1:A:353:GLN:HE22	1:A:639:LYS:HZ3	1.56	0.53
1:A:437:ALA:HB2	1:A:471:ILE:CD1	2.38	0.53
1:A:25:ASN:HB3	1:A:285:LYS:HZ3	1.73	0.53
1:A:47:GLN:NE2	6:A:1244:HOH:O	2.41	0.53
1:A:534:CYS:O	1:A:539:ALA:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:628:PRO:HA	1:A:632:CYS:SG	2.49	0.53
1:A:47:GLN:HG2	1:A:72:TYR:HE1	1.73	0.53
1:A:131:THR:HG21	1:A:247:LEU:HD13	1.91	0.53
1:A:426:ASN:ND2	1:A:426:ASN:N	2.33	0.53
1:A:554:THR:O	1:A:555:ASP:HB2	2.09	0.53
1:A:283:SER:OG	1:A:285:LYS:CD	2.56	0.52
1:A:498:ASP:OD1	1:A:500:ARG:CB	2.57	0.52
1:A:601:SER:HB2	1:A:609:LEU:CD2	2.39	0.52
1:A:652:ARG:HG2	1:A:652:ARG:NH1	2.24	0.52
1:A:379:ASP:O	1:A:383:LEU:HG	2.09	0.52
1:A:427:CYS:SG	1:A:427:CYS:O	2.68	0.52
1:A:353:GLN:NE2	1:A:639:LYS:NZ	2.57	0.52
1:A:43:ILE:HG21	6:A:1130:HOH:O	2.00	0.52
1:A:548:VAL:O	1:A:552:GLN:HG3	2.10	0.52
1:A:555:ASP:OD1	1:A:567:LYS:HD3	2.10	0.52
1:A:404:LYS:HE2	1:A:404:LYS:HA	1.92	0.52
1:A:498:ASP:OD1	1:A:500:ARG:N	2.38	0.52
1:A:277:LYS:O	1:A:282:LYS:O	2.27	0.52
1:A:97:VAL:O	1:A:207:ALA:N	2.35	0.51
1:A:349:ALA:O	1:A:373:SER:HA	2.10	0.51
1:A:133:ARG:NE	6:A:1210:HOH:O	2.35	0.51
1:A:666:GLN:CD	1:A:666:GLN:N	2.68	0.51
1:A:58:THR:HG23	6:A:1020:HOH:O	2.10	0.51
1:A:417:SER:C	1:A:419:GLN:N	2.48	0.51
5:A:696:OXL:C2	6:A:1205:HOH:O	2.56	0.51
1:A:559:ASN:C	1:A:559:ASN:OD1	2.53	0.50
1:A:691:LYS:O	6:A:1220:HOH:O	2.19	0.50
1:A:312:PRO:HB3	6:A:1160:HOH:O	2.12	0.50
1:A:522:ASN:OD1	6:A:1231:HOH:O	2.19	0.50
1:A:579:LYS:N	1:A:579:LYS:HD3	2.25	0.50
1:A:110:GLN:HB3	1:A:152:PHE:CE1	2.47	0.50
1:A:186:GLN:NE2	1:A:186:GLN:HA	2.25	0.50
1:A:113:LYS:HB3	1:A:172:LEU:HD11	1.94	0.50
1:A:105:GLN:CB	1:A:107:ASN:HD21	2.15	0.50
1:A:197:LYS:O	1:A:198:CYS:C	2.54	0.50
1:A:346:VAL:HG22	1:A:370:THR:CG2	2.41	0.50
1:A:220:ASP:CG	1:A:223:GLU:HB2	2.35	0.50
1:A:270:LEU:C	1:A:270:LEU:CD2	2.84	0.50
1:A:7:GLN:CB	1:A:37:LEU:HD21	2.40	0.49
1:A:9:CYS:HB2	1:A:54:ALA:HB1	1.94	0.49
1:A:32:PRO:CG	1:A:273:GLN:HG3	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:THR:CG2	6:A:1302:HOH:O	2.49	0.49
1:A:84:THR:HG22	1:A:85:GLU:OE2	2.12	0.49
1:A:316:SER:O	1:A:320:LEU:HG	2.12	0.49
1:A:591:LEU:O	1:A:592:ALA:HB2	2.12	0.49
1:A:8:TRP:HZ2	1:A:58:THR:HG22	1.77	0.49
1:A:437:ALA:HB3	1:A:471:ILE:HD13	1.93	0.49
1:A:3:ARG:NE	1:A:7:GLN:CG	2.67	0.49
1:A:332:ARG:HD3	6:A:1312:HOH:O	2.12	0.49
1:A:624:GLY:O	1:A:626:ASP:N	2.45	0.49
1:A:100:LYS:N	1:A:226:GLU:O	2.32	0.49
1:A:13:ASN:C	1:A:15:GLU:N	2.68	0.49
1:A:231:CYS:CB	1:A:232:PRO:CD	2.90	0.49
1:A:214:VAL:O	1:A:218:LEU:HB2	2.12	0.48
1:A:342:ARG:NH1	1:A:342:ARG:CG	2.76	0.48
1:A:427:CYS:O	1:A:649:CYS:SG	2.71	0.48
1:A:73:LYS:HE3	1:A:73:LYS:HB3	1.56	0.48
1:A:684:GLU:HG3	6:A:1256:HOH:O	2.13	0.48
1:A:432:VAL:CG1	6:A:1087:HOH:O	2.27	0.48
1:A:125:TRP:CH2	1:A:149:VAL:HG11	2.49	0.48
1:A:638:THR:HG22	6:A:1189:HOH:O	2.13	0.48
1:A:353:GLN:NE2	1:A:639:LYS:HZ3	2.12	0.47
1:A:510:ASP:C	1:A:512:GLN:H	2.22	0.47
1:A:417:SER:HA	1:A:433:GLU:OE1	2.14	0.47
1:A:3:ARG:NE	1:A:35:SER:OG	2.47	0.47
1:A:220:ASP:HB3	1:A:223:GLU:HB2	1.97	0.47
1:A:298:LEU:O	1:A:299:LEU:HB2	2.14	0.47
1:A:28:LYS:O	1:A:29:VAL:HG23	2.15	0.47
1:A:668:VAL:HG12	6:A:1226:HOH:O	2.14	0.47
1:A:218:LEU:HD23	1:A:224:ARG:HA	1.97	0.47
1:A:278:PHE:CZ	1:A:285:LYS:NZ	2.83	0.47
1:A:68:GLY:O	1:A:73:LYS:HA	2.15	0.47
1:A:263:LYS:O	1:A:266:ALA:HB3	2.15	0.47
1:A:223:GLU:OE1	1:A:223:GLU:CA	2.60	0.47
1:A:515:ASN:O	1:A:518:VAL:HB	2.15	0.47
1:A:3:ARG:HH11	1:A:3:ARG:CB	2.18	0.47
1:A:227:TYR:CD1	1:A:227:TYR:N	2.82	0.46
1:A:516:LYS:HE3	1:A:516:LYS:HB2	1.54	0.46
1:A:551:LEU:HD11	1:A:583:VAL:HG12	1.97	0.46
1:A:636:SER:O	1:A:637:GLU:O	2.33	0.46
1:A:679:THR:HG23	1:A:683:LEU:HB2	1.96	0.46
1:A:576:LEU:HD21	1:A:591:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ASN:O	1:A:16:ALA:N	2.49	0.46
1:A:111:GLY:C	1:A:154:SER:OG	2.59	0.46
1:A:679:THR:HG23	1:A:683:LEU:HD23	1.97	0.46
1:A:352:GLU:CD	1:A:522:ASN:HD21	2.23	0.46
1:A:133:ARG:CG	6:A:1210:HOH:O	2.63	0.46
1:A:231:CYS:CB	1:A:232:PRO:HD2	2.45	0.46
1:A:278:PHE:HE1	1:A:285:LYS:HZ2	1.61	0.46
1:A:636:SER:OG	1:A:645:ASP:OD1	2.34	0.46
1:A:443:ARG:HH11	1:A:443:ARG:HD3	1.31	0.46
1:A:321:GLY:O	1:A:325:PHE:CB	2.64	0.45
1:A:628:PRO:HG2	1:A:629:ASP:N	2.29	0.45
1:A:400:TYR:O	1:A:404:LYS:HG2	2.17	0.45
1:A:581:LYS:HB3	1:A:582:PRO:HD2	1.97	0.45
1:A:330:ASN:N	1:A:330:ASN:HD22	2.12	0.45
1:A:351:GLY:HA2	1:A:352:GLU:OE1	2.16	0.45
1:A:679:THR:HG22	1:A:680:SER:N	2.31	0.45
1:A:133:ARG:N	1:A:134:PRO:CD	2.79	0.45
1:A:26:MET:SD	1:A:278:PHE:HE2	2.40	0.45
1:A:37:LEU:CD2	1:A:37:LEU:H	2.17	0.45
1:A:110:GLN:HE21	1:A:110:GLN:HB2	1.45	0.45
1:A:257:ALA:HB1	6:A:1279:HOH:O	2.17	0.45
1:A:334:SER:HB2	1:A:336:GLU:OE1	2.17	0.45
1:A:525:TYR:N	1:A:525:TYR:CD1	2.78	0.45
1:A:187:GLU:HA	1:A:188:PRO:HD2	1.80	0.45
1:A:554:THR:HG22	1:A:566:LEU:HB3	1.98	0.45
1:A:58:THR:HG21	1:A:300:PHE:CD1	2.52	0.45
1:A:220:ASP:CG	1:A:221:GLU:N	2.73	0.45
1:A:551:LEU:HD11	1:A:583:VAL:CG1	2.47	0.45
1:A:404:LYS:HE3	1:A:659:TYR:OH	2.16	0.44
1:A:430:ARG:HD2	1:A:430:ARG:HH11	1.19	0.44
1:A:596:ASN:O	1:A:662:TYR:OH	2.22	0.44
1:A:270:LEU:C	1:A:270:LEU:HD22	2.42	0.44
1:A:344:ARG:CD	1:A:370:THR:HG22	2.45	0.44
1:A:26:MET:HB3	1:A:32:PRO:O	2.17	0.44
1:A:498:ASP:HA	1:A:499:PRO:HD3	1.84	0.44
1:A:84:THR:O	1:A:88:PRO:CD	2.65	0.44
1:A:133:ARG:NH1	1:A:330:ASN:O	2.49	0.44
1:A:622:ARG:HG2	6:A:1078:HOH:O	2.16	0.44
1:A:679:THR:CG2	1:A:680:SER:N	2.81	0.44
1:A:214:VAL:HG23	1:A:218:LEU:HD22	1.99	0.44
1:A:292:PRO:C	1:A:294:GLY:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:GLY:HA2	1:A:602:ARG:NH1	2.32	0.44
1:A:510:ASP:O	1:A:512:GLN:N	2.50	0.44
1:A:429:ASP:O	1:A:654:HIS:NE2	2.51	0.44
1:A:59:LEU:HG	1:A:63:PHE:CB	2.48	0.44
1:A:105:GLN:HB2	1:A:107:ASN:ND2	2.17	0.44
1:A:357:LYS:CE	1:A:633:LEU:O	2.66	0.44
1:A:34:VAL:HG13	1:A:270:LEU:HD11	1.99	0.43
1:A:314:ILE:HD13	1:A:689:LEU:HD13	2.00	0.43
1:A:49:ILE:CD1	1:A:57:VAL:HG12	2.48	0.43
1:A:51:GLU:O	1:A:52:ASN:HB2	2.18	0.43
1:A:111:GLY:O	1:A:154:SER:OG	2.35	0.43
1:A:416:LYS:HB2	6:A:1085:HOH:O	2.19	0.43
1:A:155:ALA:HB1	1:A:171:ARG:HB3	1.99	0.43
1:A:601:SER:HB2	1:A:609:LEU:HD22	2.00	0.43
1:A:437:ALA:HB2	1:A:471:ILE:HD12	2.00	0.43
1:A:619:LYS:HD3	1:A:626:ASP:OD1	2.19	0.43
1:A:117:THR:HG23	1:A:208:PHE:O	2.19	0.43
1:A:168:ASN:HD22	1:A:168:ASN:HA	1.23	0.43
1:A:191:SER:HB3	6:A:1156:HOH:O	2.19	0.43
1:A:344:ARG:HD3	1:A:370:THR:CG2	2.46	0.43
1:A:658:THR:HG23	1:A:660:GLU:H	1.80	0.43
1:A:680:SER:HB2	1:A:681:PRO:HD2	2.00	0.43
1:A:13:ASN:HB3	1:A:14:PRO:CD	2.48	0.43
1:A:224:ARG:HH11	1:A:224:ARG:HD2	1.52	0.43
1:A:236:ARG:HH11	1:A:236:ARG:HD3	1.49	0.43
1:A:342:ARG:NH1	6:A:1213:HOH:O	2.48	0.43
1:A:220:ASP:CB	1:A:223:GLU:HB2	2.49	0.43
1:A:288:LEU:HD11	1:A:300:PHE:CE2	2.54	0.43
1:A:22:TRP:HB2	1:A:286:PHE:CE2	2.54	0.42
1:A:41:SER:HB2	1:A:42:PRO:HD2	2.00	0.42
1:A:292:PRO:O	1:A:294:GLY:N	2.52	0.42
1:A:437:ALA:CB	1:A:471:ILE:HD12	2.49	0.42
1:A:453:VAL:O	1:A:456:LYS:HB2	2.19	0.42
1:A:564:LYS:HD2	1:A:564:LYS:HA	1.81	0.42
1:A:24:ARG:CZ	1:A:28:LYS:HE3	2.48	0.42
1:A:52:ASN:C	1:A:53:ARG:HG2	2.44	0.42
1:A:86:ARG:NH1	1:A:86:ARG:HG2	2.34	0.42
1:A:278:PHE:HE1	1:A:285:LYS:NZ	2.15	0.42
1:A:510:ASP:C	1:A:512:GLN:N	2.76	0.42
1:A:531:ALA:O	1:A:534:CYS:HB3	2.18	0.42
1:A:138:TRP:CE2	1:A:143:GLU:O	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:672:THR:O	1:A:673:ASN:C	2.62	0.42
1:A:59:LEU:HG	1:A:63:PHE:HB2	2.02	0.42
1:A:253:HIS:CD2	1:A:253:HIS:N	2.85	0.42
1:A:138:TRP:CD1	1:A:143:GLU:CG	3.03	0.42
1:A:463:VAL:O	1:A:464:ASP:HB2	2.19	0.42
1:A:476:LEU:O	1:A:477:PHE:C	2.60	0.42
1:A:507:CYS:HB3	1:A:523:GLU:OE1	2.19	0.42
1:A:679:THR:CG2	1:A:680:SER:H	2.33	0.42
1:A:20:PHE:O	1:A:23:GLN:HB3	2.20	0.42
1:A:36:CYS:HA	1:A:37:LEU:HD22	1.99	0.42
1:A:26:MET:HE3	1:A:32:PRO:O	2.20	0.41
1:A:62:GLY:HA3	1:A:120:ARG:O	2.19	0.41
1:A:179:ASN:ND2	1:A:186:GLN:HB3	2.34	0.41
1:A:330:ASN:OD1	6:A:1031:HOH:O	2.22	0.41
1:A:377:THR:CG2	1:A:394:LEU:CD2	2.97	0.41
1:A:684:GLU:CG	6:A:1256:HOH:O	2.67	0.41
1:A:7:GLN:HG3	1:A:35:SER:HG	1.86	0.41
1:A:321:GLY:O	1:A:325:PHE:HB2	2.21	0.41
1:A:465:ARG:H	1:A:465:ARG:HG2	1.46	0.41
1:A:112:LEU:O	1:A:153:PHE:HB3	2.20	0.41
1:A:426:ASN:HD22	1:A:426:ASN:HA	1.21	0.41
1:A:471:ILE:HB	1:A:472:PRO:CD	2.50	0.41
1:A:594:ALA:HA	1:A:595:PRO:HD3	1.94	0.41
1:A:218:LEU:O	1:A:224:ARG:NE	2.52	0.41
1:A:21:GLN:HE21	1:A:21:GLN:HB3	1.75	0.41
1:A:40:ASP:N	1:A:44:GLN:OE1	2.35	0.41
1:A:229:LEU:HA	1:A:229:LEU:HD23	1.91	0.41
1:A:424:ASP:OD1	1:A:425:PRO:N	2.53	0.41
1:A:427:CYS:C	1:A:649:CYS:SG	3.04	0.41
1:A:302:ASP:O	1:A:303:SER:HB2	2.20	0.41
1:A:410:VAL:HG21	1:A:609:LEU:HD23	2.02	0.41
1:A:508:ILE:O	1:A:509:GLY:C	2.64	0.41
1:A:174:ALA:HB3	1:A:188:PRO:CG	2.49	0.40
1:A:658:THR:HG21	1:A:660:GLU:OE1	2.21	0.40
1:A:560:GLU:CD	1:A:562:TRP:NE1	2.79	0.40
1:A:176:THR:HG21	6:A:1143:HOH:O	2.22	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%)	611 (89%)	58 (8%)	20 (3%)	3 1

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	283	SER
1	A	422	ASP
1	A	625	SER
1	A	637	GLU
1	A	29	VAL
1	A	282	LYS
1	A	678	SER
1	A	28	LYS
1	A	419	GLN
1	A	511	GLU
1	A	521	SER
1	A	293	SER
1	A	4	ARG
1	A	219	SER
1	A	423	PRO
1	A	280	LYS
1	A	418	GLN
1	A	606	VAL
1	A	260	VAL

5.3.2 Protein sidechains [i](#)

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	568/574 (99%)	509 (90%)	59 (10%)	7 4

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	5	SER
1	A	11	VAL
1	A	24	ARG
1	A	25	ASN
1	A	29	VAL
1	A	30	ARG
1	A	34	VAL
1	A	37	LEU
1	A	53	ARG
1	A	58	THR
1	A	59	LEU
1	A	71	PRO
1	A	84	THR
1	A	86	ARG
1	A	107	ASN
1	A	110	GLN
1	A	121	ARG
1	A	139	THR
1	A	149	VAL
1	A	168	ASN
1	A	181	CYS
1	A	218	LEU
1	A	220	ASP
1	A	221	GLU
1	A	223	GLU
1	A	240	ASP
1	A	241	LYS
1	A	244	ASP
1	A	270	LEU
1	A	271	LEU
1	A	281	ASP
1	A	282	LYS
1	A	301	LYS
1	A	305	ILE
1	A	326	THR

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Mol	Chain	Res	Type
1	A	352	GLU
1	A	356	ARG
1	A	384	VAL
1	A	422	ASP
1	A	436	LEU
1	A	446	THR
1	A	447	SER
1	A	448	LEU
1	A	451	ASN
1	A	463	VAL
1	A	518	VAL
1	A	575	CYS
1	A	587	ARG
1	A	593	MET
1	A	599	VAL
1	A	614	LEU
1	A	622	ARG
1	A	628	PRO
1	A	637	GLU
1	A	641	LEU
1	A	658	THR
1	A	683	LEU
1	A	689	LEU

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	25	ASN
1	A	47	GLN
1	A	52	ASN
1	A	105	GLN
1	A	107	ASN
1	A	110	GLN
1	A	168	ASN
1	A	186	GLN
1	A	234	ASN
1	A	261	ASN
1	A	273	GLN
1	A	329	GLN
1	A	330	ASN
1	A	353	GLN

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Mol	Chain	Res	Type
1	A	360	GLN
1	A	426	ASN
1	A	502	ASN
1	A	552	GLN
1	A	644	ASN
1	A	666	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 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	$\# Z > 2$
2	NAG	A	990	1	14,14,15	2.29	4 (28%)	17,19,21	5.94	9 (52%)
4	CO3	A	695	3	3,3,3	0.79	0	2,3,3	2.70	1 (50%)
5	OXL	A	696	3	5,5,5	0.81	0	6,6,6	3.34	3 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	990	1	-	3/6/23/26	0/1/1/1
5	OXL	A	696	3	-	4/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	990	NAG	O5-C5	-5.63	1.32	1.43
2	A	990	NAG	C2-N2	-4.06	1.39	1.46
2	A	990	NAG	C4-C5	2.87	1.59	1.53
2	A	990	NAG	C8-C7	-2.76	1.44	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	990	NAG	C2-N2-C7	22.48	153.02	122.90
2	A	990	NAG	C1-O5-C5	5.62	119.71	112.19
5	A	696	OXL	O4-C2-O2	5.31	136.54	123.90
5	A	696	OXL	O2-C2-C1	-4.96	110.29	120.63
4	A	695	CO3	O3-C-O1	3.82	129.44	119.68
2	A	990	NAG	C3-C4-C5	3.70	116.93	110.23
2	A	990	NAG	O6-C6-C5	3.26	122.42	111.33
5	A	696	OXL	O3-C1-C2	3.22	119.08	112.83
2	A	990	NAG	O5-C5-C6	3.06	113.62	107.66
2	A	990	NAG	O3-C3-C2	2.82	115.26	109.40
2	A	990	NAG	O5-C1-C2	-2.39	107.60	111.29
2	A	990	NAG	C6-C5-C4	-2.36	107.22	113.02
2	A	990	NAG	C8-C7-N2	2.08	119.57	116.12

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	990	NAG	C3-C2-N2-C7
2	A	990	NAG	C8-C7-N2-C2
2	A	990	NAG	O7-C7-N2-C2
5	A	696	OXL	O3-C1-C2-O4
5	A	696	OXL	O1-C1-C2-O2
5	A	696	OXL	O3-C1-C2-O2
5	A	696	OXL	O1-C1-C2-O4

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	696	OXL	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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%)	-0.43	1 (0%) 92 91	19, 37, 66, 96	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	509	GLY	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(Å ²)	Q<0.9
2	NAG	A	990	14/15	0.59	0.11	90,96,98,98	0
4	CO3	A	695	4/4	0.93	0.10	26,29,30,34	0
5	OXL	A	696	6/6	0.94	0.06	17,17,21,24	0
3	CU	A	694	1/1	0.95	0.04	28,28,28,28	0
3	CU	A	693	1/1	0.98	0.03	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.