



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2026 – 09:22 PM EDT

PDB ID : 1BKA / pdb_00001bka
Title : OXALATE-SUBSTITUTED DIFERRIC LACTOFERRIN
Authors : Baker, H.M.; Smith, C.A.; Baker, E.N.
Deposited on : 1996-04-15
Resolution : 2.40 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

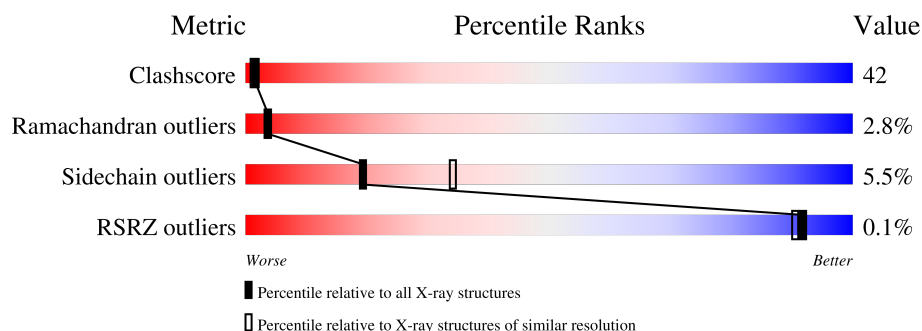
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

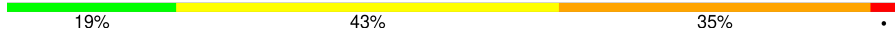
The reported resolution of this entry is 2.40 Å.

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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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
3	OXL	A	695	-	X	-	-
3	OXL	A	696	-	X	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5433 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	688	Total	C	N	O	S	0	0	0
			5298	3314	941	1006	37			

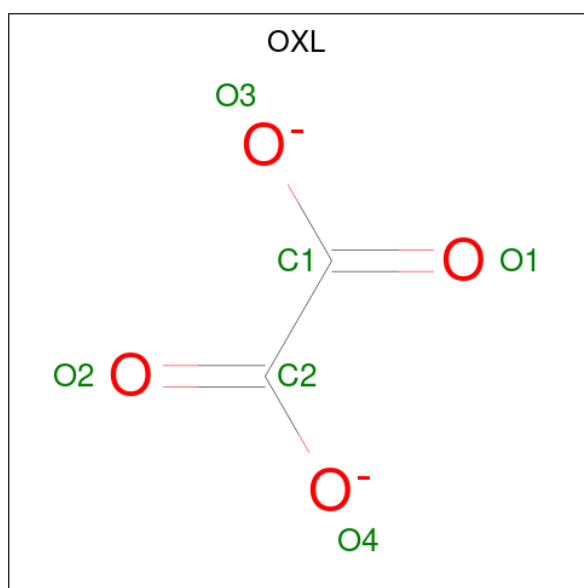
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	ARG	conflict	UNP P02788

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

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

- Molecule 3 is OXALATE ION (CCD ID: OXL) (formula: C₂O₄).



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

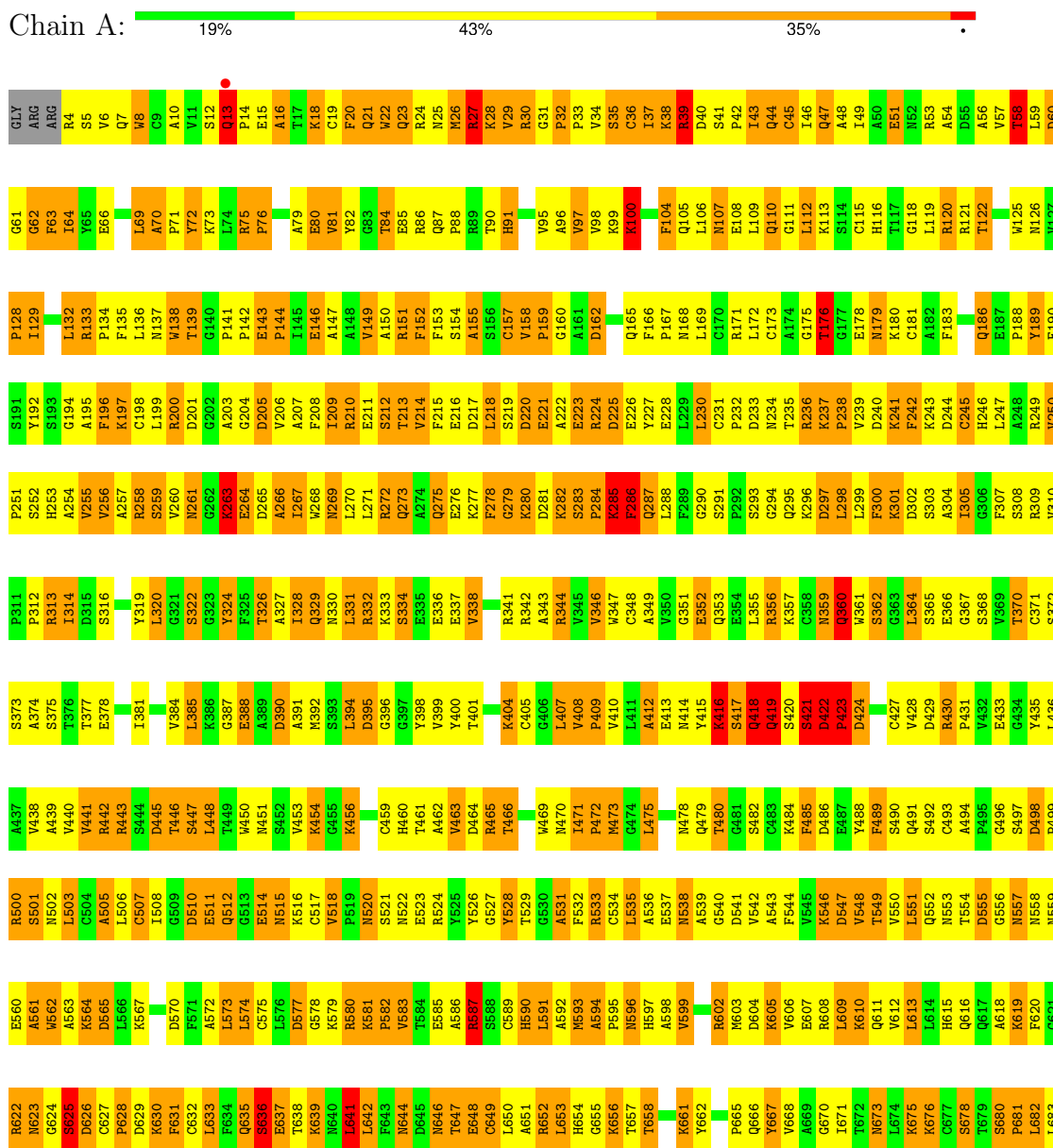
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	121	Total	O	0	0
			121	121		

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



E684
A685
C686
E687
F688
L689
R690
K691

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	155.46Å 96.92Å 55.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.40 8.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.40) 91.6 (8.00-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.20Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	(Not available) , (Not available) 0.185 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.14 , 72.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5433	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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: FE, OXL

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	1.50	33/5412 (0.6%)	3.14	772/7325 (10.5%)

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 (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	286	PHE	C-O	-20.04	0.98	1.24
1	A	284	PRO	CA-C	-18.64	1.19	1.52
1	A	79	ALA	C-O	-13.81	1.07	1.24
1	A	282	LYS	C-O	-11.85	1.06	1.24
1	A	324	TYR	C-O	10.81	1.36	1.24
1	A	282	LYS	N-CA	-9.83	1.35	1.46
1	A	421	SER	C-N	-8.64	1.15	1.33
1	A	284	PRO	C-N	-7.91	1.23	1.33
1	A	284	PRO	CA-CB	-6.81	1.44	1.53
1	A	635	GLN	C-N	-6.64	1.24	1.33
1	A	118	GLY	N-CA	6.32	1.51	1.45
1	A	471	ILE	CA-CB	6.24	1.57	1.54
1	A	639	LYS	CA-C	-6.24	1.44	1.52
1	A	514	GLU	C-O	-6.12	1.16	1.23
1	A	282	LYS	CA-C	-6.10	1.45	1.52
1	A	480	THR	CA-CB	6.07	1.62	1.54
1	A	198	CYS	N-CA	6.04	1.53	1.46
1	A	540	GLY	N-CA	5.98	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	597	HIS	ND1-CE1	5.81	1.38	1.32
1	A	560	GLU	CA-CB	-5.76	1.45	1.53
1	A	558	ASN	N-CA	5.72	1.53	1.46
1	A	281	ASP	C-N	-5.71	1.25	1.34
1	A	465	ARG	N-CA	5.67	1.52	1.45
1	A	638	THR	N-CA	5.46	1.52	1.46
1	A	422	ASP	C-N	5.40	1.46	1.33
1	A	245	CYS	N-CA	5.35	1.53	1.46
1	A	408	VAL	N-CA	5.25	1.51	1.46
1	A	176	THR	CA-CB	5.15	1.60	1.53
1	A	489	PHE	N-CA	5.13	1.52	1.45
1	A	632	CYS	N-CA	5.11	1.52	1.46
1	A	657	THR	CA-CB	5.09	1.60	1.53
1	A	290	GLY	N-CA	5.08	1.50	1.45
1	A	644	ASN	CA-C	5.04	1.59	1.52

All (772) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	ARG	CD-NE-CZ	27.14	162.39	124.40
1	A	604	ASP	CA-CB-CG	22.44	135.04	112.60
1	A	442	ARG	CD-NE-CZ	20.60	153.24	124.40
1	A	560	GLU	CA-CB-CG	18.75	151.59	114.10
1	A	553	ASN	CA-CB-CG	17.87	130.47	112.60
1	A	422	ASP	O-C-N	-15.67	103.30	121.32
1	A	673	ASN	CA-CB-CG	-14.53	98.07	112.60
1	A	151	ARG	CD-NE-CZ	-14.14	104.61	124.40
1	A	81	VAL	O-C-N	14.03	137.45	123.14
1	A	421	SER	O-C-N	13.59	140.67	122.59
1	A	300	PHE	CA-C-N	13.35	142.49	121.66
1	A	300	PHE	C-N-CA	13.35	142.49	121.66
1	A	178	GLU	CB-CG-CD	13.16	134.98	112.60
1	A	250	VAL	N-CA-C	13.08	124.15	108.45
1	A	314	ILE	N-CA-C	12.87	125.88	108.89
1	A	217	ASP	CA-CB-CG	12.79	125.39	112.60
1	A	570	ASP	O-C-N	12.69	138.20	122.34
1	A	451	ASN	CA-CB-CG	12.62	125.22	112.60
1	A	276	GLU	CA-CB-CG	12.56	139.22	114.10
1	A	599	VAL	CB-CA-C	12.03	125.83	110.91
1	A	57	VAL	O-C-N	11.64	134.36	123.19
1	A	606	VAL	N-CA-C	11.55	121.50	110.30
1	A	250	VAL	N-CA-CB	-11.52	101.88	111.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	507	CYS	O-C-N	11.30	136.20	122.86
1	A	607	GLU	CB-CA-C	11.28	128.86	110.81
1	A	673	ASN	OD1-CG-ND2	11.07	133.67	122.60
1	A	256	VAL	CA-C-O	-11.01	112.99	121.68
1	A	24	ARG	CG-CD-NE	10.97	136.14	112.00
1	A	155	ALA	CA-C-O	-10.94	108.36	121.06
1	A	284	PRO	O-C-N	10.83	136.75	122.24
1	A	507	CYS	CA-C-O	-10.55	110.06	121.56
1	A	62	GLY	O-C-N	10.53	133.40	122.24
1	A	430	ARG	NE-CZ-NH1	-10.53	110.97	121.50
1	A	408	VAL	N-CA-CB	-10.49	102.75	111.67
1	A	168	ASN	O-C-N	10.47	134.14	122.20
1	A	607	GLU	CB-CG-CD	10.41	130.31	112.60
1	A	560	GLU	N-CA-C	-10.40	91.56	108.52
1	A	352	GLU	O-C-N	10.24	133.04	122.08
1	A	70	ALA	N-CA-C	-10.22	95.64	109.84
1	A	605	LYS	CA-C-O	-10.14	107.70	119.56
1	A	484	LYS	CA-C-O	-10.06	110.07	122.64
1	A	224	ARG	NH1-CZ-NH2	10.04	132.35	119.30
1	A	442	ARG	NE-CZ-NH2	10.03	128.22	119.20
1	A	644	ASN	N-CA-CB	10.01	125.17	110.06
1	A	24	ARG	NE-CZ-NH1	9.99	131.49	121.50
1	A	451	ASN	OD1-CG-ND2	-9.99	112.61	122.60
1	A	304	ALA	N-CA-C	-9.97	97.09	110.55
1	A	429	ASP	CA-CB-CG	9.96	122.56	112.60
1	A	401	THR	CA-CB-CG2	9.96	127.43	110.50
1	A	602	ARG	N-CA-C	-9.92	98.20	110.41
1	A	155	ALA	O-C-N	9.91	134.77	123.27
1	A	259	SER	O-C-N	9.90	132.78	122.09
1	A	34	VAL	N-CA-CB	9.89	125.97	111.52
1	A	141	PRO	CB-CA-C	9.89	120.69	111.39
1	A	104	PHE	N-CA-C	-9.87	94.33	109.24
1	A	539	ALA	CA-C-N	-9.84	113.67	122.43
1	A	539	ALA	C-N-CA	-9.84	113.67	122.43
1	A	278	PHE	CA-CB-CG	-9.80	104.00	113.80
1	A	224	ARG	NE-CZ-NH2	-9.72	110.45	119.20
1	A	331	LEU	O-C-N	9.62	136.62	122.39
1	A	594	ALA	CA-C-O	-9.57	111.99	120.60
1	A	648	GLU	N-CA-C	-9.48	100.03	111.69
1	A	242	PHE	O-C-N	9.45	132.98	122.11
1	A	24	ARG	NH1-CZ-NH2	-9.44	107.03	119.30
1	A	85	GLU	CB-CG-CD	9.36	128.52	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	609	LEU	O-C-N	9.31	131.99	122.12
1	A	522	ASN	CA-CB-CG	-9.28	103.32	112.60
1	A	5	SER	CA-C-N	9.27	134.11	122.43
1	A	5	SER	C-N-CA	9.27	134.11	122.43
1	A	515	ASN	CA-CB-CG	-9.25	103.35	112.60
1	A	416	LYS	CA-C-O	9.20	131.41	120.92
1	A	304	ALA	CA-C-O	-9.19	110.96	121.81
1	A	635	GLN	CA-C-N	9.15	139.02	121.54
1	A	635	GLN	C-N-CA	9.15	139.02	121.54
1	A	610	LYS	CA-C-O	9.12	130.65	120.90
1	A	405	CYS	CA-C-N	-9.11	110.78	123.08
1	A	405	CYS	C-N-CA	-9.11	110.78	123.08
1	A	329	GLN	OE1-CD-NE2	9.10	131.70	122.60
1	A	237	LYS	CA-CB-CG	9.07	132.24	114.10
1	A	422	ASP	CA-CB-CG	-9.06	103.54	112.60
1	A	180	LYS	CA-C-O	9.06	131.23	120.81
1	A	15	GLU	N-CA-CB	9.03	123.72	110.26
1	A	665	PRO	CA-C-N	9.00	132.86	120.63
1	A	665	PRO	C-N-CA	9.00	132.86	120.63
1	A	255	VAL	CB-CA-C	8.99	120.94	111.23
1	A	121	ARG	NH1-CZ-NH2	8.99	130.99	119.30
1	A	110	GLN	CA-C-O	-8.99	111.96	120.95
1	A	518	VAL	N-CA-CB	-8.93	98.71	111.21
1	A	149	VAL	CB-CA-C	8.92	124.20	112.24
1	A	216	GLU	CA-CB-CG	8.92	131.93	114.10
1	A	450	TRP	CA-C-N	8.91	134.86	120.60
1	A	450	TRP	C-N-CA	8.91	134.86	120.60
1	A	6	VAL	CA-C-O	8.90	131.61	120.75
1	A	636	SER	O-C-N	8.86	134.37	122.59
1	A	81	VAL	N-CA-C	-8.84	95.71	108.53
1	A	265	ASP	O-C-N	8.83	131.53	122.08
1	A	391	ALA	CB-CA-C	-8.83	95.59	110.43
1	A	224	ARG	CD-NE-CZ	-8.82	112.05	124.40
1	A	546	LYS	CA-C-O	-8.81	110.50	121.78
1	A	448	LEU	CA-CB-CG	8.80	147.10	116.30
1	A	465	ARG	NE-CZ-NH2	-8.79	111.29	119.20
1	A	275	GLN	CA-C-N	8.77	132.03	120.28
1	A	275	GLN	C-N-CA	8.77	132.03	120.28
1	A	186	GLN	N-CA-C	-8.76	101.73	111.28
1	A	58	THR	CB-CA-C	8.74	123.95	109.53
1	A	100	LYS	CG-CD-CE	8.73	131.37	111.30
1	A	657	THR	CA-CB-OG1	-8.72	96.51	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	GLN	OE1-CD-NE2	8.69	131.29	122.60
1	A	551	LEU	O-C-N	-8.69	112.78	122.08
1	A	626	ASP	CA-CB-CG	-8.63	103.97	112.60
1	A	551	LEU	CB-CA-C	8.62	124.62	110.92
1	A	179	ASN	CA-CB-CG	-8.60	104.00	112.60
1	A	97	VAL	N-CA-C	8.59	120.26	107.80
1	A	240	ASP	CA-CB-CG	-8.58	104.02	112.60
1	A	657	THR	N-CA-CB	-8.55	98.85	111.51
1	A	160	GLY	CA-C-O	-8.51	110.17	119.27
1	A	493	CYS	N-CA-CB	8.50	124.64	110.79
1	A	362	SER	O-C-N	8.50	130.87	122.03
1	A	126	ASN	CB-CG-ND2	8.49	129.14	116.40
1	A	548	VAL	CB-CA-C	8.49	125.32	112.16
1	A	313	ARG	CD-NE-CZ	-8.45	112.57	124.40
1	A	524	ARG	NE-CZ-NH1	8.43	129.93	121.50
1	A	256	VAL	O-C-N	8.43	129.96	122.12
1	A	121	ARG	NE-CZ-NH2	-8.41	111.63	119.20
1	A	69	LEU	CA-C-O	8.37	131.09	121.47
1	A	580	ARG	NE-CZ-NH1	8.37	129.87	121.50
1	A	63	PHE	CA-CB-CG	-8.35	105.45	113.80
1	A	171	ARG	NE-CZ-NH1	8.30	129.80	121.50
1	A	508	ILE	N-CA-C	8.28	120.05	112.43
1	A	522	ASN	CA-C-O	-8.25	111.81	120.55
1	A	346	VAL	CA-C-O	-8.24	111.01	120.65
1	A	533	ARG	NE-CZ-NH2	-8.24	111.78	119.20
1	A	511	GLU	CA-C-N	8.23	135.25	122.49
1	A	511	GLU	C-N-CA	8.23	135.25	122.49
1	A	548	VAL	CA-CB-CG2	8.23	124.39	110.40
1	A	322	SER	CA-CB-OG	8.20	127.49	111.10
1	A	286	PHE	CB-CA-C	-8.19	94.11	110.42
1	A	388	GLU	CB-CA-C	-8.20	93.64	109.95
1	A	656	LYS	CA-C-O	-8.16	112.54	122.41
1	A	460	HIS	CA-C-O	-8.15	111.91	121.44
1	A	484	LYS	O-C-N	8.15	133.23	122.56
1	A	269	ASN	OD1-CG-ND2	8.14	130.74	122.60
1	A	152	PHE	CA-CB-CG	-8.12	105.68	113.80
1	A	337	GLU	CB-CG-CD	8.12	126.40	112.60
1	A	565	ASP	N-CA-C	8.12	123.36	113.38
1	A	210	ARG	NE-CZ-NH2	8.11	126.50	119.20
1	A	242	PHE	CA-CB-CG	8.10	121.90	113.80
1	A	497	SER	CA-CB-OG	8.10	127.29	111.10
1	A	629	ASP	N-CA-C	-8.08	101.55	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	559	ASN	OD1-CG-ND2	-8.05	114.55	122.60
1	A	378	GLU	CB-CG-CD	8.04	126.26	112.60
1	A	578	GLY	N-CA-C	-8.01	104.80	115.21
1	A	507	CYS	N-CA-CB	7.97	121.65	110.17
1	A	417	SER	CA-C-O	7.97	130.64	121.87
1	A	91	HIS	O-C-N	7.95	131.92	123.42
1	A	228	GLU	CB-CG-CD	7.94	126.09	112.60
1	A	86	ARG	O-C-N	7.93	130.65	122.09
1	A	259	SER	N-CA-C	-7.90	102.60	111.14
1	A	44	GLN	CB-CA-C	7.89	124.27	110.85
1	A	396	GLY	N-CA-C	-7.89	103.89	113.99
1	A	24	ARG	CB-CA-C	7.88	123.93	110.84
1	A	32	PRO	CB-CA-C	7.85	118.77	111.39
1	A	522	ASN	CB-CA-C	7.83	123.79	110.79
1	A	417	SER	N-CA-C	7.82	120.67	110.43
1	A	559	ASN	CA-CB-CG	7.79	120.39	112.60
1	A	241	LYS	CB-CG-CD	7.79	129.22	111.30
1	A	225	ASP	CA-CB-CG	7.77	120.37	112.60
1	A	532	PHE	CA-CB-CG	-7.77	106.03	113.80
1	A	510	ASP	O-C-N	7.76	131.76	121.83
1	A	443	ARG	CB-CG-CD	7.74	129.10	111.30
1	A	430	ARG	NH1-CZ-NH2	7.74	129.36	119.30
1	A	570	ASP	CA-C-O	-7.70	110.34	119.35
1	A	560	GLU	CB-CA-C	7.66	122.76	110.19
1	A	441	VAL	CA-C-O	-7.64	113.81	121.45
1	A	479	GLN	N-CA-C	7.63	119.60	111.28
1	A	76	PRO	CA-C-O	-7.62	112.34	121.03
1	A	465	ARG	CA-CB-CG	-7.58	98.95	114.10
1	A	649	CYS	O-C-N	7.58	132.66	122.59
1	A	31	GLY	O-C-N	7.57	129.23	122.42
1	A	537	GLU	CA-C-N	7.56	132.88	122.07
1	A	537	GLU	C-N-CA	7.56	132.88	122.07
1	A	587	ARG	N-CA-C	-7.55	103.13	111.36
1	A	687	GLU	N-CA-C	-7.55	102.99	111.07
1	A	132	LEU	N-CA-CB	-7.53	99.56	110.47
1	A	515	ASN	OD1-CG-ND2	7.53	130.13	122.60
1	A	557	ASN	CA-C-N	-7.49	111.20	122.74
1	A	557	ASN	C-N-CA	-7.49	111.20	122.74
1	A	220	ASP	CA-CB-CG	-7.48	105.12	112.60
1	A	228	GLU	CA-C-O	-7.46	113.32	121.31
1	A	531	ALA	N-CA-C	-7.46	103.08	111.14
1	A	498	ASP	O-C-N	7.46	127.80	121.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	557	ASN	CA-CB-CG	-7.42	105.18	112.60
1	A	171	ARG	CA-CB-CG	7.41	128.92	114.10
1	A	190	PHE	CA-C-O	7.41	130.55	121.81
1	A	514	GLU	CG-CD-OE1	7.40	135.41	118.40
1	A	143	GLU	CB-CG-CD	7.38	125.15	112.60
1	A	480	THR	N-CA-CB	-7.38	101.08	110.90
1	A	126	ASN	OD1-CG-ND2	-7.38	115.22	122.60
1	A	408	VAL	O-C-N	7.38	128.13	121.57
1	A	590	HIS	CA-CB-CG	-7.37	106.43	113.80
1	A	72	TYR	O-C-N	7.37	129.70	122.03
1	A	557	ASN	N-CA-C	-7.37	103.39	112.38
1	A	451	ASN	CB-CG-OD1	7.35	135.50	120.80
1	A	302	ASP	CA-CB-CG	-7.35	105.25	112.60
1	A	384	VAL	N-CA-C	-7.34	103.37	110.42
1	A	186	GLN	CB-CA-C	7.32	122.95	110.79
1	A	8	TRP	CA-C-O	-7.32	112.58	121.36
1	A	652	ARG	CG-CD-NE	7.31	128.09	112.00
1	A	360	GLN	CB-CG-CD	-7.31	100.18	112.60
1	A	454	LYS	CA-C-O	-7.30	112.91	120.80
1	A	223	GLU	N-CA-C	-7.30	103.41	111.36
1	A	212	SER	CA-CB-OG	7.28	125.66	111.10
1	A	352	GLU	CA-C-O	-7.28	113.06	121.07
1	A	272	ARG	CA-C-N	7.25	130.22	120.65
1	A	272	ARG	C-N-CA	7.25	130.22	120.65
1	A	69	LEU	N-CA-CB	-7.25	99.28	110.29
1	A	580	ARG	NE-CZ-NH2	-7.23	112.69	119.20
1	A	535	LEU	O-C-N	7.22	130.62	122.32
1	A	599	VAL	CA-C-O	-7.22	112.55	120.71
1	A	6	VAL	N-CA-CB	7.21	120.18	111.31
1	A	27	ARG	CB-CG-CD	7.20	127.86	111.30
1	A	499	PRO	N-CA-C	-7.19	105.57	114.20
1	A	176	THR	N-CA-C	7.19	120.24	108.52
1	A	461	THR	CA-C-O	-7.18	113.46	121.00
1	A	372	SER	CA-C-O	-7.17	113.26	121.58
1	A	171	ARG	CG-CD-NE	7.16	127.76	112.00
1	A	192	TYR	CA-CB-CG	7.16	126.79	113.90
1	A	310	VAL	N-CA-CB	-7.16	102.86	111.31
1	A	308	SER	CA-CB-OG	-7.16	96.79	111.10
1	A	91	HIS	CA-C-O	-7.15	113.58	121.23
1	A	366	GLU	CG-CD-OE2	-7.15	101.96	118.40
1	A	371	CYS	N-CA-C	7.14	121.30	109.95
1	A	544	PHE	CA-CB-CG	-7.13	106.67	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	ASN	CA-CB-CG	-7.12	105.48	112.60
1	A	597	HIS	CA-C-O	-7.11	114.01	121.55
1	A	670	GLY	CA-C-O	-7.11	113.32	121.00
1	A	20	PHE	N-CA-CB	7.10	120.64	110.13
1	A	260	VAL	N-CA-CB	-7.10	102.90	111.21
1	A	104	PHE	CA-C-O	-7.10	113.38	121.40
1	A	646	ASN	OD1-CG-ND2	7.09	129.69	122.60
1	A	496	GLY	O-C-N	7.09	130.74	122.30
1	A	441	VAL	O-C-N	7.09	130.55	122.82
1	A	622	ARG	O-C-N	7.07	129.44	122.09
1	A	76	PRO	CB-CA-C	-7.07	102.91	111.46
1	A	238	PRO	CA-C-N	7.06	134.68	121.97
1	A	238	PRO	C-N-CA	7.06	134.68	121.97
1	A	676	LYS	N-CA-C	7.05	119.82	111.71
1	A	303	SER	N-CA-C	7.04	121.17	112.58
1	A	493	CYS	CA-C-O	7.04	129.00	120.27
1	A	138	TRP	CA-C-N	7.04	130.41	120.28
1	A	138	TRP	C-N-CA	7.04	130.41	120.28
1	A	540	GLY	N-CA-C	-7.03	102.94	112.57
1	A	392	MET	N-CA-CB	-7.02	100.89	111.56
1	A	662	TYR	N-CA-C	7.02	118.58	111.07
1	A	284	PRO	CB-CA-C	-7.01	101.89	111.85
1	A	272	ARG	NH1-CZ-NH2	7.01	128.41	119.30
1	A	107	ASN	OD1-CG-ND2	7.00	129.60	122.60
1	A	249	ARG	O-C-N	6.99	131.52	123.27
1	A	516	LYS	CA-C-N	6.99	132.53	122.40
1	A	516	LYS	C-N-CA	6.99	132.53	122.40
1	A	186	GLN	OE1-CD-NE2	-6.97	115.63	122.60
1	A	439	ALA	CA-C-O	-6.95	113.10	120.40
1	A	261	ASN	N-CA-C	-6.95	101.79	111.52
1	A	378	GLU	CA-C-N	6.95	130.28	120.28
1	A	378	GLU	C-N-CA	6.95	130.28	120.28
1	A	691	LYS	CG-CD-CE	6.94	127.27	111.30
1	A	517	CYS	N-CA-C	6.93	121.12	112.24
1	A	51	GLU	O-C-N	6.93	131.48	122.19
1	A	395	ASP	CA-C-O	-6.93	113.84	121.87
1	A	642	LEU	CA-C-O	-6.93	110.60	120.51
1	A	610	LYS	CB-CG-CD	-6.92	95.38	111.30
1	A	206	VAL	CA-CB-CG2	6.92	122.16	110.40
1	A	375	SER	O-C-N	6.91	130.98	122.34
1	A	171	ARG	N-CA-CB	6.89	121.02	109.78
1	A	691	LYS	CA-C-O	-6.89	109.08	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	533	ARG	NE-CZ-NH1	6.88	128.38	121.50
1	A	228	GLU	CA-CB-CG	6.85	127.81	114.10
1	A	635	GLN	O-C-N	-6.85	113.95	123.34
1	A	334	SER	CA-C-O	6.84	129.76	122.03
1	A	314	ILE	O-C-N	6.83	130.39	122.81
1	A	64	ILE	CA-C-N	6.83	129.66	120.65
1	A	64	ILE	C-N-CA	6.83	129.66	120.65
1	A	314	ILE	CB-CA-C	-6.83	102.28	111.15
1	A	605	LYS	CB-CA-C	-6.82	99.03	110.56
1	A	497	SER	CA-C-O	-6.82	113.64	121.68
1	A	24	ARG	CB-CG-CD	6.81	126.97	111.30
1	A	681	PRO	O-C-N	6.81	131.00	122.22
1	A	475	LEU	CA-C-N	6.80	133.04	121.14
1	A	475	LEU	C-N-CA	6.80	133.04	121.14
1	A	629	ASP	O-C-N	6.80	130.40	122.17
1	A	613	LEU	CB-CA-C	6.80	123.14	110.70
1	A	539	ALA	CB-CA-C	6.79	122.20	110.79
1	A	151	ARG	NE-CZ-NH1	-6.79	114.71	121.50
1	A	624	GLY	CA-C-N	6.79	134.50	121.54
1	A	624	GLY	C-N-CA	6.79	134.50	121.54
1	A	362	SER	N-CA-C	-6.78	103.58	110.97
1	A	637	GLU	O-C-N	6.78	131.61	122.59
1	A	570	ASP	CB-CA-C	-6.78	98.77	110.09
1	A	116	HIS	CA-CB-CG	6.77	120.57	113.80
1	A	298	LEU	CB-CA-C	6.77	120.87	109.84
1	A	72	TYR	CA-C-N	6.76	131.72	122.19
1	A	72	TYR	C-N-CA	6.76	131.72	122.19
1	A	87	GLN	CB-CA-C	6.74	124.24	111.29
1	A	378	GLU	CA-CB-CG	6.74	127.58	114.10
1	A	259	SER	CA-C-N	6.74	131.52	122.90
1	A	259	SER	C-N-CA	6.74	131.52	122.90
1	A	309	ARG	CA-CB-CG	6.69	127.48	114.10
1	A	346	VAL	O-C-N	6.67	131.08	122.94
1	A	138	TRP	CA-C-O	6.67	127.59	120.46
1	A	392	MET	O-C-N	6.67	130.06	123.46
1	A	255	VAL	CA-C-N	-6.66	115.14	122.27
1	A	255	VAL	C-N-CA	-6.66	115.14	122.27
1	A	38	LYS	CA-CB-CG	6.65	127.40	114.10
1	A	48	ALA	N-CA-C	-6.64	103.73	110.97
1	A	250	VAL	CA-C-N	6.64	127.68	119.98
1	A	250	VAL	C-N-CA	6.64	127.68	119.98
1	A	137	ASN	OD1-CG-ND2	6.64	129.24	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	351	GLY	CA-C-N	6.62	130.00	120.79
1	A	351	GLY	C-N-CA	6.62	130.00	120.79
1	A	15	GLU	N-CA-C	-6.61	103.26	112.45
1	A	493	CYS	CA-C-N	6.61	129.75	122.74
1	A	493	CYS	C-N-CA	6.61	129.75	122.74
1	A	273	GLN	O-C-N	6.61	128.90	122.03
1	A	572	ALA	CA-C-O	-6.60	114.20	121.33
1	A	390	ASP	N-CA-CB	-6.60	100.57	111.06
1	A	144	PRO	O-C-N	6.59	130.89	122.85
1	A	314	ILE	CA-CB-CG1	-6.59	99.20	110.40
1	A	435	TYR	CA-CB-CG	6.59	125.76	113.90
1	A	329	GLN	O-C-N	6.59	128.94	122.09
1	A	59	LEU	N-CA-C	6.58	119.08	109.07
1	A	454	LYS	CA-CB-CG	6.58	127.25	114.10
1	A	630	LYS	N-CA-C	6.57	121.61	111.56
1	A	443	ARG	NE-CZ-NH2	6.54	125.09	119.20
1	A	273	GLN	OE1-CD-NE2	6.53	129.13	122.60
1	A	420	SER	O-C-N	6.53	131.47	122.46
1	A	647	THR	O-C-N	6.52	131.18	122.96
1	A	290	GLY	N-CA-C	-6.51	99.66	110.80
1	A	377	THR	O-C-N	6.51	128.87	122.09
1	A	670	GLY	O-C-N	6.51	128.43	122.18
1	A	21	GLN	N-CA-C	-6.51	104.19	111.28
1	A	488	TYR	CA-CB-CG	6.51	125.61	113.90
1	A	651	ALA	N-CA-C	6.51	120.30	109.95
1	A	427	CYS	CA-CB-SG	6.50	129.36	114.40
1	A	309	ARG	N-CA-CB	6.49	119.52	110.17
1	A	219	SER	N-CA-CB	-6.49	98.69	109.72
1	A	294	GLY	N-CA-C	-6.47	106.22	113.79
1	A	22	TRP	CA-CB-CG	6.46	125.88	113.60
1	A	388	GLU	CB-CG-CD	-6.46	101.62	112.60
1	A	305	ILE	CB-CA-C	6.46	117.59	110.62
1	A	249	ARG	CG-CD-NE	-6.43	97.85	112.00
1	A	261	ASN	N-CA-CB	6.43	121.68	111.91
1	A	328	ILE	N-CA-C	-6.42	104.50	110.53
1	A	412	ALA	N-CA-CB	-6.42	100.58	110.85
1	A	668	VAL	O-C-N	6.42	128.20	121.91
1	A	245	CYS	N-CA-CB	-6.41	100.35	110.79
1	A	366	GLU	CB-CA-C	-6.40	103.63	111.82
1	A	24	ARG	CA-CB-CG	6.40	126.90	114.10
1	A	522	ASN	O-C-N	6.39	128.90	122.12
1	A	139	THR	CA-CB-CG2	6.38	121.35	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	661	LYS	N-CA-C	-6.37	104.25	111.07
1	A	162	ASP	CA-CB-CG	-6.36	106.24	112.60
1	A	688	PHE	CA-C-O	-6.36	113.81	120.55
1	A	129	ILE	O-C-N	6.35	128.28	121.87
1	A	471	ILE	O-C-N	6.34	124.48	120.42
1	A	492	SER	CA-C-N	6.34	131.48	121.72
1	A	492	SER	C-N-CA	6.34	131.48	121.72
1	A	460	HIS	CA-CB-CG	-6.33	107.47	113.80
1	A	276	GLU	CG-CD-OE1	6.33	132.96	118.40
1	A	419	GLN	CB-CG-CD	6.33	123.35	112.60
1	A	36	CYS	CB-CA-C	-6.32	99.09	109.53
1	A	622	ARG	NE-CZ-NH1	6.32	127.81	121.50
1	A	223	GLU	CA-C-O	6.31	127.11	120.42
1	A	562	TRP	O-C-N	6.31	128.81	122.12
1	A	272	ARG	NE-CZ-NH2	-6.31	113.52	119.20
1	A	423	PRO	N-CA-C	-6.30	99.48	112.47
1	A	173	CYS	CB-CA-C	6.30	119.84	109.70
1	A	417	SER	CA-C-N	6.29	133.56	121.54
1	A	417	SER	C-N-CA	6.29	133.56	121.54
1	A	668	VAL	CA-C-O	-6.29	114.51	121.17
1	A	421	SER	N-CA-C	6.27	124.15	110.80
1	A	567	LYS	N-CA-C	-6.27	99.59	109.50
1	A	448	LEU	N-CA-CB	6.27	119.66	109.95
1	A	60	ASP	CA-CB-CG	-6.26	106.34	112.60
1	A	466	THR	CA-CB-OG1	-6.26	100.22	109.60
1	A	334	SER	N-CA-CB	-6.25	101.78	110.29
1	A	39	ARG	O-C-N	6.25	130.11	123.42
1	A	438	VAL	CA-C-O	-6.24	115.05	121.67
1	A	367	GLY	CA-C-O	-6.24	112.02	119.00
1	A	656	LYS	N-CA-CB	-6.23	101.61	110.58
1	A	237	LYS	CB-CG-CD	6.21	125.58	111.30
1	A	304	ALA	CA-C-N	-6.20	115.26	122.14
1	A	304	ALA	C-N-CA	-6.20	115.26	122.14
1	A	603	MET	CB-CG-SD	-6.20	94.11	112.70
1	A	555	ASP	CA-CB-CG	6.20	118.80	112.60
1	A	290	GLY	O-C-N	6.19	128.25	123.23
1	A	296	LYS	CA-CB-CG	6.19	126.48	114.10
1	A	336	GLU	CB-CG-CD	6.19	123.13	112.60
1	A	63	PHE	CA-C-N	-6.19	111.98	120.46
1	A	63	PHE	C-N-CA	-6.19	111.98	120.46
1	A	478	ASN	N-CA-C	-6.19	104.45	111.07
1	A	30	ARG	N-CA-CB	-6.18	107.13	114.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	THR	CB-CA-C	-6.18	100.06	110.19
1	A	599	VAL	CA-CB-CG1	6.18	120.90	110.40
1	A	424	ASP	N-CA-C	6.18	120.62	109.44
1	A	501	SER	CA-C-N	6.17	129.06	120.29
1	A	501	SER	C-N-CA	6.17	129.06	120.29
1	A	653	LEU	N-CA-C	6.17	120.00	112.23
1	A	359	ASN	O-C-N	6.16	130.79	122.59
1	A	631	PHE	CA-CB-CG	6.16	119.96	113.80
1	A	680	SER	N-CA-CB	6.14	119.08	110.11
1	A	374	ALA	N-CA-CB	6.14	120.91	111.46
1	A	652	ARG	CA-C-O	-6.14	114.81	121.44
1	A	146	GLU	O-C-N	6.13	129.16	122.11
1	A	207	ALA	N-CA-CB	6.12	120.96	110.68
1	A	512	GLN	CB-CA-C	-6.11	99.85	110.17
1	A	456	LYS	CG-CD-CE	6.10	125.32	111.30
1	A	16	ALA	CA-C-O	6.10	127.01	120.55
1	A	201	ASP	CB-CA-C	-6.09	98.82	110.57
1	A	240	ASP	CB-CA-C	6.09	120.24	109.65
1	A	242	PHE	CA-C-O	-6.09	114.10	120.92
1	A	212	SER	N-CA-C	6.08	117.71	111.14
1	A	244	ASP	CA-C-N	-6.08	112.35	121.72
1	A	244	ASP	C-N-CA	-6.08	112.35	121.72
1	A	300	PHE	N-CA-C	-6.08	100.09	109.52
1	A	254	ALA	N-CA-C	6.08	119.39	109.06
1	A	137	ASN	CA-C-N	-6.07	114.49	123.11
1	A	137	ASN	C-N-CA	-6.07	114.49	123.11
1	A	520	ASN	N-CA-CB	6.07	120.97	111.56
1	A	62	GLY	CA-C-O	-6.07	113.84	120.40
1	A	236	ARG	NH1-CZ-NH2	6.07	127.19	119.30
1	A	427	CYS	CA-C-O	-6.06	112.73	120.31
1	A	20	PHE	CA-C-N	-6.06	112.16	120.28
1	A	20	PHE	C-N-CA	-6.06	112.16	120.28
1	A	157	CYS	N-CA-CB	6.06	120.05	110.84
1	A	258	ARG	CD-NE-CZ	6.06	132.88	124.40
1	A	241	LYS	CG-CD-CE	6.05	125.23	111.30
1	A	230	LEU	CA-C-N	-6.04	112.25	121.92
1	A	230	LEU	C-N-CA	-6.04	112.25	121.92
1	A	454	LYS	CA-C-N	-6.04	116.25	123.44
1	A	454	LYS	C-N-CA	-6.04	116.25	123.44
1	A	237	LYS	CA-C-O	6.04	126.62	120.64
1	A	75	ARG	O-C-N	6.04	128.28	121.94
1	A	543	ALA	CA-C-O	-6.03	113.72	120.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	ARG	CA-CB-CG	-6.03	102.04	114.10
1	A	486	ASP	CA-CB-CG	6.03	118.62	112.60
1	A	27	ARG	NE-CZ-NH1	6.02	127.52	121.50
1	A	683	LEU	N-CA-C	-6.02	104.64	112.23
1	A	146	GLU	CB-CG-CD	6.01	122.82	112.60
1	A	310	VAL	O-C-N	6.00	125.15	121.37
1	A	416	LYS	CA-C-N	6.00	131.00	120.87
1	A	416	LYS	C-N-CA	6.00	131.00	120.87
1	A	642	LEU	O-C-N	5.99	130.56	122.59
1	A	22	TRP	N-CA-CB	5.99	118.86	109.94
1	A	212	SER	CA-C-O	5.98	126.86	120.70
1	A	564	LYS	N-CA-C	5.98	118.28	111.11
1	A	461	THR	CA-CB-OG1	-5.97	100.64	109.60
1	A	666	GLN	O-C-N	5.97	128.48	122.03
1	A	687	GLU	O-C-N	5.97	128.22	122.07
1	A	424	ASP	CA-C-N	5.96	125.35	118.85
1	A	424	ASP	C-N-CA	5.96	125.35	118.85
1	A	522	ASN	N-CA-C	-5.96	104.79	111.28
1	A	235	THR	O-C-N	5.96	130.18	123.27
1	A	375	SER	CA-C-O	-5.96	112.38	119.35
1	A	87	GLN	O-C-N	5.94	126.72	121.37
1	A	446	THR	N-CA-C	5.93	120.06	112.34
1	A	331	LEU	N-CA-C	-5.93	106.03	113.20
1	A	556	GLY	N-CA-C	-5.93	107.77	115.59
1	A	429	ASP	CA-C-O	5.92	126.28	119.35
1	A	538	ASN	CB-CG-ND2	-5.92	107.53	116.40
1	A	282	LYS	CA-C-O	-5.91	112.92	119.78
1	A	337	GLU	CG-CD-OE1	5.91	132.00	118.40
1	A	388	GLU	CA-C-N	5.91	131.51	122.11
1	A	388	GLU	C-N-CA	5.91	131.51	122.11
1	A	407	LEU	CA-C-O	-5.91	115.11	121.56
1	A	360	GLN	N-CA-CB	-5.91	100.50	110.49
1	A	266	ALA	O-C-N	5.91	128.18	122.03
1	A	203	ALA	N-CA-CB	5.91	118.57	110.01
1	A	370	THR	CA-CB-OG1	-5.90	100.75	109.60
1	A	320	LEU	N-CA-C	5.90	117.71	111.28
1	A	356	ARG	CA-C-N	-5.90	111.35	120.31
1	A	356	ARG	C-N-CA	-5.90	111.35	120.31
1	A	236	ARG	NE-CZ-NH1	-5.89	115.61	121.50
1	A	585	GLU	CB-CG-CD	5.88	122.60	112.60
1	A	667	TYR	CA-C-O	5.88	126.78	120.55
1	A	654	HIS	CA-CB-CG	-5.87	107.93	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	260	VAL	N-CA-C	5.87	116.56	107.99
1	A	27	ARG	NH1-CZ-NH2	-5.85	111.69	119.30
1	A	658	THR	N-CA-C	-5.85	99.11	109.06
1	A	239	VAL	CA-CB-CG1	5.84	120.33	110.40
1	A	602	ARG	CA-C-O	-5.84	115.33	121.99
1	A	221	GLU	CB-CA-C	-5.84	101.47	110.81
1	A	135	PHE	CB-CA-C	-5.83	99.58	109.38
1	A	197	LYS	N-CA-C	-5.83	105.01	111.36
1	A	26	MET	N-CA-C	-5.83	102.65	111.56
1	A	478	ASN	CA-CB-CG	5.83	118.43	112.60
1	A	520	ASN	O-C-N	5.82	129.65	123.42
1	A	563	ALA	N-CA-C	5.82	120.38	113.28
1	A	249	ARG	CA-C-O	-5.82	113.92	120.32
1	A	549	THR	N-CA-CB	5.81	118.44	110.01
1	A	329	GLN	CA-CB-CG	-5.81	102.49	114.10
1	A	351	GLY	CA-C-O	5.81	127.91	122.57
1	A	21	GLN	CA-C-O	-5.80	114.40	120.55
1	A	80	GLU	CB-CG-CD	-5.80	102.73	112.60
1	A	547	ASP	OD1-CG-OD2	5.80	136.82	122.90
1	A	286	PHE	CA-C-O	5.79	128.78	120.51
1	A	415	TYR	N-CA-CB	-5.79	102.37	111.05
1	A	394	LEU	CA-C-O	5.78	128.20	121.44
1	A	215	PHE	O-C-N	5.77	130.06	122.33
1	A	539	ALA	N-CA-C	-5.77	104.36	111.40
1	A	356	ARG	NE-CZ-NH1	5.76	127.26	121.50
1	A	558	ASN	O-C-N	5.76	130.05	123.31
1	A	560	GLU	CB-CG-CD	5.75	122.37	112.60
1	A	23	GLN	CA-C-N	5.74	130.32	121.19
1	A	23	GLN	C-N-CA	5.74	130.32	121.19
1	A	54	ALA	O-C-N	-5.74	118.25	123.41
1	A	348	CYS	N-CA-CB	5.74	119.78	110.43
1	A	13	GLN	CA-C-N	5.74	125.44	119.82
1	A	13	GLN	C-N-CA	5.74	125.44	119.82
1	A	272	ARG	CD-NE-CZ	-5.73	116.38	124.40
1	A	447	SER	CA-C-O	-5.73	112.36	119.18
1	A	45	CYS	N-CA-C	-5.73	105.04	111.28
1	A	95	VAL	CA-C-O	5.72	128.62	121.92
1	A	344	ARG	CA-C-O	5.72	127.00	120.54
1	A	647	THR	CB-CA-C	-5.72	101.68	110.26
1	A	372	SER	CA-C-N	-5.71	112.50	121.87
1	A	372	SER	C-N-CA	-5.71	112.50	121.87
1	A	118	GLY	N-CA-C	-5.71	103.50	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	554	THR	CA-CB-CG2	5.71	120.21	110.50
1	A	255	VAL	CA-C-O	-5.71	113.74	120.76
1	A	494	ALA	N-CA-CB	-5.70	104.02	111.09
1	A	591	LEU	CB-CA-C	-5.70	101.93	110.88
1	A	122	THR	CA-C-N	-5.69	111.66	120.31
1	A	122	THR	C-N-CA	-5.69	111.66	120.31
1	A	349	ALA	N-CA-CB	-5.69	101.64	110.57
1	A	215	PHE	CA-C-O	-5.69	113.08	119.79
1	A	537	GLU	CG-CD-OE2	-5.68	105.33	118.40
1	A	624	GLY	CA-C-O	5.68	126.51	120.94
1	A	141	PRO	O-C-N	-5.68	118.70	121.31
1	A	213	THR	CA-CB-OG1	-5.68	101.08	109.60
1	A	326	THR	O-C-N	5.68	130.04	122.43
1	A	280	LYS	O-C-N	5.68	130.14	122.59
1	A	465	ARG	N-CA-CB	-5.68	101.38	110.46
1	A	399	VAL	N-CA-C	-5.67	104.00	111.09
1	A	139	THR	O-C-N	5.67	128.86	122.22
1	A	629	ASP	CB-CA-C	5.67	120.32	110.79
1	A	551	LEU	CA-C-O	5.67	127.31	121.07
1	A	391	ALA	N-CA-CB	-5.67	102.94	111.56
1	A	585	GLU	CG-CD-OE1	5.67	131.43	118.40
1	A	652	ARG	CB-CA-C	5.66	119.67	109.64
1	A	20	PHE	N-CA-C	-5.66	104.50	111.40
1	A	596	ASN	O-C-N	5.66	129.77	122.81
1	A	632	CYS	CB-CA-C	5.66	119.47	110.19
1	A	43	ILE	CB-CG1-CD1	-5.65	101.94	113.80
1	A	329	GLN	CB-CG-CD	-5.63	103.03	112.60
1	A	415	TYR	CA-C-O	-5.63	115.03	121.68
1	A	218	LEU	N-CA-C	5.63	118.70	107.62
1	A	421	SER	CB-CA-C	-5.62	99.24	110.42
1	A	128	PRO	O-C-N	5.62	128.52	122.17
1	A	485	PHE	N-CA-CB	5.62	119.86	110.32
1	A	15	GLU	CA-CB-CG	5.61	125.32	114.10
1	A	456	LYS	N-CA-CB	5.61	118.12	110.38
1	A	625	SER	N-CA-CB	-5.61	101.02	110.49
1	A	57	VAL	CA-C-O	-5.60	115.69	120.96
1	A	84	THR	CA-CB-OG1	-5.60	101.20	109.60
1	A	171	ARG	CD-NE-CZ	5.59	132.23	124.40
1	A	259	SER	CA-C-O	-5.59	114.94	120.70
1	A	690	ARG	CD-NE-CZ	5.58	132.21	124.40
1	A	139	THR	OG1-CB-CG2	5.58	120.45	109.30
1	A	540	GLY	CA-C-O	-5.58	116.14	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	489	PHE	CA-CB-CG	-5.57	108.23	113.80
1	A	676	LYS	CA-C-N	5.56	130.00	120.72
1	A	676	LYS	C-N-CA	5.56	130.00	120.72
1	A	430	ARG	CA-C-O	5.56	124.70	119.76
1	A	18	LYS	CA-C-O	5.55	126.83	120.90
1	A	514	GLU	CG-CD-OE2	-5.55	105.64	118.40
1	A	5	SER	O-C-N	5.54	129.67	123.19
1	A	276	GLU	CG-CD-OE2	-5.54	105.66	118.40
1	A	135	PHE	CA-C-O	5.53	124.98	118.90
1	A	581	LYS	CA-C-O	5.53	125.52	120.26
1	A	512	GLN	O-C-N	5.53	128.93	122.24
1	A	387	GLY	O-C-N	5.52	128.61	122.31
1	A	656	LYS	N-CA-C	-5.52	98.92	108.52
1	A	183	PHE	CB-CA-C	5.52	119.66	111.88
1	A	256	VAL	N-CA-C	-5.52	101.85	109.46
1	A	641	LEU	CA-C-N	5.52	132.08	121.54
1	A	641	LEU	C-N-CA	5.52	132.08	121.54
1	A	361	TRP	CA-C-O	5.52	126.05	119.60
1	A	451	ASN	N-CA-C	5.51	119.11	112.38
1	A	655	GLY	N-CA-C	5.51	122.68	115.40
1	A	22	TRP	N-CA-C	-5.51	104.50	111.11
1	A	243	LYS	CA-CB-CG	5.51	125.12	114.10
1	A	205	ASP	O-C-N	5.51	130.18	122.36
1	A	553	ASN	O-C-N	5.51	128.86	122.19
1	A	189	TYR	CA-CB-CG	-5.51	103.99	113.90
1	A	392	MET	CA-C-O	-5.51	115.04	121.10
1	A	287	GLN	OE1-CD-NE2	5.50	128.10	122.60
1	A	573	LEU	CA-C-N	5.50	129.73	122.30
1	A	573	LEU	C-N-CA	5.50	129.73	122.30
1	A	676	LYS	CA-CB-CG	5.50	125.10	114.10
1	A	90	THR	CB-CA-C	5.50	120.58	111.23
1	A	370	THR	CA-C-O	-5.50	115.21	121.58
1	A	312	PRO	CA-C-N	-5.49	111.55	120.72
1	A	312	PRO	C-N-CA	-5.49	111.55	120.72
1	A	312	PRO	CB-CA-C	5.48	120.61	111.56
1	A	32	PRO	O-C-N	-5.47	118.79	121.31
1	A	44	GLN	N-CA-C	-5.47	105.40	111.36
1	A	515	ASN	CA-C-O	-5.47	114.01	120.57
1	A	244	ASP	O-C-N	5.47	129.81	122.49
1	A	583	VAL	N-CA-C	5.47	116.85	110.62
1	A	503	LEU	CB-CA-C	5.46	121.05	110.46
1	A	482	SER	CA-CB-OG	-5.45	100.20	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324	TYR	N-CA-C	5.44	117.29	111.36
1	A	550	VAL	N-CA-C	-5.44	105.30	110.42
1	A	633	LEU	CD1-CG-CD2	5.44	122.77	110.80
1	A	412	ALA	CA-C-O	-5.44	115.01	121.16
1	A	166	PHE	N-CA-C	5.44	119.70	110.02
1	A	597	HIS	N-CA-C	-5.44	102.95	110.35
1	A	528	TYR	N-CA-C	5.44	117.63	111.11
1	A	122	THR	O-C-N	5.43	129.81	122.59
1	A	644	ASN	N-CA-C	-5.42	101.63	110.20
1	A	561	ALA	O-C-N	5.42	129.80	122.59
1	A	366	GLU	O-C-N	5.42	128.79	122.67
1	A	505	ALA	CA-C-O	-5.41	113.98	120.10
1	A	180	LYS	CA-C-N	5.41	130.25	122.40
1	A	180	LYS	C-N-CA	5.41	130.25	122.40
1	A	480	THR	CA-C-O	5.41	124.77	118.77
1	A	35	SER	CA-CB-OG	5.40	121.91	111.10
1	A	56	ALA	N-CA-CB	-5.40	102.29	111.69
1	A	171	ARG	N-CA-C	5.40	120.27	111.37
1	A	158	VAL	CA-C-O	5.39	127.17	119.95
1	A	332	ARG	CD-NE-CZ	5.39	131.94	124.40
1	A	120	ARG	N-CA-C	5.38	119.79	113.23
1	A	420	SER	N-CA-C	-5.38	106.56	113.01
1	A	293	SER	N-CA-CB	5.38	117.86	109.85
1	A	242	PHE	N-CA-CB	5.37	118.53	109.78
1	A	86	ARG	CB-CA-C	-5.37	102.42	110.90
1	A	502	ASN	O-C-N	5.37	128.27	122.15
1	A	593	MET	CA-CB-CG	-5.37	103.37	114.10
1	A	378	GLU	O-C-N	-5.36	116.44	122.12
1	A	577	ASP	CA-C-N	-5.34	113.70	122.20
1	A	577	ASP	C-N-CA	-5.34	113.70	122.20
1	A	241	LYS	CA-C-O	5.34	129.02	119.36
1	A	450	TRP	CA-CB-CG	-5.34	103.46	113.60
1	A	223	GLU	CB-CG-CD	5.33	121.67	112.60
1	A	21	GLN	N-CA-CB	5.33	117.95	110.12
1	A	235	THR	N-CA-CB	5.33	121.44	111.53
1	A	421	SER	CA-C-N	5.32	134.78	121.80
1	A	421	SER	C-N-CA	5.32	134.78	121.80
1	A	419	GLN	N-CA-CB	5.32	120.16	112.13
1	A	47	GLN	CA-C-O	-5.31	113.06	119.27
1	A	32	PRO	CA-C-O	5.31	124.72	120.90
1	A	166	PHE	CA-C-N	5.30	126.47	119.84
1	A	166	PHE	C-N-CA	5.30	126.47	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	ARG	N-CA-CB	5.30	118.03	110.67
1	A	195	ALA	O-C-N	-5.30	115.55	122.59
1	A	96	ALA	CA-C-O	-5.29	114.79	120.46
1	A	84	THR	O-C-N	5.29	130.03	123.15
1	A	471	ILE	CA-C-N	5.29	126.45	119.84
1	A	471	ILE	C-N-CA	5.29	126.45	119.84
1	A	618	ALA	CB-CA-C	-5.29	100.52	110.67
1	A	602	ARG	CA-CB-CG	5.29	124.67	114.10
1	A	143	GLU	CG-CD-OE1	5.28	130.54	118.40
1	A	418	GLN	N-CA-C	-5.28	99.56	110.80
1	A	97	VAL	CB-CA-C	-5.27	103.27	110.96
1	A	57	VAL	CB-CA-C	-5.27	103.69	111.80
1	A	85	GLU	CA-CB-CG	5.26	124.63	114.10
1	A	200	ARG	NE-CZ-NH2	5.26	123.94	119.20
1	A	157	CYS	N-CA-C	-5.26	98.65	108.02
1	A	615	HIS	CA-C-O	-5.25	115.28	120.80
1	A	263	LYS	N-CA-CB	5.25	119.37	110.49
1	A	637	GLU	CA-C-N	5.25	132.63	123.91
1	A	637	GLU	C-N-CA	5.25	132.63	123.91
1	A	558	ASN	CA-C-O	-5.25	114.49	120.32
1	A	190	PHE	CA-C-N	5.25	131.56	121.54
1	A	190	PHE	C-N-CA	5.25	131.56	121.54
1	A	296	LYS	CB-CG-CD	5.25	123.37	111.30
1	A	381	ILE	CA-C-N	5.25	127.74	120.29
1	A	381	ILE	C-N-CA	5.25	127.74	120.29
1	A	151	ARG	N-CA-C	-5.24	107.26	113.97
1	A	104	PHE	CB-CA-C	5.24	121.60	110.07
1	A	459	CYS	CA-CB-SG	5.24	126.45	114.40
1	A	243	LYS	CG-CD-CE	5.24	123.34	111.30
1	A	682	LEU	CA-C-O	-5.24	114.87	120.42
1	A	368	SER	N-CA-CB	5.23	118.93	110.40
1	A	505	ALA	N-CA-C	5.23	117.72	111.71
1	A	404	LYS	CA-C-O	5.23	125.82	119.49
1	A	207	ALA	N-CA-C	-5.22	100.39	108.90
1	A	253	HIS	CA-C-N	5.22	131.35	122.37
1	A	253	HIS	C-N-CA	5.22	131.35	122.37
1	A	297	ASP	CA-C-N	-5.22	114.03	121.50
1	A	297	ASP	C-N-CA	-5.22	114.03	121.50
1	A	691	LYS	CB-CG-CD	5.22	123.30	111.30
1	A	196	PHE	CB-CA-C	5.21	120.23	110.70
1	A	531	ALA	CB-CA-C	5.21	119.13	110.90
1	A	629	ASP	N-CA-CB	5.20	117.83	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	305	ILE	O-C-N	5.20	128.68	122.03
1	A	407	LEU	CA-C-N	-5.20	113.41	121.88
1	A	407	LEU	C-N-CA	-5.20	113.41	121.88
1	A	97	VAL	CA-CB-CG2	5.20	119.23	110.40
1	A	72	TYR	N-CA-CB	-5.19	102.33	109.91
1	A	613	LEU	CA-C-O	-5.19	114.48	120.24
1	A	650	LEU	CD1-CG-CD2	-5.19	99.38	110.80
1	A	673	ASN	CB-CG-OD1	-5.19	110.42	120.80
1	A	675	LYS	CA-C-O	-5.19	113.22	119.49
1	A	211	GLU	CA-C-N	5.18	127.49	120.44
1	A	211	GLU	C-N-CA	5.18	127.49	120.44
1	A	623	ASN	OD1-CG-ND2	-5.18	117.42	122.60
1	A	139	THR	CA-CB-OG1	-5.18	101.83	109.60
1	A	631	PHE	O-C-N	5.17	129.21	123.52
1	A	133	ARG	O-C-N	5.17	125.46	120.55
1	A	619	LYS	CA-CB-CG	-5.17	103.76	114.10
1	A	129	ILE	CB-CA-C	-5.16	104.16	112.16
1	A	373	SER	N-CA-CB	-5.16	103.42	111.56
1	A	461	THR	N-CA-C	-5.15	105.35	110.97
1	A	239	VAL	N-CA-CB	-5.15	102.73	111.23
1	A	470	ASN	CA-C-O	-5.15	115.39	120.90
1	A	656	LYS	O-C-N	5.15	129.18	122.38
1	A	460	HIS	O-C-N	5.14	129.84	123.15
1	A	12	SER	CA-C-O	5.14	127.02	121.26
1	A	66	GLU	N-CA-CB	5.14	117.63	109.82
1	A	178	GLU	CA-CB-CG	5.14	124.37	114.10
1	A	500	ARG	CB-CA-C	5.14	118.64	109.29
1	A	121	ARG	CB-CG-CD	5.13	123.11	111.30
1	A	157	CYS	CA-C-O	-5.13	114.79	120.33
1	A	602	ARG	NE-CZ-NH2	-5.12	114.59	119.20
1	A	392	MET	N-CA-C	-5.12	100.53	108.42
1	A	466	THR	N-CA-C	5.12	116.55	110.97
1	A	582	PRO	CB-CA-C	5.12	117.95	110.63
1	A	255	VAL	N-CA-CB	-5.12	105.45	111.39
1	A	427	CYS	N-CA-C	-5.11	104.68	112.04
1	A	198	CYS	CA-CB-SG	5.11	126.14	114.40
1	A	118	GLY	CA-C-O	-5.10	116.75	121.96
1	A	607	GLU	O-C-N	-5.10	116.78	122.09
1	A	408	VAL	CA-C-O	-5.10	114.01	120.95
1	A	490	SER	CA-C-N	5.10	130.77	121.89
1	A	490	SER	C-N-CA	5.10	130.77	121.89
1	A	395	ASP	O-C-N	5.09	128.60	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	496	GLY	CA-C-O	-5.09	113.45	119.46
1	A	486	ASP	CB-CG-OD1	5.09	130.11	118.40
1	A	118	GLY	O-C-N	5.09	129.51	123.46
1	A	430	ARG	N-CA-CB	5.09	118.30	110.01
1	A	465	ARG	NH1-CZ-NH2	5.09	125.91	119.30
1	A	327	ALA	O-C-N	5.08	128.52	122.27
1	A	445	ASP	CA-CB-CG	5.07	117.67	112.60
1	A	267	ILE	O-C-N	5.06	127.43	121.96
1	A	8	TRP	O-C-N	5.06	128.73	123.06
1	A	175	GLY	CA-C-N	5.06	130.14	123.05
1	A	175	GLY	C-N-CA	5.06	130.14	123.05
1	A	8	TRP	CA-C-N	-5.06	116.04	122.77
1	A	8	TRP	C-N-CA	-5.06	116.04	122.77
1	A	529	THR	N-CA-C	-5.06	105.67	111.14
1	A	538	ASN	OD1-CG-ND2	5.04	127.64	122.60
1	A	370	THR	CA-CB-CG2	5.04	119.07	110.50
1	A	384	VAL	CA-CB-CG2	5.04	118.96	110.40
1	A	385	LEU	CA-C-O	-5.03	115.22	120.55
1	A	574	LEU	O-C-N	5.03	128.91	123.13
1	A	416	LYS	N-CA-CB	5.02	117.37	109.69
1	A	433	GLU	N-CA-C	5.02	120.25	113.72
1	A	13	GLN	O-C-N	5.02	127.09	121.32
1	A	264	GLU	CA-C-N	5.02	127.77	120.79
1	A	264	GLU	C-N-CA	5.02	127.77	120.79
1	A	322	SER	N-CA-CB	5.02	117.42	109.94
1	A	524	ARG	CG-CD-NE	5.02	123.05	112.00
1	A	430	ARG	CD-NE-CZ	-5.01	117.38	124.40
1	A	24	ARG	CA-C-O	-5.01	115.16	121.02
1	A	80	GLU	CA-C-O	5.01	126.86	121.55
1	A	409	PRO	O-C-N	-5.01	117.49	123.10
1	A	639	LYS	O-C-N	5.01	129.32	122.46
1	A	503	LEU	CA-C-N	-5.01	114.79	122.60
1	A	503	LEU	C-N-CA	-5.01	114.79	122.60
1	A	15	GLU	CG-CD-OE2	-5.00	106.90	118.40
1	A	635	GLN	CB-CG-CD	-5.00	104.10	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	285	LYS	Mainchain
1	A	587	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	5298	0	5142	435	0
2	A	2	0	0	0	0
3	A	12	0	0	0	0
4	A	121	0	0	31	0
All	All	5433	0	5142	435	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 (435) 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:291:SER:HB3	1:A:298:LEU:HD23	1.19	1.19
1:A:417:SER:C	1:A:419:GLN:H	1.42	1.13
1:A:462:ALA:HB3	1:A:465:ARG:HD2	1.31	1.08
1:A:13:GLN:HB3	1:A:14:PRO:HD3	1.35	1.05
1:A:119:LEU:HG	1:A:120:ARG:HD3	1.30	1.05
1:A:100:LYS:HD2	1:A:225:ASP:O	1.59	1.03
1:A:295:GLN:HB3	1:A:298:LEU:HD21	1.33	1.03
1:A:231:CYS:SG	1:A:237:LYS:HD3	2.00	1.02
1:A:220:ASP:OD1	1:A:221:GLU:N	2.00	0.95
1:A:283:SER:OG	1:A:285:LYS:NZ	2.00	0.94
1:A:626:ASP:HB3	1:A:630:LYS:HB2	1.51	0.93
1:A:257:ALA:HB1	4:A:713:HOH:O	1.67	0.93
1:A:686:CYS:O	1:A:690:ARG:HG2	1.69	0.92
1:A:259:SER:O	4:A:835:HOH:O	1.88	0.92
1:A:36:CYS:C	1:A:37:ILE:HD12	1.96	0.91
1:A:422:ASP:O	1:A:424:ASP:N	2.04	0.90
1:A:13:GLN:HB3	1:A:14:PRO:CD	2.02	0.90
1:A:417:SER:C	1:A:419:GLN:N	2.24	0.89
1:A:113:LYS:O	1:A:205:ASP:HB2	1.71	0.89
1:A:658:THR:HG21	1:A:661:LYS:HG3	1.52	0.89
1:A:291:SER:HB3	1:A:298:LEU:CD2	2.02	0.89
1:A:443:ARG:CD	4:A:868:HOH:O	2.21	0.88
1:A:238:PRO:HD2	1:A:241:LYS:HG3	1.54	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:647:THR:HG22	1:A:649:CYS:O	1.75	0.85
1:A:138:TRP:NE1	1:A:143:GLU:O	2.09	0.85
1:A:58:THR:HG23	4:A:704:HOH:O	1.76	0.84
1:A:295:GLN:HB3	1:A:298:LEU:CD2	2.06	0.84
1:A:214:VAL:HG12	4:A:934:HOH:O	1.77	0.84
1:A:646:ASN:OD1	4:A:886:HOH:O	1.95	0.83
1:A:622:ARG:HD3	1:A:622:ARG:O	1.76	0.82
1:A:443:ARG:HD2	4:A:868:HOH:O	1.77	0.82
1:A:561:ALA:HA	1:A:564:LYS:HD3	1.61	0.82
1:A:41:SER:HB2	1:A:42:PRO:HD2	1.62	0.82
1:A:70:ALA:HA	1:A:73:LYS:HE3	1.62	0.82
1:A:295:GLN:CB	1:A:298:LEU:HD21	2.10	0.82
1:A:176:THR:HG22	1:A:176:THR:O	1.77	0.81
1:A:446:THR:N	4:A:784:HOH:O	2.12	0.81
1:A:352:GLU:H	1:A:352:GLU:CD	1.87	0.81
1:A:680:SER:HB2	1:A:681:PRO:HD2	1.62	0.81
1:A:322:SER:HB3	1:A:385:LEU:O	1.78	0.81
1:A:647:THR:CG2	1:A:649:CYS:O	2.29	0.81
1:A:658:THR:CG2	1:A:661:LYS:HG3	2.10	0.81
1:A:291:SER:CB	1:A:298:LEU:HD23	2.09	0.81
1:A:443:ARG:NE	4:A:868:HOH:O	2.13	0.81
1:A:658:THR:HG23	1:A:661:LYS:H	1.45	0.80
1:A:39:ARG:HH11	1:A:39:ARG:CG	1.94	0.80
1:A:27:ARG:HD2	1:A:28:LYS:N	1.96	0.80
1:A:430:ARG:HG2	1:A:431:PRO:HD2	1.63	0.79
1:A:446:THR:CA	4:A:784:HOH:O	2.31	0.79
1:A:385:LEU:HD23	1:A:407:LEU:HD21	1.64	0.78
1:A:26:MET:HE2	1:A:270:LEU:HD12	1.66	0.78
1:A:104:PHE:HA	1:A:108:GLU:OE1	1.84	0.78
1:A:667:TYR:CE2	1:A:671:ILE:HD11	2.20	0.76
1:A:115:CYS:SG	1:A:204:GLY:HA3	2.26	0.76
1:A:4:ARG:HG3	1:A:4:ARG:HH11	1.48	0.76
1:A:39:ARG:HH11	1:A:39:ARG:HG2	1.49	0.76
1:A:214:VAL:O	1:A:218:LEU:HB2	1.86	0.75
1:A:99:LYS:HG2	1:A:227:TYR:CE1	2.22	0.74
1:A:359:ASN:O	1:A:362:SER:HB3	1.87	0.74
1:A:326:THR:HG22	1:A:329:GLN:HE22	1.52	0.73
1:A:595:PRO:O	4:A:918:HOH:O	2.05	0.73
1:A:40:ASP:HB2	1:A:44:GLN:OE1	1.87	0.73
1:A:385:LEU:CD2	1:A:407:LEU:HD21	2.17	0.73
1:A:447:SER:N	4:A:784:HOH:O	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ARG:NH1	1:A:263:LYS:HE3	2.05	0.72
1:A:533:ARG:NH1	4:A:914:HOH:O	2.17	0.72
1:A:462:ALA:HB3	1:A:465:ARG:CD	2.17	0.72
1:A:220:ASP:HB3	1:A:223:GLU:HG3	1.72	0.71
1:A:622:ARG:HD3	1:A:622:ARG:C	2.15	0.71
1:A:417:SER:O	1:A:419:GLN:N	2.19	0.71
1:A:186:GLN:O	1:A:188:PRO:HD3	1.91	0.70
1:A:47:GLN:HG2	1:A:72:TYR:CE1	2.26	0.70
1:A:573:LEU:HD11	1:A:586:ALA:HB2	1.72	0.70
1:A:344:ARG:HD3	1:A:370:THR:HG21	1.73	0.70
1:A:612:VAL:O	1:A:616:GLN:HG2	1.90	0.70
1:A:446:THR:CB	4:A:784:HOH:O	2.40	0.69
1:A:7:GLN:HG2	1:A:35:SER:OG	1.92	0.69
1:A:282:LYS:O	1:A:283:SER:HB2	1.91	0.69
1:A:413:GLU:OE2	4:A:774:HOH:O	2.11	0.69
1:A:38:LYS:O	1:A:39:ARG:HG2	1.93	0.69
1:A:13:GLN:CB	1:A:14:PRO:CD	2.69	0.68
1:A:352:GLU:O	1:A:355:LEU:HB3	1.93	0.68
1:A:422:ASP:O	1:A:423:PRO:C	2.32	0.68
1:A:220:ASP:OD1	1:A:220:ASP:C	2.36	0.68
1:A:436:LEU:CD2	1:A:593:MET:HE2	2.24	0.67
1:A:119:LEU:HG	1:A:120:ARG:CD	2.19	0.67
1:A:223:GLU:HB3	4:A:921:HOH:O	1.94	0.67
1:A:622:ARG:C	1:A:622:ARG:CD	2.68	0.67
1:A:98:VAL:HG11	1:A:230:LEU:HD21	1.76	0.67
1:A:445:ASP:O	1:A:580:ARG:NH2	2.28	0.67
1:A:18:LYS:O	1:A:22:TRP:N	2.17	0.66
1:A:480:THR:HG21	4:A:936:HOH:O	1.94	0.66
1:A:547:ASP:OD1	1:A:547:ASP:N	2.28	0.66
1:A:133:ARG:N	1:A:134:PRO:CD	2.59	0.66
1:A:4:ARG:HH22	1:A:266:ALA:HB2	1.59	0.65
1:A:107:ASN:OD1	1:A:107:ASN:N	2.15	0.65
1:A:330:ASN:C	1:A:332:ARG:H	2.05	0.65
1:A:430:ARG:HH22	1:A:648:GLU:CD	2.04	0.65
1:A:4:ARG:HG3	1:A:4:ARG:NH1	2.12	0.65
1:A:29:VAL:O	1:A:30:ARG:HB2	1.96	0.64
1:A:441:VAL:HG13	1:A:574:LEU:HD13	1.79	0.64
1:A:436:LEU:HD21	1:A:593:MET:HE2	1.80	0.64
1:A:658:THR:CG2	1:A:661:LYS:CG	2.76	0.64
1:A:288:LEU:HD11	1:A:300:PHE:CE2	2.33	0.64
1:A:122:THR:HG21	1:A:250:VAL:HG21	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:MET:HE2	1:A:270:LEU:CD1	2.29	0.63
1:A:409:PRO:HB2	1:A:653:LEU:HD11	1.81	0.63
1:A:430:ARG:HG2	1:A:431:PRO:CD	2.28	0.63
1:A:359:ASN:O	1:A:362:SER:CB	2.47	0.63
1:A:13:GLN:CB	1:A:14:PRO:HD3	2.20	0.63
1:A:250:VAL:HB	1:A:251:PRO:HD2	1.80	0.63
1:A:258:ARG:NH1	1:A:261:ASN:O	2.33	0.62
1:A:473:MET:HE3	1:A:485:PHE:HB3	1.81	0.62
1:A:132:LEU:O	1:A:136:LEU:HG	1.99	0.62
1:A:456:LYS:N	1:A:456:LYS:HD2	2.15	0.61
1:A:51:GLU:HG3	1:A:53:ARG:CG	2.30	0.61
1:A:442:ARG:HD3	1:A:538:ASN:OD1	2.01	0.61
1:A:360:GLN:NE2	1:A:631:PHE:HE1	1.98	0.61
1:A:644:ASN:HB3	4:A:886:HOH:O	2.01	0.61
1:A:42:PRO:O	1:A:46:ILE:HG13	2.01	0.60
1:A:436:LEU:HD21	1:A:593:MET:CE	2.30	0.60
1:A:448:LEU:HD11	1:A:456:LYS:HG2	1.83	0.60
1:A:352:GLU:CD	1:A:352:GLU:N	2.58	0.60
1:A:636:SER:HB3	1:A:641:LEU:HD22	1.83	0.60
1:A:133:ARG:HB3	1:A:134:PRO:HD3	1.83	0.60
1:A:346:VAL:HG22	1:A:370:THR:CG2	2.32	0.60
1:A:446:THR:HB	4:A:784:HOH:O	2.00	0.60
1:A:36:CYS:O	1:A:37:ILE:HD12	2.02	0.60
1:A:71:PRO:C	1:A:73:LYS:HD2	2.26	0.60
1:A:247:LEU:HD12	1:A:247:LEU:N	2.17	0.60
1:A:416:LYS:HD2	1:A:416:LYS:C	2.27	0.59
1:A:4:ARG:NH2	1:A:266:ALA:HB2	2.18	0.59
1:A:288:LEU:HD11	1:A:300:PHE:HE2	1.68	0.59
1:A:88:PRO:HB3	1:A:305:ILE:HD11	1.85	0.59
1:A:581:LYS:HB3	1:A:582:PRO:CD	2.33	0.58
1:A:181:CYS:SG	1:A:181:CYS:O	2.61	0.58
1:A:76:PRO:HA	1:A:256:VAL:HA	1.86	0.58
1:A:20:PHE:O	1:A:23:GLN:HB3	2.03	0.58
1:A:313:ARG:NH1	1:A:313:ARG:HG3	2.18	0.58
1:A:410:VAL:HG21	1:A:609:LEU:HD23	1.85	0.58
1:A:272:ARG:O	1:A:275:GLN:HB3	2.04	0.58
1:A:359:ASN:O	1:A:362:SER:N	2.37	0.57
1:A:58:THR:HG21	1:A:300:PHE:CD1	2.39	0.57
1:A:551:LEU:HD11	1:A:583:VAL:HG12	1.84	0.57
1:A:58:THR:HB	1:A:255:VAL:HG22	1.87	0.57
1:A:122:THR:HA	1:A:324:TYR:OH	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:ASP:OD1	1:A:579:LYS:N	2.30	0.57
1:A:41:SER:HB2	1:A:42:PRO:CD	2.33	0.57
1:A:220:ASP:OD1	1:A:222:ALA:N	2.37	0.57
1:A:221:GLU:HG3	4:A:761:HOH:O	2.04	0.57
1:A:271:LEU:O	1:A:275:GLN:HB2	2.05	0.57
1:A:413:GLU:HB3	1:A:647:THR:HG23	1.85	0.57
1:A:440:VAL:HG12	1:A:535:LEU:CD2	2.35	0.57
1:A:346:VAL:HG22	1:A:370:THR:HG23	1.87	0.57
1:A:471:ILE:HD13	1:A:592:ALA:HB3	1.87	0.57
1:A:442:ARG:HH12	1:A:541:ASP:HA	1.69	0.57
1:A:605:LYS:O	1:A:605:LYS:HG3	2.05	0.56
1:A:47:GLN:HG2	1:A:72:TYR:HE1	1.67	0.56
1:A:81:VAL:HG11	1:A:88:PRO:HB2	1.88	0.56
1:A:271:LEU:HB3	1:A:307:PHE:CD2	2.41	0.56
1:A:334:SER:HA	4:A:705:HOH:O	2.04	0.56
1:A:100:LYS:HG3	1:A:226:GLU:C	2.30	0.56
1:A:330:ASN:C	1:A:332:ARG:N	2.62	0.56
1:A:196:PHE:O	1:A:200:ARG:HB2	2.06	0.56
1:A:580:ARG:O	1:A:581:LYS:HG3	2.06	0.56
1:A:360:GLN:HE21	1:A:631:PHE:HE1	1.54	0.56
1:A:25:ASN:HA	1:A:28:LYS:HB2	1.87	0.55
1:A:332:ARG:C	1:A:333:LYS:HG2	2.31	0.55
1:A:514:GLU:O	1:A:515:ASN:HB2	2.07	0.55
1:A:324:TYR:O	1:A:328:ILE:HG13	2.06	0.55
1:A:445:ASP:HB3	1:A:448:LEU:HD23	1.87	0.55
1:A:129:ILE:HG22	1:A:129:ILE:O	2.06	0.55
1:A:286:PHE:CG	1:A:287:GLN:N	2.74	0.55
1:A:417:SER:OG	1:A:418:GLN:N	2.38	0.55
1:A:268:TRP:HA	1:A:268:TRP:CE3	2.43	0.55
1:A:301:LYS:HD3	1:A:301:LYS:C	2.31	0.55
1:A:51:GLU:CD	1:A:53:ARG:HH11	2.14	0.54
1:A:214:VAL:CG1	4:A:934:HOH:O	2.46	0.54
1:A:297:ASP:OD2	4:A:768:HOH:O	2.18	0.54
1:A:221:GLU:O	1:A:224:ARG:HB2	2.07	0.54
1:A:436:LEU:HD22	1:A:590:HIS:ND1	2.23	0.54
1:A:133:ARG:NH1	1:A:330:ASN:O	2.40	0.54
1:A:362:SER:O	1:A:365:SER:OG	2.26	0.54
1:A:680:SER:HB2	1:A:681:PRO:CD	2.35	0.54
1:A:346:VAL:O	1:A:390:ASP:HB2	2.08	0.54
1:A:81:VAL:CG1	1:A:88:PRO:HB2	2.38	0.54
1:A:42:PRO:O	1:A:46:ILE:N	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LYS:HG3	1:A:226:GLU:O	2.08	0.54
1:A:507:CYS:HB3	1:A:523:GLU:CD	2.33	0.53
1:A:37:ILE:HD12	1:A:37:ILE:N	2.19	0.53
1:A:129:ILE:HD13	1:A:129:ILE:N	2.22	0.53
1:A:510:ASP:N	1:A:514:GLU:O	2.35	0.53
1:A:47:GLN:O	1:A:51:GLU:HG2	2.08	0.53
1:A:231:CYS:HB2	1:A:233:ASP:OD1	2.09	0.53
1:A:344:ARG:HD3	1:A:370:THR:CG2	2.39	0.53
1:A:551:LEU:HD11	1:A:583:VAL:CG1	2.39	0.53
1:A:97:VAL:O	1:A:199:LEU:HD22	2.09	0.53
1:A:352:GLU:N	1:A:352:GLU:OE1	2.22	0.52
1:A:436:LEU:HD22	1:A:590:HIS:CG	2.44	0.52
1:A:639:LYS:HB2	1:A:641:LEU:HD13	1.92	0.52
1:A:680:SER:HB2	4:A:820:HOH:O	2.08	0.52
1:A:111:GLY:N	1:A:152:PHE:O	2.32	0.52
1:A:575:CYS:HB2	1:A:577:ASP:OD1	2.08	0.52
1:A:10:ALA:HB3	1:A:37:ILE:O	2.09	0.52
1:A:75:ARG:NH1	1:A:314:ILE:O	2.42	0.52
1:A:97:VAL:HG23	1:A:209:ILE:HD13	1.92	0.52
1:A:71:PRO:O	1:A:73:LYS:HD2	2.10	0.52
1:A:343:ALA:O	1:A:608:ARG:NE	2.41	0.52
1:A:360:GLN:NE2	1:A:631:PHE:CE1	2.78	0.52
1:A:40:ASP:O	1:A:41:SER:HB3	2.11	0.51
1:A:133:ARG:N	1:A:134:PRO:HD2	2.24	0.51
1:A:189:TYR:C	1:A:194:GLY:HA3	2.35	0.51
1:A:231:CYS:SG	1:A:237:LYS:CD	2.88	0.51
1:A:316:SER:O	1:A:320:LEU:HG	2.11	0.51
1:A:580:ARG:NH1	4:A:785:HOH:O	1.94	0.51
1:A:51:GLU:HG3	1:A:53:ARG:HG3	1.93	0.51
1:A:332:ARG:C	1:A:333:LYS:CG	2.84	0.51
1:A:577:ASP:OD1	1:A:579:LYS:HB2	2.10	0.51
1:A:247:LEU:N	1:A:247:LEU:CD1	2.73	0.51
1:A:400:TYR:O	1:A:404:LYS:HG2	2.10	0.51
1:A:581:LYS:CB	1:A:582:PRO:CD	2.89	0.51
1:A:111:GLY:O	1:A:154:SER:OG	2.24	0.51
1:A:313:ARG:HB3	1:A:685:ALA:HB2	1.91	0.51
1:A:466:THR:HG21	1:A:594:ALA:HB1	1.93	0.50
1:A:38:LYS:O	1:A:39:ARG:CG	2.58	0.50
1:A:128:PRO:HG2	1:A:129:ILE:H	1.76	0.50
1:A:91:HIS:HA	1:A:250:VAL:O	2.11	0.50
1:A:13:GLN:N	1:A:38:LYS:HE2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ALA:CA	1:A:73:LYS:HE3	2.37	0.50
1:A:70:ALA:CB	1:A:73:LYS:HE3	2.42	0.49
1:A:491:GLN:HB2	1:A:505:ALA:HB3	1.94	0.49
1:A:347:TRP:CH2	1:A:613:LEU:HD11	2.47	0.49
1:A:620:PHE:CE1	1:A:626:ASP:HB2	2.47	0.49
1:A:221:GLU:HA	1:A:224:ARG:HD2	1.94	0.49
1:A:72:TYR:HE2	4:A:714:HOH:O	1.95	0.49
1:A:528:TYR:O	1:A:549:THR:HG21	2.12	0.49
1:A:581:LYS:HD2	1:A:589:CYS:HB2	1.93	0.48
1:A:491:GLN:HG3	1:A:506:LEU:HD21	1.95	0.48
1:A:104:PHE:H	1:A:236:ARG:HH11	1.60	0.48
1:A:210:ARG:HD2	1:A:212:SER:OG	2.12	0.48
1:A:241:LYS:O	1:A:242:PHE:C	2.53	0.48
1:A:441:VAL:HG11	1:A:574:LEU:HD11	1.96	0.48
1:A:471:ILE:N	1:A:472:PRO:CD	2.76	0.48
1:A:27:ARG:HD2	1:A:28:LYS:CA	2.44	0.48
1:A:264:GLU:HA	1:A:267:ILE:HD12	1.94	0.48
1:A:4:ARG:HH11	1:A:4:ARG:CG	2.16	0.48
1:A:22:TRP:O	1:A:23:GLN:C	2.56	0.48
1:A:313:ARG:HG3	1:A:313:ARG:HH11	1.78	0.48
1:A:469:TRP:O	1:A:472:PRO:HD2	2.13	0.48
1:A:555:ASP:C	1:A:557:ASN:H	2.20	0.48
1:A:428:VAL:HG12	1:A:652:ARG:HG3	1.95	0.48
1:A:43:ILE:HD12	1:A:43:ILE:HG23	1.64	0.48
1:A:194:GLY:O	1:A:197:LYS:N	2.47	0.47
1:A:436:LEU:CD2	1:A:593:MET:CE	2.91	0.47
1:A:619:LYS:HA	1:A:625:SER:HB3	1.95	0.47
1:A:275:GLN:O	1:A:279:GLY:HA3	2.14	0.47
1:A:341:ARG:O	1:A:341:ARG:HG3	2.12	0.47
1:A:644:ASN:O	1:A:647:THR:OG1	2.26	0.47
1:A:147:ALA:O	1:A:151:ARG:HG3	2.13	0.47
1:A:37:ILE:N	1:A:37:ILE:CD1	2.76	0.47
1:A:220:ASP:CB	1:A:223:GLU:HG3	2.40	0.47
1:A:332:ARG:O	1:A:333:LYS:HG2	2.13	0.47
1:A:353:GLN:HG2	1:A:356:ARG:NH1	2.29	0.47
1:A:326:THR:HG22	1:A:329:GLN:NE2	2.25	0.47
1:A:653:LEU:HD13	1:A:656:LYS:O	2.15	0.47
1:A:673:ASN:O	1:A:676:LYS:HB2	2.14	0.47
1:A:38:LYS:O	1:A:39:ARG:NH1	2.46	0.47
1:A:241:LYS:O	1:A:245:CYS:N	2.47	0.47
1:A:110:GLN:HA	1:A:152:PHE:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:GLN:HE21	1:A:105:GLN:HB3	1.40	0.47
1:A:440:VAL:O	1:A:542:VAL:HA	2.14	0.47
1:A:586:ALA:O	1:A:590:HIS:ND1	2.33	0.47
1:A:639:LYS:CB	1:A:641:LEU:HD13	2.45	0.47
1:A:498:ASP:HB3	1:A:501:SER:HB3	1.95	0.47
1:A:680:SER:CB	1:A:681:PRO:HD2	2.36	0.47
1:A:18:LYS:NZ	1:A:288:LEU:O	2.39	0.46
1:A:97:VAL:HG23	1:A:209:ILE:CD1	2.44	0.46
1:A:220:ASP:HB3	1:A:223:GLU:CG	2.43	0.46
1:A:364:LEU:HB3	1:A:620:PHE:CZ	2.50	0.46
1:A:419:GLN:C	1:A:421:SER:N	2.72	0.46
1:A:21:GLN:HG3	1:A:286:PHE:CE1	2.51	0.46
1:A:463:VAL:O	1:A:464:ASP:HB2	2.14	0.46
1:A:627:CYS:HA	1:A:628:PRO:HA	1.57	0.46
1:A:680:SER:OG	4:A:792:HOH:O	2.21	0.46
1:A:80:GLU:OE1	1:A:301:LYS:HB2	2.15	0.46
1:A:220:ASP:HB3	1:A:223:GLU:OE2	2.15	0.46
1:A:162:ASP:OD1	1:A:162:ASP:C	2.56	0.46
1:A:441:VAL:CG1	1:A:574:LEU:HD13	2.45	0.46
1:A:40:ASP:CB	1:A:44:GLN:OE1	2.59	0.46
1:A:58:THR:HG23	1:A:299:LEU:O	2.15	0.46
1:A:347:TRP:CZ3	1:A:613:LEU:HD11	2.50	0.46
1:A:39:ARG:HH11	1:A:39:ARG:HG3	1.77	0.46
1:A:119:LEU:O	1:A:120:ARG:HB2	2.14	0.46
1:A:453:VAL:CG1	1:A:454:LYS:N	2.79	0.46
1:A:466:THR:HG21	1:A:594:ALA:CB	2.46	0.46
1:A:656:LYS:HA	1:A:661:LYS:HB3	1.98	0.46
1:A:41:SER:CB	1:A:42:PRO:CD	2.94	0.45
1:A:157:CYS:C	1:A:159:PRO:HD3	2.40	0.45
1:A:20:PHE:HD1	1:A:23:GLN:OE1	1.99	0.45
1:A:106:LEU:HD12	1:A:106:LEU:HA	1.69	0.45
1:A:619:LYS:HB3	1:A:619:LYS:HE2	1.58	0.45
1:A:688:PHE:CD1	1:A:689:LEU:HD23	2.50	0.45
1:A:97:VAL:CG2	1:A:209:ILE:HD11	2.46	0.45
1:A:546:LYS:HE3	1:A:548:VAL:CG2	2.47	0.45
1:A:385:LEU:HD21	1:A:407:LEU:HD21	1.96	0.45
1:A:512:GLN:HG3	4:A:907:HOH:O	2.15	0.45
1:A:60:ASP:CG	1:A:61:GLY:N	2.75	0.45
1:A:70:ALA:HA	1:A:73:LYS:CE	2.39	0.45
1:A:561:ALA:CA	1:A:564:LYS:HD3	2.41	0.45
1:A:636:SER:HB3	1:A:641:LEU:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ARG:HG2	1:A:39:ARG:NH1	2.24	0.45
1:A:286:PHE:CD1	1:A:287:GLN:N	2.84	0.45
1:A:688:PHE:HD1	1:A:689:LEU:HD23	1.82	0.45
1:A:271:LEU:O	1:A:275:GLN:CB	2.65	0.45
1:A:456:LYS:O	1:A:489:PHE:HB3	2.17	0.45
1:A:62:GLY:HA3	1:A:120:ARG:O	2.17	0.44
1:A:498:ASP:C	1:A:500:ARG:N	2.75	0.44
1:A:441:VAL:CG1	1:A:574:LEU:CD1	2.95	0.44
1:A:548:VAL:O	1:A:552:GLN:HG3	2.17	0.44
1:A:97:VAL:HG21	1:A:209:ILE:HD11	1.99	0.44
1:A:40:ASP:N	1:A:44:GLN:OE1	2.50	0.44
1:A:125:TRP:O	1:A:128:PRO:HG2	2.18	0.44
1:A:440:VAL:HG12	1:A:535:LEU:HD21	1.99	0.44
1:A:469:TRP:C	1:A:472:PRO:HD2	2.42	0.44
1:A:498:ASP:C	1:A:500:ARG:H	2.24	0.44
1:A:688:PHE:HD1	1:A:689:LEU:CD2	2.30	0.44
1:A:45:CYS:O	1:A:49:ILE:HG13	2.18	0.44
1:A:112:LEU:O	1:A:153:PHE:HB3	2.18	0.44
1:A:208:PHE:C	1:A:209:ILE:HG23	2.43	0.44
1:A:507:CYS:HB3	1:A:523:GLU:OE1	2.17	0.44
1:A:573:LEU:CD2	1:A:583:VAL:HG22	2.48	0.44
1:A:690:ARG:HA	1:A:690:ARG:HD2	1.72	0.44
1:A:20:PHE:O	1:A:21:GLN:C	2.61	0.44
1:A:150:ALA:HB2	1:A:169:LEU:HG	2.00	0.44
1:A:587:ARG:O	1:A:590:HIS:CE1	2.70	0.44
1:A:637:GLU:O	1:A:639:LYS:HG2	2.18	0.44
1:A:29:VAL:HG11	1:A:277:LYS:HD3	2.00	0.44
1:A:51:GLU:O	1:A:53:ARG:HG2	2.18	0.44
1:A:142:PRO:O	1:A:144:PRO:HD3	2.18	0.44
1:A:285:LYS:NZ	1:A:285:LYS:HB3	2.33	0.44
1:A:498:ASP:HB3	1:A:501:SER:CB	2.48	0.44
1:A:520:ASN:HB2	4:A:727:HOH:O	2.17	0.43
1:A:503:LEU:HD23	1:A:503:LEU:HA	1.76	0.43
1:A:32:PRO:HA	1:A:33:PRO:HD3	1.82	0.43
1:A:551:LEU:CD1	1:A:583:VAL:HG11	2.48	0.43
1:A:591:LEU:N	1:A:591:LEU:HD23	2.32	0.43
1:A:43:ILE:HD13	1:A:46:ILE:HD12	2.01	0.43
1:A:555:ASP:C	1:A:557:ASN:N	2.77	0.43
1:A:682:LEU:O	1:A:682:LEU:HG	2.16	0.43
1:A:143:GLU:HA	1:A:144:PRO:HD2	1.75	0.43
1:A:263:LYS:O	1:A:267:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:LEU:HD12	1:A:633:LEU:HA	1.78	0.43
1:A:390:ASP:OD1	1:A:602:ARG:NH2	2.43	0.43
1:A:394:LEU:HB3	1:A:398:TYR:HB2	1.99	0.43
1:A:564:LYS:NZ	1:A:565:ASP:OD2	2.44	0.43
1:A:680:SER:CB	1:A:681:PRO:CD	2.97	0.43
1:A:82:TYR:CE2	1:A:252:SER:HB2	2.53	0.43
1:A:404:LYS:HE3	1:A:404:LYS:HB3	1.69	0.43
1:A:395:ASP:OD2	1:A:465:ARG:HA	2.18	0.43
1:A:19:CYS:C	1:A:36:CYS:SG	3.02	0.42
1:A:125:TRP:O	1:A:129:ILE:HG12	2.19	0.42
1:A:208:PHE:C	1:A:209:ILE:CG2	2.92	0.42
1:A:430:ARG:NH2	1:A:648:GLU:CD	2.76	0.42
1:A:675:LYS:O	1:A:678:SER:O	2.37	0.42
1:A:231:CYS:HB3	1:A:232:PRO:HD2	2.00	0.42
1:A:28:LYS:HB3	1:A:29:VAL:H	1.37	0.42
1:A:91:HIS:CA	1:A:250:VAL:O	2.66	0.42
1:A:531:ALA:O	1:A:534:CYS:HB3	2.20	0.42
1:A:30:ARG:HA	1:A:30:ARG:HD3	1.77	0.42
1:A:51:GLU:CG	1:A:53:ARG:HH11	2.33	0.42
1:A:129:ILE:O	1:A:129:ILE:CG2	2.65	0.42
1:A:430:ARG:NH2	1:A:648:GLU:OE2	2.53	0.42
1:A:286:PHE:C	1:A:287:GLN:HG3	2.43	0.42
1:A:526:TYR:CG	1:A:527:GLY:N	2.87	0.42
1:A:8:TRP:CD1	1:A:299:LEU:HD22	2.54	0.42
1:A:112:LEU:N	1:A:112:LEU:CD1	2.82	0.42
1:A:412:ALA:HA	1:A:598:ALA:HA	2.01	0.42
1:A:593:MET:HE3	1:A:593:MET:HB2	1.92	0.42
1:A:18:LYS:HA	1:A:21:GLN:HG2	2.02	0.42
1:A:110:GLN:HB2	1:A:152:PHE:CE1	2.54	0.42
1:A:158:VAL:O	1:A:159:PRO:C	2.62	0.42
1:A:283:SER:C	1:A:285:LYS:N	2.71	0.42
1:A:469:TRP:CZ3	1:A:473:MET:HE2	2.54	0.42
1:A:109:LEU:O	1:A:110:GLN:C	2.63	0.42
1:A:314:ILE:HD13	1:A:689:LEU:HD21	2.01	0.42
1:A:105:GLN:NE2	4:A:928:HOH:O	2.53	0.41
1:A:246:HIS:C	1:A:247:LEU:HD12	2.45	0.41
1:A:251:PRO:HB2	1:A:319:TYR:CE2	2.55	0.41
1:A:408:VAL:HG12	4:A:778:HOH:O	2.19	0.41
1:A:430:ARG:HA	1:A:431:PRO:HD3	1.77	0.41
1:A:16:ALA:O	1:A:19:CYS:HB3	2.19	0.41
1:A:43:ILE:HD13	1:A:43:ILE:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ASN:O	1:A:273:GLN:HG2	2.18	0.41
1:A:561:ALA:O	1:A:564:LYS:HG2	2.19	0.41
1:A:658:THR:HG23	1:A:661:LYS:N	2.25	0.41
1:A:510:ASP:HB2	1:A:511:GLU:H	1.55	0.41
1:A:110:GLN:N	1:A:152:PHE:CZ	2.89	0.41
1:A:128:PRO:HG2	1:A:129:ILE:N	2.36	0.41
1:A:331:LEU:HD23	1:A:331:LEU:HA	1.83	0.41
1:A:338:VAL:O	1:A:342:ARG:HG3	2.20	0.41
1:A:688:PHE:CD1	1:A:688:PHE:C	2.97	0.41
1:A:231:CYS:HB3	1:A:232:PRO:CD	2.51	0.41
1:A:533:ARG:HB2	1:A:562:TRP:CH2	2.56	0.41
1:A:69:LEU:O	1:A:70:ALA:C	2.64	0.41
1:A:75:ARG:HA	1:A:76:PRO:HD3	1.82	0.41
1:A:111:GLY:O	1:A:154:SER:CB	2.69	0.41
1:A:472:PRO:O	1:A:475:LEU:N	2.50	0.41
1:A:581:LYS:CB	1:A:582:PRO:HD3	2.50	0.41
1:A:84:THR:O	1:A:88:PRO:N	2.54	0.41
1:A:165:GLN:C	1:A:167:PRO:HD2	2.44	0.41
1:A:284:PRO:C	1:A:286:PHE:N	2.78	0.41
1:A:596:ASN:OD1	1:A:596:ASN:N	2.54	0.41
1:A:611:GLN:O	1:A:612:VAL:C	2.64	0.41
1:A:25:ASN:ND2	1:A:25:ASN:H	2.18	0.41
1:A:28:LYS:C	1:A:30:ARG:H	2.28	0.41
1:A:82:TYR:O	1:A:88:PRO:HA	2.21	0.41
1:A:179:ASN:CG	1:A:186:GLN:HB3	2.46	0.41
1:A:414:ASN:O	1:A:648:GLU:N	2.42	0.41
1:A:19:CYS:O	1:A:36:CYS:SG	2.79	0.40
1:A:105:GLN:NE2	1:A:105:GLN:HA	2.35	0.40
1:A:214:VAL:HG12	1:A:214:VAL:H	1.38	0.40
1:A:63:PHE:O	1:A:64:ILE:C	2.63	0.40
1:A:104:PHE:H	1:A:236:ARG:NH1	2.19	0.40
1:A:106:LEU:HD12	1:A:230:LEU:HD13	2.03	0.40
1:A:469:TRP:CH2	1:A:473:MET:HE2	2.56	0.40
1:A:526:TYR:CD1	1:A:526:TYR:C	2.98	0.40
1:A:155:ALA:CB	1:A:172:LEU:HD21	2.51	0.40
1:A:357:LYS:NZ	1:A:633:LEU:O	2.37	0.40
1:A:475:LEU:HD23	1:A:475:LEU:HA	1.89	0.40
1:A:551:LEU:CD1	1:A:583:VAL:CG1	2.99	0.40
1:A:625:SER:OG	1:A:626:ASP:OD1	2.35	0.40
1:A:329:GLN:HE21	1:A:329:GLN:HB2	1.27	0.40
1:A:268:TRP:HA	1:A:268:TRP:HE3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:LYS:HB2	1:A:278:PHE:CE2	2.56	0.40
1:A:280:LYS:O	1:A:282:LYS:HG3	2.21	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	686/691 (99%)	594 (87%)	73 (11%)	19 (3%)	4 3

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	283	SER
1	A	418	GLN
1	A	421	SER
1	A	279	GLY
1	A	286	PHE
1	A	472	PRO
1	A	625	SER
1	A	678	SER
1	A	473	MET
1	A	521	SER
1	A	642	LEU
1	A	28	LYS
1	A	29	VAL
1	A	213	THR
1	A	263	LYS
1	A	360	GLN
1	A	422	ASP
1	A	536	ALA
1	A	423	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	568/574 (99%)	537 (94%)	31 (6%)	19	34

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	27	ARG
1	A	37	ILE
1	A	39	ARG
1	A	58	THR
1	A	100	LYS
1	A	112	LEU
1	A	139	THR
1	A	146	GLU
1	A	149	VAL
1	A	159	PRO
1	A	176	THR
1	A	209	ILE
1	A	214	VAL
1	A	285	LYS
1	A	301	LYS
1	A	338	VAL
1	A	364	LEU
1	A	388	GLU
1	A	416	LYS
1	A	419	GLN
1	A	422	ASP
1	A	463	VAL
1	A	518	VAL
1	A	599	VAL
1	A	610	LYS
1	A	623	ASN
1	A	628	PRO
1	A	635	GLN
1	A	636	SER

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Mol	Chain	Res	Type
1	A	641	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	25	ASN
1	A	47	GLN
1	A	52	ASN
1	A	105	GLN
1	A	261	ASN
1	A	329	GLN
1	A	330	ASN
1	A	360	GLN
1	A	491	GLN
1	A	635	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OXL	A	696	2	5,5,5	1.83	3 (60%)	6,6,6	2.95	5 (83%)
3	OXL	A	695	2	5,5,5	1.94	2 (40%)	6,6,6	2.49	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
3	OXL	A	696	2	-	4/4/4/4	-
3	OXL	A	695	2	-	4/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	695	OXL	O1-C1	2.60	1.29	1.22
3	A	695	OXL	O2-C2	2.55	1.28	1.22
3	A	696	OXL	O1-C1	2.40	1.28	1.22
3	A	696	OXL	O2-C2	2.31	1.28	1.22
3	A	696	OXL	C2-C1	2.28	1.58	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	696	OXL	O1-C1-C2	-3.87	112.57	120.63
3	A	695	OXL	O2-C2-C1	-3.71	112.91	120.63
3	A	696	OXL	O2-C2-C1	-3.61	113.11	120.63
3	A	696	OXL	O4-C2-O2	3.10	131.27	123.90
3	A	695	OXL	O4-C2-C1	3.07	118.78	112.83
3	A	695	OXL	O3-C1-O1	2.76	130.48	123.90
3	A	696	OXL	O3-C1-C2	2.73	118.13	112.83
3	A	696	OXL	O3-C1-O1	2.25	129.25	123.90

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	695	OXL	O3-C1-C2-O4
3	A	696	OXL	O3-C1-C2-O4
3	A	695	OXL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	A	696	OXL	O1-C1-C2-O2
3	A	696	OXL	O3-C1-C2-O2
3	A	695	OXL	O1-C1-C2-O4
3	A	695	OXL	O3-C1-C2-O2
3	A	696	OXL	O1-C1-C2-O4

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	421:SER	C	422:ASP	N	1.15

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	688/691 (99%)	-1.04	1 (0%) 92 90	23, 45, 80, 99	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	13	GLN	3.6

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
3	OXL	A	695	6/6	0.96	0.07	37,40,43,46	0
2	FE	A	693	1/1	0.99	0.02	38,38,38,38	0
3	OXL	A	696	6/6	0.99	0.03	19,22,31,33	0
2	FE	A	694	1/1	1.00	0.02	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.