



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2025 – 11:17 AM EDT

PDB ID : 1C1G / pdb_00001c1g
Title : CRYSTAL STRUCTURE OF TROPOMYOSIN AT 7 ANGSTROMS RESOLUTION IN THE SPERMINE-INDUCED CRYSTAL FORM
Authors : Whitby, F.G.; Phillips Jr., G.N.
Deposited on : 1999-07-22
Resolution : 7.00 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 Phenix2.0rc1
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

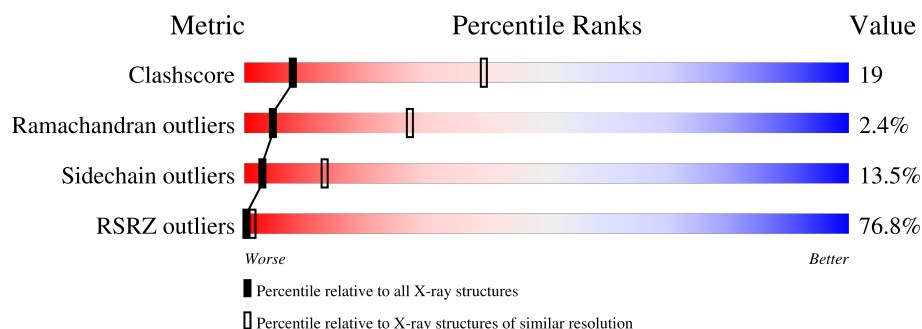
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.00 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	180529	1146 (10.00-4.00)
Ramachandran outliers	177936	1014 (10.00-4.00)
Sidechain outliers	177891	1035 (10.00-3.96)
RSRZ outliers	164620	1102 (10.00-4.00)

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	284	
1	B	284	
1	C	284	
1	D	284	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9160 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.

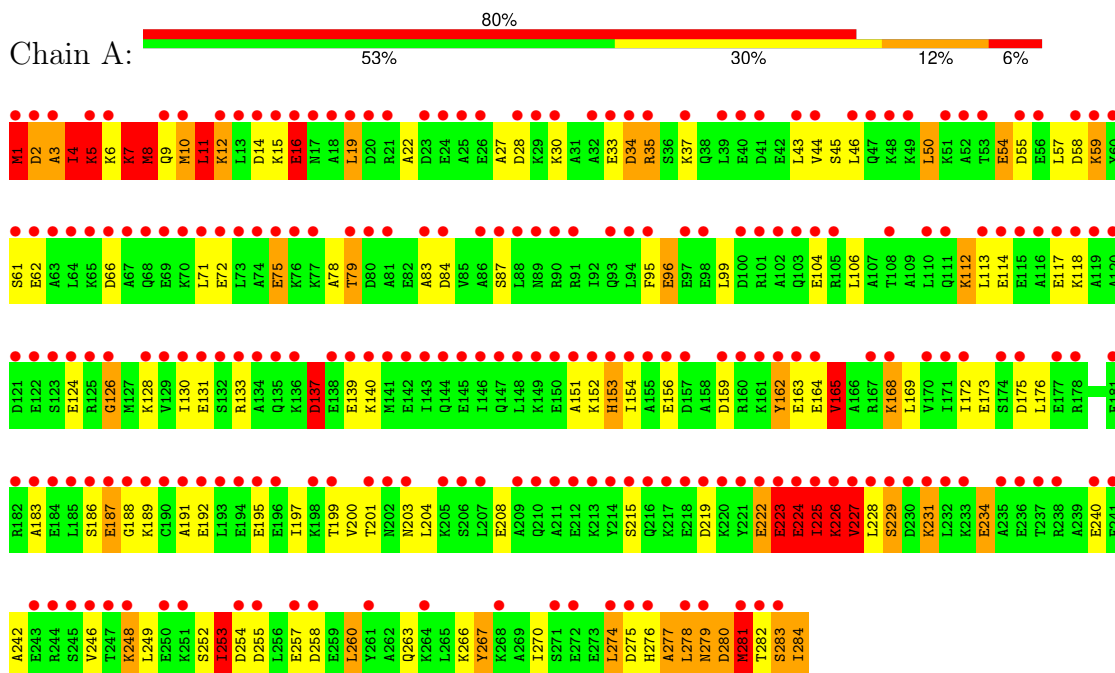
- Molecule 1 is a protein called TROPOMYOSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	0	0
			2290	1402	387	494	7			
1	B	284	Total	C	N	O	S	0	0	0
			2290	1402	387	494	7			
1	C	284	Total	C	N	O	S	0	0	0
			2290	1402	387	494	7			
1	D	284	Total	C	N	O	S	0	0	0
			2290	1402	387	494	7			

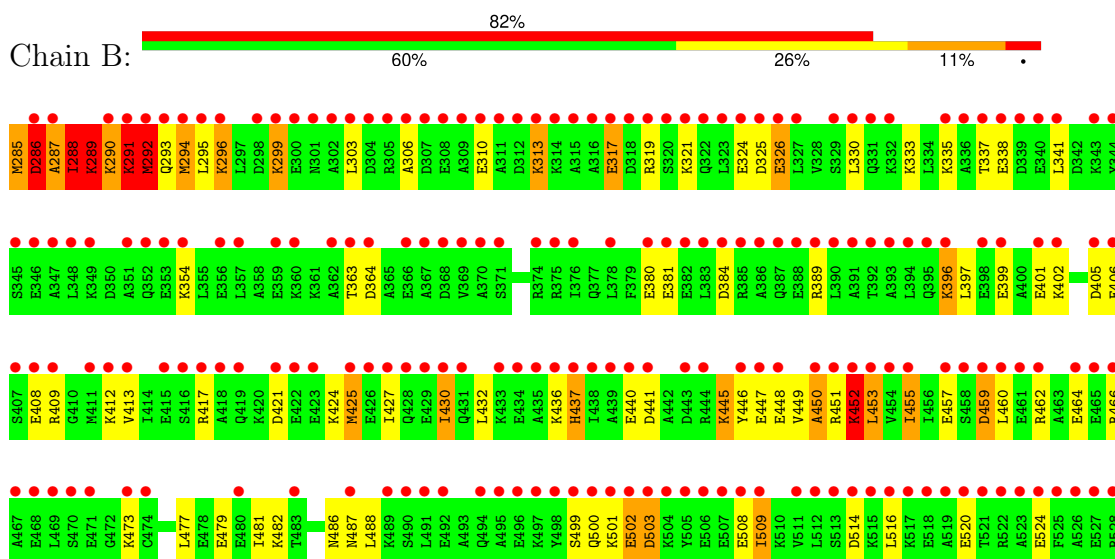
3 Residue-property plots

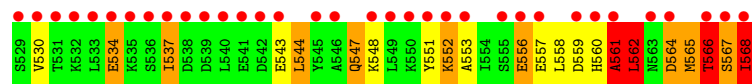
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: TROPOMYOSIN

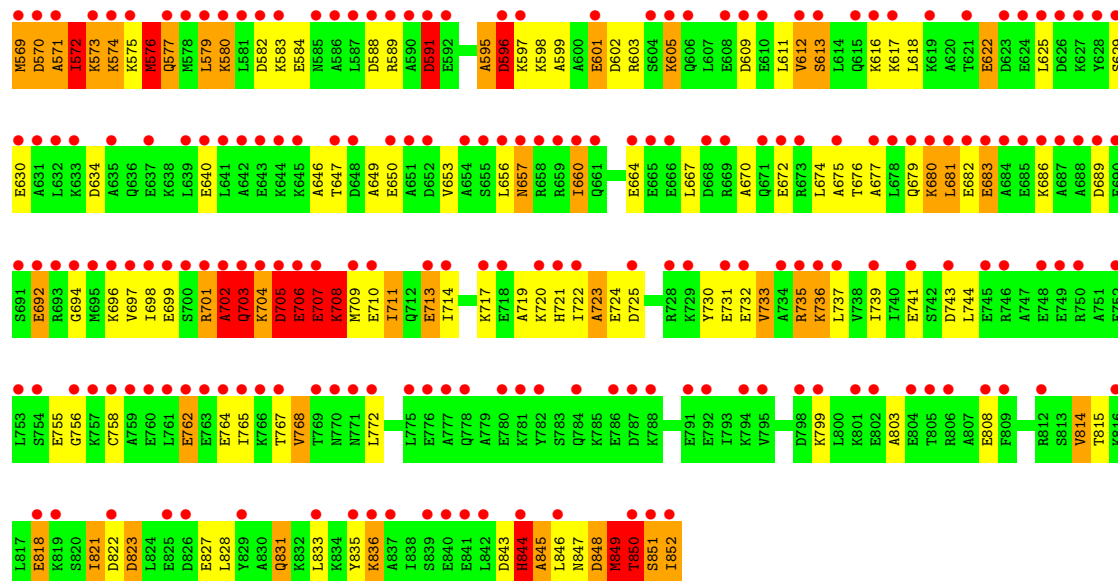


• Molecule 1: TROPOMYOSIN

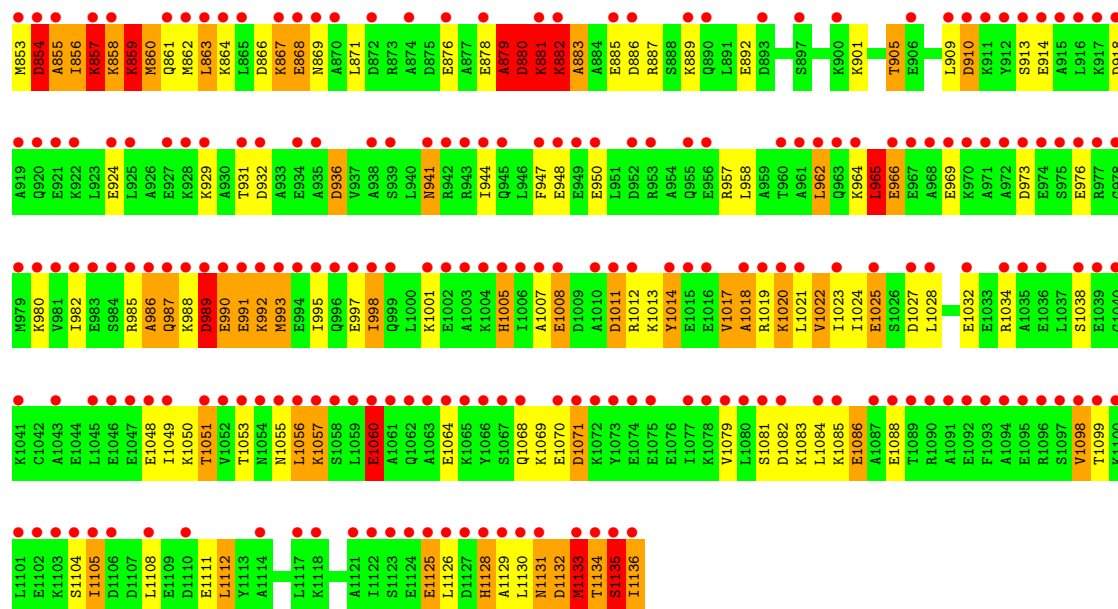
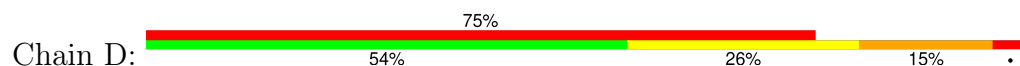




• Molecule 1: TROPOMYOSIN



• Molecule 1: TROPOMYOSIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	259.74Å 55.30Å 136.26Å 90.00° 97.42° 90.00°	Depositor
Resolution (Å)	100.00 – 7.00 100.00 – 7.00	Depositor EDS
% Data completeness (in resolution range)	96.4 (100.00-7.00) 96.4 (100.00-7.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 6.73Å)	Xtriage
Refinement program	XTALVIEW, X-PLOR	Depositor
R, R_{free}	0.404 , (Not available) 0.450 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	210.9	Xtriage
Anisotropy	1.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.12 , 999.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	9160	wwPDB-VP
Average B, all atoms (Å ²)	174.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.35% 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

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	1.04	12/2299 (0.5%)	2.36	126/3062 (4.1%)
1	B	0.93	7/2299 (0.3%)	2.16	90/3062 (2.9%)
1	C	1.60	27/2299 (1.2%)	2.52	137/3062 (4.5%)
1	D	1.21	20/2299 (0.9%)	2.48	118/3062 (3.9%)
All	All	1.22	66/9196 (0.7%)	2.39	471/12248 (3.8%)

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	3
1	C	0	5
1	D	0	5
All	All	0	13

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	852	ILE	N-CA	32.64	2.08	1.46
1	C	851	SER	C-N	26.63	1.70	1.33
1	C	572	ILE	CA-CB	19.78	1.81	1.54
1	C	852	ILE	CA-CB	18.49	2.04	1.54
1	C	705	ASP	CA-C	17.17	1.76	1.52
1	D	859	LYS	N-CA	16.78	1.67	1.46
1	D	860	MET	N-CA	15.44	1.64	1.46
1	C	851	SER	CA-C	14.27	1.71	1.52
1	C	705	ASP	C-N	14.18	1.53	1.33
1	C	705	ASP	N-CA	14.14	1.65	1.46
1	D	858	LYS	C-N	13.42	1.52	1.33
1	D	859	LYS	CA-C	11.70	1.68	1.52
1	A	224	GLU	CA-CB	11.26	1.72	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	860	MET	CA-C	10.42	1.66	1.53
1	A	223	GLU	N-CA	9.05	1.57	1.46
1	D	858	LYS	C-O	8.93	1.35	1.24
1	D	860	MET	C-N	8.55	1.46	1.33
1	D	879	ALA	N-CA	8.10	1.56	1.46
1	B	565	MET	N-CA	7.95	1.56	1.46
1	A	222	GLU	C-N	7.89	1.44	1.33
1	C	704	LYS	C-N	7.88	1.45	1.33
1	A	223	GLU	CA-C	7.78	1.63	1.52
1	B	288	ILE	CA-CB	-7.63	1.44	1.54
1	C	706	GLU	N-CA	6.96	1.54	1.46
1	D	878	GLU	C-N	6.96	1.43	1.33
1	C	721	HIS	CD2-NE2	-6.90	1.30	1.37
1	B	562	LEU	N-CA	-6.72	1.38	1.46
1	B	560	HIS	CD2-NE2	-6.71	1.30	1.37
1	C	706	GLU	C-N	6.66	1.42	1.33
1	D	856	ILE	CA-CB	6.63	1.63	1.54
1	D	862	MET	C-N	6.61	1.42	1.33
1	C	849	MET	N-CA	6.52	1.54	1.46
1	D	882	LYS	C-N	6.48	1.42	1.33
1	D	857	LYS	C-O	6.44	1.32	1.24
1	C	708	LYS	CG-CD	6.30	1.71	1.52
1	A	153	HIS	CD2-NE2	-6.29	1.30	1.37
1	D	1128	HIS	CD2-NE2	-6.27	1.30	1.37
1	C	572	ILE	N-CA	6.25	1.54	1.46
1	C	708	LYS	N-CA	-6.22	1.38	1.46
1	A	276	HIS	CD2-NE2	-6.22	1.31	1.37
1	C	844	HIS	CD2-NE2	-6.18	1.31	1.37
1	C	852	ILE	CA-C	6.14	1.65	1.52
1	B	437	HIS	CD2-NE2	-6.12	1.31	1.37
1	C	576	MET	CA-C	-5.97	1.45	1.52
1	D	862	MET	N-CA	5.96	1.53	1.46
1	D	879	ALA	CA-C	5.96	1.60	1.52
1	C	573	LYS	CA-C	5.95	1.60	1.52
1	C	848	ASP	N-CA	-5.94	1.39	1.46
1	A	226	LYS	C-N	5.91	1.41	1.33
1	C	704	LYS	N-CA	5.85	1.53	1.46
1	A	3	ALA	N-CA	-5.81	1.39	1.46
1	D	856	ILE	CA-C	5.80	1.61	1.52
1	C	702	ALA	C-O	5.76	1.31	1.24
1	C	706	GLU	CA-C	5.75	1.60	1.52
1	D	1005	HIS	CD2-NE2	-5.72	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	11	LEU	N-CA	5.68	1.53	1.46
1	A	281	MET	CA-C	5.66	1.60	1.52
1	A	8	MET	CA-CB	-5.37	1.45	1.53
1	C	708	LYS	CB-CG	5.35	1.68	1.52
1	A	222	GLU	C-O	5.23	1.30	1.24
1	D	882	LYS	CA-C	5.17	1.59	1.52
1	B	289	LYS	N-CA	-5.10	1.39	1.46
1	B	568	ILE	CB-CG2	-5.09	1.35	1.52
1	D	861	GLN	C-N	5.08	1.41	1.33
1	C	703	GLN	C-N	5.04	1.40	1.33
1	C	847	ASN	C-O	5.02	1.30	1.24

All (471) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	572	ILE	N-CA-CB	-30.61	60.73	111.23
1	B	568	ILE	N-CA-CB	-28.89	62.38	111.50
1	A	4	ILE	CA-CB-CG2	-25.50	67.14	110.50
1	D	856	ILE	N-CA-C	-25.42	79.32	111.09
1	D	880	ASP	CA-CB-CG	25.17	137.77	112.60
1	D	858	LYS	CA-C-O	-20.69	90.92	120.51
1	C	851	SER	CA-C-O	-19.71	92.32	120.51
1	B	564	ASP	CA-CB-CG	19.09	131.69	112.60
1	D	856	ILE	CB-CA-C	18.65	142.47	112.26
1	A	225	ILE	N-CA-C	-18.45	91.80	110.62
1	C	847	ASN	CA-C-N	-18.33	93.22	122.73
1	C	847	ASN	C-N-CA	-18.33	93.22	122.73
1	D	861	GLN	N-CA-C	-18.29	87.03	112.45
1	C	852	ILE	CB-CA-C	-18.23	75.14	111.60
1	D	861	GLN	CA-C-N	-17.97	90.13	120.68
1	D	861	GLN	C-N-CA	-17.97	90.13	120.68
1	D	880	ASP	N-CA-C	17.93	148.99	110.80
1	C	708	LYS	CA-CB-CG	17.12	148.34	114.10
1	C	572	ILE	N-CA-C	-16.61	74.79	109.34
1	D	856	ILE	N-CA-CB	-16.55	80.82	110.77
1	A	224	GLU	CA-CB-CG	15.38	144.85	114.10
1	A	226	LYS	CA-C-O	-15.21	105.03	120.70
1	C	851	SER	CA-C-N	14.86	148.44	121.70
1	C	851	SER	C-N-CA	14.86	148.44	121.70
1	C	708	LYS	CG-CD-CE	14.83	145.40	111.30
1	C	572	ILE	CA-CB-CG2	14.53	135.20	110.50
1	D	990	GLU	N-CA-C	-14.39	95.05	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	851	SER	N-CA-C	14.18	141.00	110.80
1	A	4	ILE	CA-CB-CG1	14.13	134.42	110.40
1	A	223	GLU	CA-C-O	13.92	140.41	120.51
1	C	848	ASP	N-CA-C	13.61	128.23	112.72
1	C	852	ILE	N-CA-CB	13.18	133.91	111.50
1	A	224	GLU	N-CA-C	12.95	138.38	110.80
1	C	571	ALA	CA-C-N	12.77	144.96	121.97
1	C	571	ALA	C-N-CA	12.77	144.96	121.97
1	C	705	ASP	N-CA-C	12.76	128.71	112.89
1	A	280	ASP	N-CA-C	-12.63	97.60	111.36
1	D	878	GLU	O-C-N	12.61	135.70	122.09
1	D	857	LYS	N-CA-C	12.53	127.78	111.75
1	D	862	MET	CA-C-O	-12.46	105.09	119.79
1	D	856	ILE	CA-C-O	-12.26	107.23	120.47
1	B	568	ILE	N-CA-C	-12.06	77.23	111.00
1	C	849	MET	N-CA-C	-11.94	96.47	111.75
1	B	565	MET	N-CA-C	-11.90	96.87	112.34
1	D	860	MET	N-CA-C	11.88	127.94	112.26
1	A	3	ALA	CA-C-O	-11.81	108.74	120.90
1	A	7	LYS	CA-CB-CG	11.79	137.68	114.10
1	C	848	ASP	CA-CB-CG	11.76	124.36	112.60
1	D	859	LYS	O-C-N	-11.71	107.02	122.59
1	A	12	LYS	N-CA-C	-11.62	99.10	113.97
1	D	998	ILE	N-CA-C	-11.41	99.75	110.82
1	D	881	LYS	N-CA-C	-11.39	97.68	111.69
1	C	703	GLN	CA-C-O	-11.38	108.38	120.55
1	C	708	LYS	CB-CG-CD	11.04	136.70	111.30
1	B	288	ILE	CA-CB-CG2	-11.01	91.78	110.50
1	D	879	ALA	CA-C-O	11.00	136.24	120.51
1	D	965	LEU	N-CA-C	-10.87	98.97	111.03
1	D	858	LYS	CA-C-N	10.80	142.16	121.54
1	D	858	LYS	C-N-CA	10.80	142.16	121.54
1	A	281	MET	O-C-N	-10.78	108.26	122.59
1	C	818	GLU	N-CA-C	-10.65	99.21	111.03
1	D	878	GLU	CA-C-N	10.45	141.49	121.54
1	D	878	GLU	C-N-CA	10.45	141.49	121.54
1	B	565	MET	CG-SD-CE	10.34	123.65	100.90
1	C	701	ARG	CA-C-N	10.27	135.92	120.31
1	C	701	ARG	C-N-CA	10.27	135.92	120.31
1	C	572	ILE	CA-C-O	-10.22	108.00	120.78
1	D	859	LYS	N-CA-C	10.15	132.43	110.80
1	C	708	LYS	N-CA-CB	-10.15	93.34	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	ASP	CA-CB-CG	10.14	122.74	112.60
1	C	591	ASP	CA-CB-CG	10.12	122.72	112.60
1	C	701	ARG	O-C-N	9.89	133.42	122.15
1	A	281	MET	CB-CA-C	-9.81	90.89	110.42
1	C	572	ILE	CB-CA-C	9.80	127.36	111.29
1	B	397	LEU	N-CA-C	-9.80	100.15	111.03
1	D	993	MET	N-CA-C	-9.77	100.19	111.03
1	A	7	LYS	CA-C-N	-9.75	102.76	122.55
1	A	7	LYS	C-N-CA	-9.75	102.76	122.55
1	A	283	SER	CA-C-O	-9.72	107.61	119.18
1	A	280	ASP	N-CA-CB	-9.66	95.86	110.16
1	C	852	ILE	CA-CB-CG2	9.62	126.85	110.50
1	D	936	ASP	CA-CB-CG	9.62	122.22	112.60
1	A	222	GLU	O-C-N	9.59	134.70	122.23
1	A	284	ILE	CA-CB-CG2	-9.47	94.39	110.50
1	B	565	MET	CA-CB-CG	9.45	133.01	114.10
1	C	851	SER	N-CA-CB	-9.44	94.53	110.49
1	A	9	GLN	N-CA-C	-9.39	101.00	111.14
1	B	294	MET	CA-C-O	-9.38	111.05	120.89
1	C	702	ALA	O-C-N	9.37	133.80	122.27
1	C	704	LYS	CA-C-O	-9.31	107.19	120.51
1	A	281	MET	N-CA-CB	9.28	126.17	110.49
1	C	848	ASP	N-CA-CB	-9.22	96.97	110.70
1	C	708	LYS	N-CA-C	9.20	130.39	110.80
1	D	1056	LEU	N-CA-C	-9.20	101.23	111.07
1	A	5	LYS	CB-CA-C	-9.17	96.33	110.92
1	C	741	GLU	N-CA-C	-9.16	98.84	112.04
1	D	882	LYS	CA-C-O	-9.15	107.42	120.51
1	A	5	LYS	CA-CB-CG	9.12	132.35	114.10
1	C	849	MET	N-CA-CB	9.12	124.55	110.14
1	C	852	ILE	N-CA-C	9.12	136.53	111.00
1	C	576	MET	CB-CA-C	-9.11	96.50	110.90
1	D	867	LYS	N-CA-C	-9.09	100.99	112.90
1	C	576	MET	N-CA-CB	9.05	123.20	110.07
1	D	862	MET	N-CA-C	9.03	123.60	112.23
1	C	702	ALA	N-CA-C	8.99	122.25	111.82
1	A	279	ASN	CA-C-O	8.96	130.58	119.11
1	B	564	ASP	CA-C-O	-8.95	107.60	120.13
1	D	962	LEU	N-CA-C	-8.93	100.50	111.40
1	B	564	ASP	N-CA-CB	-8.91	95.36	110.33
1	A	284	ILE	CA-CB-CG1	8.83	125.41	110.40
1	C	823	ASP	CA-CB-CG	8.69	121.29	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	858	LYS	N-CA-C	-8.66	92.36	110.80
1	B	565	MET	N-CA-CB	8.65	125.75	110.18
1	B	564	ASP	CB-CA-C	8.64	124.67	110.24
1	D	854	ASP	N-CA-C	8.59	129.10	110.80
1	C	852	ILE	CG1-CB-CG2	-8.57	84.97	110.70
1	A	1	MET	N-CA-C	-8.50	87.21	111.00
1	D	857	LYS	CA-C-O	8.48	129.70	120.20
1	A	225	ILE	CA-C-N	-8.46	108.94	120.44
1	A	225	ILE	C-N-CA	-8.46	108.94	120.44
1	B	453	LEU	N-CA-C	-8.44	101.77	110.97
1	B	405	ASP	CA-CB-CG	8.41	121.01	112.60
1	D	855	ALA	CA-C-N	8.38	134.04	120.30
1	D	855	ALA	C-N-CA	8.38	134.04	120.30
1	C	681	LEU	N-CA-C	-8.35	100.85	112.45
1	D	862	MET	O-C-N	-8.34	111.16	122.33
1	A	224	GLU	O-C-N	8.34	133.68	122.59
1	D	989	ASP	CA-CB-CG	8.30	120.90	112.60
1	A	275	ASP	N-CA-C	-8.28	102.21	111.07
1	D	1135	SER	N-CA-C	-8.22	99.15	111.81
1	C	707	GLU	N-CA-C	-8.20	100.67	111.24
1	A	253	ILE	N-CA-C	-8.18	100.82	112.35
1	A	226	LYS	O-C-N	-8.16	113.27	122.09
1	D	1071	ASP	CA-CB-CG	8.16	120.76	112.60
1	C	609	ASP	CA-CB-CG	8.15	120.75	112.60
1	B	568	ILE	CB-CA-C	8.15	127.90	111.60
1	A	255	ASP	CA-CB-CG	8.13	120.73	112.60
1	C	596	ASP	CA-CB-CG	8.11	120.71	112.60
1	C	580	LYS	N-CA-C	-8.10	102.53	111.36
1	C	572	ILE	CG1-CB-CG2	-8.09	86.43	110.70
1	C	730	TYR	N-CA-C	-8.09	103.20	113.23
1	B	288	ILE	CA-CB-CG1	8.07	124.13	110.40
1	D	861	GLN	CA-C-O	-8.06	110.17	120.00
1	D	860	MET	O-C-N	-8.05	111.89	122.20
1	D	1082	ASP	N-CA-C	-8.02	102.48	111.14
1	C	598	LYS	N-CA-C	-7.99	102.52	111.07
1	C	702	ALA	CA-C-N	7.97	134.02	120.71
1	C	702	ALA	C-N-CA	7.97	134.02	120.71
1	D	878	GLU	CA-C-O	-7.97	112.49	120.70
1	D	886	ASP	N-CA-C	-7.94	103.38	113.23
1	B	364	ASP	N-CA-C	-7.92	102.33	110.97
1	C	706	GLU	CA-C-O	-7.90	112.10	120.55
1	C	705	ASP	CA-C-N	7.88	133.88	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	705	ASP	C-N-CA	7.88	133.88	120.71
1	A	139	GLU	N-CA-C	-7.88	102.63	111.14
1	D	1014	TYR	CA-CB-CG	7.82	127.97	113.90
1	B	303	LEU	N-CA-C	-7.78	102.39	111.03
1	D	858	LYS	O-C-N	7.78	132.94	122.59
1	B	514	ASP	N-CA-C	-7.75	102.43	111.03
1	B	294	MET	O-C-N	-7.73	112.99	122.11
1	B	287	ALA	N-CA-C	7.73	119.70	111.28
1	B	446	TYR	CA-CB-CG	7.72	127.80	113.90
1	A	222	GLU	CA-C-N	7.72	136.28	121.54
1	A	222	GLU	C-N-CA	7.72	136.28	121.54
1	A	223	GLU	N-CA-C	7.72	127.23	110.80
1	C	701	ARG	CA-C-O	-7.71	112.24	120.42
1	A	280	ASP	CB-CA-C	7.68	123.91	110.85
1	B	566	THR	O-C-N	-7.54	112.06	122.46
1	B	330	LEU	N-CA-C	-7.53	103.16	111.36
1	C	664	GLU	N-CA-C	-7.50	102.71	111.03
1	A	96	GLU	N-CA-C	-7.49	102.26	111.40
1	D	1132	ASP	CA-CB-CG	7.48	120.08	112.60
1	A	165	VAL	N-CA-CB	-7.45	101.16	110.47
1	A	2	ASP	CA-C-O	7.44	131.15	120.51
1	C	704	LYS	CA-C-N	7.43	134.15	121.14
1	C	704	LYS	C-N-CA	7.43	134.15	121.14
1	B	291	LYS	N-CA-C	7.43	122.34	113.28
1	D	879	ALA	N-CA-C	7.42	126.60	110.80
1	B	481	ILE	N-CA-C	-7.41	102.20	112.50
1	B	290	LYS	CA-C-N	-7.39	108.31	122.06
1	B	290	LYS	C-N-CA	-7.39	108.31	122.06
1	A	162	TYR	N-CA-C	-7.39	104.07	113.23
1	C	705	ASP	O-C-N	-7.38	112.27	122.46
1	B	450	ALA	N-CA-C	-7.38	101.41	112.04
1	B	567	SER	CA-C-N	7.38	134.98	121.70
1	B	567	SER	C-N-CA	7.38	134.98	121.70
1	C	576	MET	N-CA-C	-7.36	103.19	111.14
1	C	699	GLU	N-CA-C	-7.36	102.86	111.03
1	C	850	THR	CA-CB-CG2	7.32	122.94	110.50
1	D	880	ASP	O-C-N	7.31	132.32	122.59
1	D	880	ASP	CA-C-O	7.30	130.95	120.51
1	A	45	SER	N-CA-C	-7.30	103.34	112.90
1	C	710	GLU	N-CA-C	-7.29	102.72	111.69
1	C	721	HIS	CB-CG-CD2	-7.27	121.75	131.20
1	D	859	LYS	CA-C-N	-7.27	111.74	122.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	859	LYS	C-N-CA	-7.27	111.74	122.86
1	C	847	ASN	O-C-N	7.24	129.80	122.12
1	D	856	ILE	O-C-N	-7.24	113.62	121.80
1	C	848	ASP	O-C-N	-7.23	113.45	122.35
1	B	448	GLU	N-CA-C	-7.13	103.19	110.97
1	C	573	LYS	CA-CB-CG	7.13	128.37	114.10
1	D	853	MET	O-C-N	-7.13	111.59	123.00
1	D	1032	GLU	N-CA-C	-7.13	102.70	111.40
1	D	854	ASP	O-C-N	-7.12	113.11	122.59
1	D	991	GLU	N-CA-C	7.12	121.23	112.54
1	A	224	GLU	CA-C-O	7.10	130.67	120.51
1	A	7	LYS	N-CA-CB	7.09	122.48	110.49
1	B	561	ALA	O-C-N	7.04	131.95	122.59
1	A	4	ILE	CA-C-N	-7.03	111.03	120.79
1	A	4	ILE	C-N-CA	-7.03	111.03	120.79
1	D	1069	LYS	N-CA-C	-6.99	104.49	113.16
1	B	299	LYS	N-CA-C	-6.99	103.09	111.69
1	D	1060	GLU	N-CA-C	-6.99	101.98	112.04
1	D	948	GLU	N-CA-C	-6.98	102.88	111.40
1	A	173	GLU	CA-CB-CG	6.94	127.98	114.10
1	C	835	TYR	N-CA-C	-6.94	103.48	112.23
1	D	1128	HIS	CB-CG-CD2	-6.93	122.19	131.20
1	B	464	GLU	N-CA-C	-6.89	103.00	111.40
1	B	417	ARG	N-CA-C	-6.88	103.39	111.03
1	A	188	GLY	N-CA-C	-6.87	104.18	112.49
1	D	860	MET	CA-CB-CG	6.84	127.78	114.10
1	A	276	HIS	CB-CG-CD2	-6.81	122.35	131.20
1	A	126	GLY	N-CA-C	-6.79	104.27	112.49
1	C	588	ASP	N-CA-C	-6.79	103.12	111.40
1	C	703	GLN	CA-C-N	6.77	134.47	121.54
1	C	703	GLN	C-N-CA	6.77	134.47	121.54
1	A	283	SER	CA-C-N	-6.75	109.56	121.70
1	A	283	SER	C-N-CA	-6.75	109.56	121.70
1	C	573	LYS	CA-C-O	6.74	128.11	120.90
1	B	565	MET	CB-CA-C	-6.72	95.12	110.18
1	A	16	GLU	CA-C-O	-6.70	113.97	121.00
1	B	566	THR	N-CA-C	6.70	121.20	112.89
1	D	855	ALA	O-C-N	-6.70	113.26	122.30
1	D	1018	ALA	N-CA-C	-6.69	104.14	112.90
1	A	284	ILE	CB-CG1-CD1	6.67	127.81	113.80
1	C	707	GLU	CA-C-N	-6.67	108.80	121.54
1	C	707	GLU	C-N-CA	-6.67	108.80	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	918	ASP	CA-CB-CG	6.64	119.24	112.60
1	C	706	GLU	N-CA-C	6.64	119.50	111.40
1	D	856	ILE	CG1-CB-CG2	-6.64	90.79	110.70
1	B	292	MET	N-CA-C	-6.63	103.15	111.11
1	C	576	MET	O-C-N	6.63	129.25	122.09
1	D	1128	HIS	CB-CG-ND1	6.62	132.62	122.70
1	A	27	ALA	N-CA-C	-6.61	103.33	111.40
1	A	153	HIS	CB-CG-CD2	-6.61	122.61	131.20
1	B	292	MET	CB-CA-C	-6.60	100.25	110.81
1	C	613	SER	N-CA-C	-6.58	103.37	111.40
1	A	281	MET	CA-C-O	6.58	129.91	120.51
1	C	630	GLU	N-CA-C	-6.56	103.75	111.03
1	C	849	MET	CB-CA-C	-6.55	97.75	110.46
1	A	104	GLU	N-CA-C	-6.54	104.07	111.14
1	D	882	LYS	O-C-N	-6.54	113.89	122.59
1	B	380	GLU	N-CA-C	-6.54	103.77	111.03
1	A	258	ASP	CA-C-O	-6.51	114.19	120.90
1	A	254	ASP	CA-C-O	-6.49	114.07	120.89
1	A	8	MET	CA-CB-CG	6.49	127.07	114.10
1	B	310	GLU	N-CA-C	-6.49	105.52	113.50
1	A	279	ASN	N-CA-C	6.47	121.00	113.18
1	C	569	MET	O-C-N	-6.46	112.66	123.00
1	D	973	ASP	CA-CB-CG	6.44	119.04	112.60
1	A	75	GLU	CA-CB-CG	-6.43	101.24	114.10
1	A	22	ALA	CA-C-O	-6.41	114.16	120.89
1	C	595	ALA	N-CA-C	-6.36	104.22	112.68
1	C	848	ASP	CB-CA-C	6.33	121.39	110.94
1	B	566	THR	CA-CB-OG1	-6.33	100.11	109.60
1	D	857	LYS	O-C-N	6.33	129.42	122.20
1	B	289	LYS	N-CA-C	6.31	119.83	111.75
1	C	706	GLU	O-C-N	-6.31	114.54	122.17
1	A	78	ALA	N-CA-C	-6.30	104.04	111.03
1	D	860	MET	N-CA-CB	-6.29	100.85	111.17
1	C	843	ASP	N-CA-CB	6.29	119.39	109.82
1	D	863	LEU	N-CA-C	6.29	120.05	112.38
1	C	629	SER	CA-C-N	6.28	129.17	120.63
1	C	629	SER	C-N-CA	6.28	129.17	120.63
1	B	303	LEU	CA-C-O	-6.26	114.45	120.90
1	B	551	TYR	N-CA-C	-6.26	104.53	111.36
1	C	605	LYS	N-CA-C	-6.26	103.98	111.69
1	B	452	LYS	N-CA-C	-6.24	105.79	113.41
1	A	4	ILE	O-C-N	6.23	130.36	122.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	576	MET	CA-C-N	-6.22	111.30	120.38
1	C	576	MET	C-N-CA	-6.22	111.30	120.38
1	B	547	GLN	CA-C-O	-6.21	114.30	120.70
1	A	62	GLU	N-CA-C	-6.21	104.20	110.97
1	D	856	ILE	CA-CB-CG2	6.20	121.03	110.50
1	A	229	SER	CA-C-N	6.16	129.01	120.63
1	A	229	SER	C-N-CA	6.16	129.01	120.63
1	D	932	ASP	N-CA-C	-6.16	104.49	111.14
1	D	1098	VAL	N-CA-C	-6.15	96.55	109.34
1	A	83	ALA	N-CA-C	-6.14	104.67	111.36
1	C	732	GLU	CA-C-N	6.11	128.78	120.77
1	C	732	GLU	C-N-CA	6.11	128.78	120.77
1	A	277	ALA	O-C-N	-6.11	115.54	122.08
1	C	831	GLN	CA-C-O	-6.10	114.61	120.90
1	A	283	SER	N-CA-C	6.09	120.71	113.28
1	A	10	MET	N-CA-C	-6.06	103.99	111.33
1	D	861	GLN	N-CA-CB	6.06	119.29	110.26
1	D	987	GLN	N-CA-C	-6.05	105.55	113.12
1	A	75	GLU	CB-CG-CD	6.05	122.88	112.60
1	D	857	LYS	CB-CA-C	-6.03	98.76	110.46
1	A	8	MET	CA-C-N	6.02	128.63	120.44
1	A	8	MET	C-N-CA	6.02	128.63	120.44
1	B	564	ASP	N-CA-C	6.02	120.69	112.68
1	B	486	ASN	N-CA-C	-6.02	104.64	111.14
1	B	286	ASP	N-CA-C	6.02	123.62	110.80
1	B	562	LEU	N-CA-C	6.02	117.51	111.07
1	B	292	MET	CA-CB-CG	6.01	126.13	114.10
1	A	258	ASP	N-CA-C	-6.01	104.36	111.03
1	A	117	GLU	N-CA-C	-6.01	104.65	111.14
1	B	482	LYS	CA-CB-CG	6.00	126.11	114.10
1	A	223	GLU	CB-CG-CD	6.00	122.80	112.60
1	D	881	LYS	CA-CB-CG	5.98	126.06	114.10
1	D	883	ALA	N-CA-C	5.97	123.51	110.80
1	C	843	ASP	CB-CA-C	-5.95	101.46	110.92
1	C	850	THR	CA-CB-OG1	-5.94	100.69	109.60
1	D	941	ASN	OD1-CG-ND2	-5.94	116.66	122.60
1	D	887	ARG	N-CA-C	-5.92	104.75	111.14
1	A	5	LYS	N-CA-CB	5.91	118.81	109.82
1	B	561	ALA	CA-C-O	5.91	128.96	120.51
1	A	284	ILE	CG1-CB-CG2	-5.91	92.97	110.70
1	A	34	ASP	N-CA-C	-5.91	105.57	112.89
1	C	733	VAL	N-CA-CB	-5.91	104.42	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	LYS	N-CA-C	-5.90	101.89	111.04
1	A	137	ASP	CA-C-O	-5.89	114.25	120.55
1	B	547	GLN	CA-CB-CG	-5.88	102.34	114.10
1	C	601	GLU	N-CA-C	-5.88	104.79	111.14
1	C	822	ASP	CA-C-O	-5.88	114.85	120.90
1	A	187	GLU	N-CA-C	-5.87	106.66	113.88
1	A	137	ASP	CA-CB-CG	-5.86	106.74	112.60
1	A	192	GLU	N-CA-C	-5.86	104.80	111.07
1	B	560	HIS	O-C-N	5.84	129.24	122.17
1	A	10	MET	CA-C-O	-5.83	114.33	120.63
1	D	966	GLU	N-CA-C	5.81	118.09	111.11
1	A	215	SER	CA-C-O	-5.80	114.92	120.90
1	B	534	GLU	N-CA-C	-5.80	104.32	111.40
1	C	723	ALA	N-CA-C	-5.76	104.69	110.97
1	C	689	ASP	N-CA-C	5.76	117.56	111.28
1	C	756	GLY	N-CA-C	-5.76	105.82	112.50
1	C	706	GLU	CB-CA-C	-5.76	101.11	110.79
1	B	445	LYS	N-CA-C	-5.75	104.93	111.14
1	B	501	LYS	N-CA-C	-5.75	105.15	111.82
1	C	589	ARG	NE-CZ-NH1	-5.74	115.77	121.50
1	C	847	ASN	CA-C-O	5.74	126.82	120.63
1	D	914	GLU	N-CA-C	-5.73	104.95	111.14
1	A	4	ILE	CG1-CB-CG2	-5.73	93.50	110.70
1	B	503	ASP	CA-CB-CG	5.73	118.33	112.60
1	C	630	GLU	CA-C-O	-5.73	115.00	120.90
1	C	844	HIS	CB-CG-CD2	-5.73	123.75	131.20
1	A	128	LYS	N-CA-C	5.70	119.05	111.75
1	B	566	THR	CA-CB-CG2	5.70	120.18	110.50
1	A	164	GLU	CA-C-N	5.69	128.56	120.53
1	A	164	GLU	C-N-CA	5.69	128.56	120.53
1	B	289	LYS	CA-CB-CG	5.68	125.47	114.10
1	B	425	MET	N-CA-C	-5.68	104.70	111.69
1	A	204	LEU	N-CA-C	-5.67	105.01	111.14
1	D	1028	LEU	N-CA-C	-5.67	105.09	111.28
1	A	35	ARG	NE-CZ-NH1	-5.66	115.84	121.50
1	C	672	GLU	N-CA-C	-5.66	104.59	112.45
1	D	858	LYS	CB-CA-C	5.65	121.67	110.42
1	B	306	ALA	N-CA-C	5.64	118.28	111.40
1	C	572	ILE	CA-CB-CG1	-5.64	100.81	110.40
1	A	275	ASP	CA-C-O	-5.63	114.90	120.82
1	D	965	LEU	CA-C-N	5.57	128.05	120.54
1	D	965	LEU	C-N-CA	5.57	128.05	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	871	LEU	CA-C-O	-5.56	115.16	121.00
1	D	1014	TYR	N-CA-CB	-5.56	101.67	110.28
1	A	224	GLU	CB-CG-CD	5.55	122.04	112.60
1	A	195	GLU	N-CA-C	-5.53	105.16	111.14
1	D	1105	ILE	N-CA-C	-5.53	104.97	111.00
1	C	762	GLU	CA-CB-CG	-5.50	103.11	114.10
1	A	276	HIS	CB-CG-ND1	5.49	130.94	122.70
1	B	409	ARG	CA-C-N	5.49	126.08	119.98
1	B	409	ARG	C-N-CA	5.49	126.08	119.98
1	D	1131	ASN	O-C-N	-5.49	114.94	122.46
1	B	363	THR	N-CA-C	5.49	118.03	111.71
1	C	724	GLU	N-CA-C	5.47	117.94	111.33
1	A	10	MET	O-C-N	-5.46	116.34	122.12
1	A	19	LEU	CA-C-O	-5.46	114.64	120.42
1	A	225	ILE	CA-C-O	-5.45	115.28	120.95
1	B	441	ASP	N-CA-C	-5.44	104.99	111.03
1	A	61	SER	CA-C-N	5.44	127.83	120.65
1	A	61	SER	C-N-CA	5.44	127.83	120.65
1	C	849	MET	CA-C-N	-5.42	111.46	120.68
1	C	849	MET	C-N-CA	-5.42	111.46	120.68
1	C	622	GLU	N-CA-C	-5.42	104.92	112.45
1	A	79	THR	N-CA-C	5.41	118.68	111.75
1	B	319	ARG	N-CA-C	-5.39	105.32	111.14
1	C	850	THR	CA-C-N	-5.39	111.25	121.54
1	C	850	THR	C-N-CA	-5.39	111.25	121.54
1	D	1133	MET	CA-CB-CG	5.38	124.87	114.10
1	C	683	GLU	N-CA-C	-5.35	105.61	111.82
1	D	855	ALA	N-CA-C	5.35	119.75	112.04
1	A	176	LEU	N-CA-C	-5.34	105.37	111.14
1	B	288	ILE	CA-C-O	5.34	127.45	120.78
1	C	772	LEU	N-CA-C	-5.34	105.54	111.36
1	D	1070	GLU	N-CA-C	-5.32	104.91	111.40
1	D	853	MET	N-CA-C	5.31	125.87	111.00
1	C	601	GLU	CA-C-N	5.30	127.65	120.44
1	C	601	GLU	C-N-CA	5.30	127.65	120.44
1	D	1007	ALA	N-CA-C	-5.30	105.51	111.28
1	B	445	LYS	CA-C-N	5.29	128.76	120.82
1	B	445	LYS	C-N-CA	5.29	128.76	120.82
1	A	191	ALA	CA-C-N	5.28	127.30	120.44
1	A	191	ALA	C-N-CA	5.28	127.30	120.44
1	A	168	LYS	N-CA-C	-5.27	105.64	111.71
1	C	577	GLN	OE1-CD-NE2	-5.26	117.34	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1011	ASP	N-CA-C	-5.25	105.63	111.36
1	B	430	ILE	N-CA-C	-5.25	105.59	110.53
1	B	502	GLU	CA-C-O	-5.25	114.86	120.42
1	A	153	HIS	CB-CG-ND1	5.24	130.57	122.70
1	A	19	LEU	CA-C-N	5.24	127.25	120.44
1	A	19	LEU	C-N-CA	5.24	127.25	120.44
1	A	131	GLU	N-CA-C	-5.24	105.17	112.45
1	C	574	LYS	N-CA-C	5.23	117.07	111.36
1	D	1128	HIS	CA-CB-CG	5.23	119.03	113.80
1	B	447	GLU	N-CA-C	5.23	118.12	111.69
1	A	124	GLU	N-CA-C	-5.22	106.75	113.23
1	C	602	ASP	N-CA-C	-5.22	105.50	111.14
1	C	737	LEU	CA-C-O	-5.20	115.54	120.90
1	B	556	GLU	CA-C-O	5.20	126.06	120.55
1	C	850	THR	O-C-N	-5.20	115.36	122.33
1	C	803	ALA	CA-C-N	5.20	127.67	120.29
1	C	803	ALA	C-N-CA	5.20	127.67	120.29
1	C	721	HIS	CB-CG-ND1	5.19	130.48	122.70
1	A	164	GLU	N-CA-C	-5.18	104.56	111.24
1	D	998	ILE	CA-C-O	-5.17	114.81	120.96
1	C	703	GLN	OE1-CD-NE2	-5.16	117.44	122.60
1	C	768	VAL	N-CA-CB	-5.16	104.23	112.07
1	B	405	ASP	N-CA-C	-5.16	105.66	111.28
1	C	831	GLN	N-CA-C	-5.15	105.31	111.03
1	B	437	HIS	CB-CG-CD2	-5.15	124.51	131.20
1	D	868	GLU	CA-CB-CG	-5.15	103.81	114.10
1	A	267	TYR	N-CA-C	-5.14	106.27	112.54
1	D	1008	GLU	N-CA-C	5.13	116.68	111.14
1	B	487	ASN	OD1-CG-ND2	-5.12	117.48	122.60
1	D	871	LEU	N-CA-C	-5.12	105.39	110.97
1	B	384	ASP	CA-C-O	-5.12	115.62	121.00
1	D	1032	GLU	CA-C-N	5.12	127.45	120.54
1	D	1032	GLU	C-N-CA	5.12	127.45	120.54
1	A	240	GLU	CB-CG-CD	5.11	121.29	112.60
1	D	861	GLN	O-C-N	5.11	129.79	122.28
1	B	296	LYS	N-CA-C	-5.11	105.17	111.40
1	B	464	GLU	CA-C-N	5.11	127.08	120.44
1	B	464	GLU	C-N-CA	5.11	127.08	120.44
1	B	401	GLU	N-CA-C	-5.10	105.41	110.97
1	B	453	LEU	CA-CB-CG	5.10	134.13	116.30
1	A	183	ALA	CA-C-N	5.09	127.36	120.38
1	A	183	ALA	C-N-CA	5.09	127.36	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1132	ASP	CA-C-N	5.09	131.26	121.54
1	D	1132	ASP	C-N-CA	5.09	131.26	121.54
1	B	381	GLU	N-CA-C	5.08	117.48	111.33
1	C	570	ASP	N-CA-C	5.08	121.62	110.80
1	C	814	VAL	CA-C-O	-5.08	115.79	121.17
1	A	260	LEU	N-CA-C	-5.08	105.40	112.45
1	C	570	ASP	O-C-N	-5.07	115.84	122.59
1	C	725	ASP	N-CA-C	-5.07	105.75	111.28
1	A	163	GLU	N-CA-C	-5.06	107.11	113.28
1	C	850	THR	N-CA-CB	5.06	118.09	110.30
1	D	862	MET	CA-CB-CG	5.05	124.21	114.10
1	A	227	VAL	N-CA-C	5.05	119.84	109.34
1	B	486	ASN	CA-C-O	-5.05	115.50	120.70
1	A	208	GLU	N-CA-C	-5.04	105.43	111.03
1	D	985	ARG	N-CA-C	-5.04	100.06	110.80
1	D	1024	ILE	CA-C-N	5.04	126.99	120.44
1	D	1024	ILE	C-N-CA	5.04	126.99	120.44
1	D	1055	ASN	OD1-CG-ND2	-5.04	117.56	122.60
1	D	1098	VAL	CA-C-O	-5.01	114.52	120.78
1	C	704	LYS	N-CA-C	5.01	121.47	110.80
1	D	1013	LYS	CA-C-N	5.01	127.93	120.31
1	D	1013	LYS	C-N-CA	5.01	127.93	120.31
1	A	222	GLU	CA-C-O	-5.01	114.68	120.24
1	B	325	ASP	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	223	GLU	Mainchain,Peptide
1	A	224	GLU	Mainchain
1	C	702	ALA	Mainchain
1	C	703	GLN	Mainchain
1	C	705	ASP	Peptide
1	C	707	GLU	Peptide
1	C	850	THR	Peptide
1	D	1135	SER	Mainchain
1	D	859	LYS	Mainchain,Peptide
1	D	879	ALA	Mainchain,Peptide

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	2290	0	2295	101	0
1	B	2290	0	2292	88	0
1	C	2290	0	2291	134	3
1	D	2290	0	2292	94	3
All	All	9160	0	9170	353	3

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 19.

All (353) 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:C:572:ILE:CB	1:C:572:ILE:CA	1.81	1.58
1:C:705:ASP:C	1:C:705:ASP:CA	1.76	1.54
1:D:859:LYS:N	1:D:859:LYS:CA	1.67	1.51
1:C:851:SER:C	1:C:852:ILE:N	1.70	1.49
1:C:572:ILE:CB	1:C:572:ILE:N	1.71	1.46
1:C:852:ILE:CB	1:C:852:ILE:CA	2.04	1.35
1:C:572:ILE:N	1:C:572:ILE:HB	1.29	1.29
1:A:280:ASP:HB3	1:B:565:MET:SD	1.80	1.22
1:C:852:ILE:N	1:C:852:ILE:CA	2.08	1.17
1:C:852:ILE:CB	1:C:852:ILE:C	2.27	1.08
1:C:705:ASP:N	1:C:708:LYS:HD2	1.74	1.02
1:D:880:ASP:HB3	1:D:882:LYS:N	1.74	1.01
1:B:567:SER:HB2	1:B:568:ILE:HD12	1.44	0.97
1:C:852:ILE:N	1:C:852:ILE:HA	1.79	0.97
1:C:572:ILE:HB	1:C:572:ILE:H	1.28	0.95
1:C:703:GLN:C	1:C:708:LYS:HG2	1.92	0.94
1:D:860:MET:HA	1:D:863:LEU:H	1.32	0.93
1:C:705:ASP:HB3	1:D:993:MET:HB2	1.50	0.90
1:C:571:ALA:C	1:C:572:ILE:HB	1.96	0.89
1:C:702:ALA:HA	1:C:708:LYS:HE2	1.53	0.88
1:D:880:ASP:HB2	1:D:883:ALA:N	1.90	0.87
1:A:224:GLU:HB2	1:A:227:VAL:N	1.90	0.86
1:A:8:MET:SD	1:B:292:MET:HA	2.15	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ILE:HD12	1:B:288:ILE:HB	1.58	0.86
1:C:576:MET:SD	1:D:859:LYS:HE2	2.16	0.85
1:A:224:GLU:HB2	1:A:227:VAL:H	1.44	0.82
1:C:572:ILE:CA	1:C:572:ILE:CG1	2.57	0.81
1:C:569:MET:C	1:C:572:ILE:HG22	2.05	0.80
1:A:223:GLU:HA	1:A:224:GLU:HG2	1.64	0.79
1:C:571:ALA:C	1:C:572:ILE:CB	2.53	0.79
1:D:880:ASP:HB2	1:D:883:ALA:H	1.46	0.78
1:C:703:GLN:O	1:C:708:LYS:HG2	1.85	0.77
1:C:705:ASP:C	1:C:705:ASP:CB	2.60	0.74
1:C:707:GLU:N	1:C:708:LYS:HG3	2.03	0.74
1:D:1017:VAL:HA	1:D:1020:LYS:HB2	1.71	0.73
1:C:706:GLU:H	1:C:708:LYS:HE3	1.54	0.73
1:C:705:ASP:CA	1:C:708:LYS:HB3	2.20	0.72
1:D:860:MET:SD	1:D:864:LYS:HB2	2.29	0.72
1:C:571:ALA:O	1:C:575:LYS:HB3	1.89	0.72
1:A:224:GLU:HB2	1:A:226:LYS:C	2.14	0.72
1:B:449:VAL:HA	1:B:452:LYS:HB2	1.72	0.71
1:C:707:GLU:H	1:C:708:LYS:HG3	1.53	0.70
1:A:4:ILE:HD12	1:B:288:ILE:CB	2.22	0.70
1:A:8:MET:HE1	1:B:295:LEU:C	2.17	0.70
1:C:706:GLU:C	1:C:708:LYS:HB2	2.18	0.69
1:D:859:LYS:N	1:D:859:LYS:HA	1.95	0.69
1:A:43:LEU:HD11	1:B:326:GLU:HB3	1.76	0.68
1:A:219:ASP:HA	1:A:222:GLU:HG3	1.77	0.67
1:A:222:GLU:O	1:A:224:GLU:HB3	1.94	0.67
1:C:848:ASP:HA	1:C:851:SER:H	1.60	0.67
1:C:705:ASP:H	1:C:708:LYS:HD2	1.56	0.67
1:A:57:LEU:HD22	1:B:337:THR:HG22	1.77	0.66
1:B:558:LEU:O	1:B:561:ALA:HB3	1.96	0.66
1:D:856:ILE:O	1:D:859:LYS:N	2.28	0.65
1:D:855:ALA:O	1:D:858:LYS:HB2	1.97	0.65
1:C:702:ALA:C	1:C:708:LYS:HD3	2.22	0.65
1:A:2:ASP:O	1:A:5:LYS:HB3	1.97	0.65
1:A:8:MET:SD	1:B:292:MET:CA	2.84	0.65
1:C:702:ALA:O	1:C:708:LYS:HG3	1.96	0.64
1:C:706:GLU:H	1:C:708:LYS:CE	2.10	0.64
1:B:285:MET:C	1:B:288:ILE:HG13	2.23	0.64
1:C:706:GLU:N	1:C:708:LYS:CG	2.60	0.64
1:C:852:ILE:CA	1:C:852:ILE:HB	2.21	0.64
1:D:860:MET:HA	1:D:863:LEU:N	2.09	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ALA:O	1:A:280:ASP:HB2	1.97	0.64
1:D:854:ASP:O	1:D:857:LYS:HB3	1.98	0.63
1:B:286:ASP:O	1:B:289:LYS:HB3	1.97	0.63
1:C:704:LYS:N	1:C:708:LYS:HG2	2.13	0.63
1:A:7:LYS:CE	1:B:292:MET:HB2	2.27	0.63
1:C:846:LEU:O	1:C:849:MET:N	2.31	0.63
1:A:1:MET:H2	1:A:4:ILE:HG12	1.64	0.63
1:C:828:LEU:HD11	1:D:1111:GLU:HG3	1.80	0.63
1:C:831:GLN:HE22	1:D:1112:LEU:HG	1.64	0.62
1:D:989:ASP:HA	1:D:992:LYS:HB2	1.81	0.62
1:D:859:LYS:N	1:D:859:LYS:CB	2.58	0.62
1:A:8:MET:HE1	1:B:296:LYS:N	2.14	0.62
1:C:703:GLN:O	1:C:707:GLU:HB3	2.00	0.62
1:C:705:ASP:N	1:C:708:LYS:CD	2.59	0.61
1:C:852:ILE:HG22	1:D:1136:ILE:HD13	1.81	0.61
1:B:291:LYS:NZ	1:B:291:LYS:HB3	2.16	0.61
1:D:1130:LEU:HA	1:D:1133:MET:SD	2.40	0.61
1:A:1:MET:H2	1:A:4:ILE:H	1.46	0.61
1:A:224:GLU:HB3	1:A:226:LYS:H	1.66	0.61
1:C:705:ASP:O	1:C:709:MET:HB2	2.00	0.61
1:C:852:ILE:C	1:C:852:ILE:CG2	2.73	0.61
1:C:705:ASP:C	1:C:708:LYS:HB3	2.26	0.61
1:A:4:ILE:HD11	1:B:288:ILE:HD12	1.83	0.60
1:B:285:MET:O	1:B:288:ILE:HG13	2.01	0.60
1:D:857:LYS:O	1:D:858:LYS:O	2.20	0.60
1:C:848:ASP:O	1:C:851:SER:N	2.35	0.60
1:B:421:ASP:O	1:B:425:MET:HB2	2.03	0.59
1:D:880:ASP:HB3	1:D:882:LYS:H	1.66	0.59
1:B:287:ALA:O	1:B:290:LYS:HB2	2.02	0.59
1:D:856:ILE:HA	1:D:859:LYS:HB3	1.84	0.59
1:B:557:GLU:O	1:B:561:ALA:HB2	2.02	0.59
1:A:7:LYS:CD	1:A:8:MET:HG2	2.33	0.59
1:A:253:ILE:O	1:A:257:GLU:HB2	2.02	0.59
1:B:530:VAL:O	1:B:534:GLU:HB2	2.02	0.59
1:A:3:ALA:O	1:A:6:LYS:N	2.36	0.59
1:B:459:ASP:OD1	1:B:462:ARG:NH2	2.36	0.58
1:C:731:GLU:O	1:C:735:ARG:HB2	2.02	0.58
1:A:4:ILE:CD1	1:B:288:ILE:HD12	2.33	0.58
1:A:186:SER:HA	1:A:189:LYS:HB2	1.86	0.58
1:D:880:ASP:CG	1:D:882:LYS:HB2	2.29	0.58
1:A:1:MET:N	1:A:4:ILE:HG12	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:TYR:HE2	1:B:547:GLN:HB3	1.69	0.57
1:C:848:ASP:CA	1:C:851:SER:H	2.17	0.57
1:C:705:ASP:C	1:C:708:LYS:CB	2.78	0.57
1:A:260:LEU:HD11	1:B:543:GLU:HB3	1.86	0.57
1:C:601:GLU:HB3	1:C:605:LYS:NZ	2.19	0.57
1:C:706:GLU:H	1:C:708:LYS:CD	2.17	0.57
1:C:848:ASP:O	1:C:851:SER:CA	2.53	0.57
1:A:278:LEU:O	1:A:281:MET:HB3	2.04	0.57
1:B:408:GLU:O	1:B:412:LYS:HG3	2.05	0.57
1:D:986:ALA:HA	1:D:989:ASP:OD1	2.05	0.57
1:A:224:GLU:CB	1:A:227:VAL:H	2.17	0.56
1:C:596:ASP:CG	1:D:881:LYS:HZ3	2.13	0.56
1:A:224:GLU:HB3	1:A:226:LYS:N	2.20	0.56
1:C:706:GLU:N	1:C:708:LYS:HE3	2.21	0.56
1:C:848:ASP:C	1:C:850:THR:N	2.62	0.56
1:D:1019:ARG:HA	1:D:1022:VAL:HG12	1.87	0.56
1:D:1084:LEU:O	1:D:1088:GLU:HB2	2.05	0.56
1:D:1133:MET:HG2	1:D:1134:THR:N	2.19	0.56
1:A:7:LYS:HD2	1:A:8:MET:HG2	1.88	0.55
1:C:706:GLU:N	1:C:708:LYS:CD	2.69	0.55
1:D:1056:LEU:HG	1:D:1060:GLU:OE2	2.07	0.55
1:A:8:MET:SD	1:B:291:LYS:O	2.65	0.55
1:B:436:LYS:HZ3	1:B:440:GLU:CD	2.14	0.55
1:B:445:LYS:O	1:B:449:VAL:HG12	2.07	0.55
1:C:569:MET:O	1:C:572:ILE:HG22	2.07	0.55
1:C:572:ILE:CA	1:C:572:ILE:HG13	2.37	0.55
1:D:1131:ASN:O	1:D:1135:SER:HB2	2.07	0.55
1:B:289:LYS:HB2	1:B:289:LYS:NZ	2.22	0.54
1:B:499:SER:HA	1:B:502:GLU:HB3	1.88	0.54
1:A:7:LYS:HE3	1:B:292:MET:HB2	1.89	0.54
1:A:165:VAL:HG23	1:B:453:LEU:HD23	1.90	0.54
1:A:224:GLU:CB	1:A:226:LYS:N	2.71	0.54
1:C:711:ILE:O	1:C:714:ILE:HG22	2.08	0.54
1:A:225:ILE:HD11	1:B:508:GLU:HB3	1.89	0.53
1:B:500:GLN:HA	1:B:503:ASP:OD1	2.09	0.53
1:C:677:ALA:O	1:C:681:LEU:HB2	2.08	0.53
1:A:8:MET:CG	1:B:292:MET:HA	2.38	0.53
1:C:625:LEU:HD22	1:D:905:THR:HG22	1.90	0.53
1:C:701:ARG:O	1:C:708:LYS:CD	2.56	0.53
1:D:854:ASP:C	1:D:857:LYS:HB3	2.33	0.53
1:D:1048:GLU:HA	1:D:1051:THR:OG1	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:GLU:HA	1:A:224:GLU:CG	2.36	0.52
1:B:548:LYS:O	1:B:552:LYS:HD2	2.10	0.52
1:B:565:MET:CA	1:B:568:ILE:HG22	2.40	0.52
1:A:263:GLN:NE2	1:B:544:LEU:HG	2.25	0.52
1:B:285:MET:HA	1:B:288:ILE:HD12	1.91	0.51
1:C:571:ALA:HA	1:C:574:LYS:HB3	1.92	0.51
1:A:280:ASP:C	1:A:282:THR:H	2.18	0.51
1:C:702:ALA:CA	1:C:708:LYS:HD3	2.41	0.51
1:D:995:ILE:O	1:D:998:ILE:HG22	2.10	0.51
1:C:705:ASP:C	1:C:705:ASP:HA	2.15	0.51
1:A:55:ASP:O	1:A:59:LYS:HG2	2.11	0.51
1:A:283:SER:O	1:A:284:ILE:HD13	2.10	0.51
1:C:576:MET:HE3	1:D:863:LEU:HD11	1.93	0.51
1:A:274:LEU:O	1:A:277:ALA:HB3	2.11	0.50
1:C:827:GLU:HG3	1:C:831:GLN:NE2	2.25	0.50
1:A:4:ILE:HG13	1:B:288:ILE:HG21	1.94	0.50
1:A:263:GLN:HE22	1:B:544:LEU:HG	1.75	0.50
1:B:291:LYS:HE2	1:B:294:MET:HB3	1.93	0.50
1:C:713:GLU:CD	1:C:717:LYS:HZ1	2.19	0.50
1:D:876:GLU:O	1:D:879:ALA:HB3	2.11	0.50
1:D:1050:LYS:HA	1:D:1053:THR:OG1	2.11	0.50
1:A:242:ALA:O	1:A:246:VAL:HG23	2.12	0.50
1:C:582:ASP:CG	1:D:867:LYS:HZ3	2.20	0.50
1:C:764:GLU:O	1:C:768:VAL:HG12	2.11	0.50
1:D:880:ASP:CB	1:D:883:ALA:N	2.70	0.50
1:B:564:ASP:O	1:B:568:ILE:HB	2.12	0.49
1:C:733:VAL:HG22	1:D:1021:LEU:HD23	1.94	0.49
1:A:1:MET:O	1:A:4:ILE:N	2.45	0.49
1:A:75:GLU:CD	1:B:354:LYS:HZ3	2.20	0.49
1:A:114:GLU:HG2	1:A:118:LYS:NZ	2.27	0.49
1:B:402:LYS:O	1:B:406:GLU:HG3	2.11	0.49
1:B:564:ASP:C	1:B:566:THR:N	2.69	0.49
1:C:656:LEU:O	1:C:660:ILE:HD13	2.12	0.49
1:C:705:ASP:HA	1:C:708:LYS:HB3	1.94	0.49
1:D:976:GLU:O	1:D:980:LYS:HG3	2.13	0.49
1:A:172:ILE:HD11	1:B:460:LEU:HD22	1.95	0.49
1:C:667:LEU:HD11	1:D:950:GLU:HB3	1.95	0.49
1:C:680:LYS:HA	1:C:683:GLU:HB2	1.94	0.49
1:B:291:LYS:HB3	1:B:291:LYS:HZ3	1.77	0.48
1:C:844:HIS:O	1:C:845:ALA:C	2.56	0.48
1:B:317:GLU:O	1:B:321:LYS:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:558:LEU:O	1:B:562:LEU:HB2	2.12	0.48
1:A:7:LYS:HG3	1:A:8:MET:H	1.79	0.48
1:A:280:ASP:HB3	1:B:565:MET:CE	2.43	0.48
1:C:597:LYS:NZ	1:C:601:GLU:OE2	2.47	0.48
1:C:702:ALA:O	1:C:708:LYS:CD	2.62	0.48
1:B:451:ARG:O	1:B:455:ILE:HB	2.14	0.48
1:C:702:ALA:HA	1:C:708:LYS:CE	2.34	0.48
1:D:987:GLN:HA	1:D:990:GLU:HB2	1.95	0.48
1:D:1064:GLU:O	1:D:1068:GLN:HG3	2.14	0.47
1:A:3:ALA:O	1:A:4:ILE:C	2.57	0.47
1:C:848:ASP:C	1:C:851:SER:N	2.72	0.47
1:D:941:ASN:O	1:D:944:ILE:HG22	2.14	0.47
1:D:1126:LEU:O	1:D:1129:ALA:HB3	2.14	0.47
1:A:133:ARG:O	1:A:137:ASP:HB2	2.14	0.47
1:A:162:TYR:HA	1:A:165:VAL:HG12	1.97	0.47
1:A:228:LEU:HD12	1:B:509:ILE:HG12	1.96	0.47
1:C:576:MET:HG3	1:D:859:LYS:HG3	1.95	0.47
1:A:137:ASP:CG	1:A:140:LYS:HZ1	2.23	0.47
1:D:856:ILE:HA	1:D:859:LYS:CB	2.44	0.47
1:A:225:ILE:HD12	1:B:509:ILE:HG13	1.95	0.47
1:B:543:GLU:HG3	1:B:547:GLN:HE21	1.80	0.47
1:C:703:GLN:O	1:C:708:LYS:N	2.48	0.47
1:C:646:ALA:O	1:C:650:GLU:HB2	2.15	0.47
1:C:670:ALA:O	1:C:674:LEU:HB2	2.14	0.47
1:D:866:ASP:HA	1:D:869:ASN:HB3	1.97	0.47
1:A:222:GLU:O	1:A:224:GLU:CB	2.63	0.46
1:A:249:LEU:HD22	1:B:537:ILE:HG21	1.97	0.46
1:A:203:ASN:HB3	1:B:488:LEU:HD11	1.98	0.46
1:C:701:ARG:O	1:C:708:LYS:HD3	2.16	0.46
1:A:106:LEU:HD21	1:B:389:ARG:HD3	1.96	0.46
1:B:396:LYS:HZ2	1:B:399:GLU:CD	2.23	0.46
1:C:601:GLU:O	1:C:605:LYS:HG3	2.15	0.46
1:C:818:GLU:O	1:C:821:ILE:HG22	2.16	0.46
1:C:579:LEU:HG	1:D:860:MET:HG3	1.96	0.46
1:D:880:ASP:HB3	1:D:882:LYS:CA	2.45	0.46
1:C:674:LEU:HD21	1:D:957:ARG:HD3	1.97	0.46
1:C:705:ASP:CA	1:C:708:LYS:HD2	2.45	0.46
1:C:612:VAL:HG22	1:C:616:LYS:NZ	2.31	0.46
1:C:694:GLY:O	1:C:697:VAL:HG12	2.16	0.46
1:D:1014:TYR:O	1:D:1018:ALA:HB2	2.15	0.46
1:C:650:GLU:CD	1:D:929:LYS:HZ1	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:704:LYS:C	1:C:708:LYS:CG	2.89	0.45
1:A:4:ILE:CG1	1:B:288:ILE:HG21	2.45	0.45
1:A:16:GLU:O	1:A:19:LEU:HB2	2.16	0.45
1:B:292:MET:HG2	1:B:293:GLN:HG3	1.99	0.45
1:A:7:LYS:NZ	1:B:292:MET:HB2	2.31	0.45
1:A:224:GLU:HB2	1:A:226:LYS:CA	2.47	0.45
1:B:290:LYS:O	1:B:293:GLN:HB2	2.15	0.45
1:B:473:LYS:HZ3	1:B:477:LEU:HD11	1.81	0.45
1:C:653:VAL:O	1:C:657:ASN:HB2	2.16	0.45
1:B:450:ALA:O	1:B:453:LEU:HG	2.17	0.45
1:A:95:PHE:O	1:A:99:LEU:HD13	2.16	0.45
1:C:622:GLU:OE1	1:D:901:LYS:NZ	2.50	0.45
1:D:880:ASP:CB	1:D:883:ALA:H	2.23	0.45
1:D:958:LEU:O	1:D:962:LEU:HB2	2.16	0.45
1:A:223:GLU:O	1:A:227:VAL:HB	2.16	0.45
1:A:266:LYS:O	1:A:270:ILE:HG13	2.17	0.45
1:A:112:LYS:HB2	1:A:112:LYS:NZ	2.32	0.45
1:B:285:MET:N	1:B:288:ILE:HD11	2.32	0.45
1:C:576:MET:HE2	1:C:577:GLN:HA	1.98	0.45
1:D:859:LYS:CA	1:D:859:LYS:H	2.07	0.45
1:A:4:ILE:HG22	1:A:7:LYS:HG2	1.99	0.45
1:A:248:LYS:NZ	1:A:252:SER:OG	2.50	0.45
1:B:424:LYS:HA	1:B:427:ILE:HB	1.99	0.44
1:C:704:LYS:O	1:C:708:LYS:CA	2.65	0.44
1:A:7:LYS:HD3	1:A:8:MET:HG2	1.99	0.44
1:D:856:ILE:HD13	1:D:856:ILE:HG21	1.62	0.44
1:D:885:GLU:O	1:D:889:LYS:HG3	2.17	0.44
1:D:1021:LEU:HD12	1:D:1022:VAL:N	2.33	0.44
1:B:285:MET:SD	1:B:289:LYS:NZ	2.88	0.44
1:C:675:ALA:O	1:C:679:GLN:HB2	2.18	0.44
1:C:849:MET:HE2	1:D:1132:ASP:HB3	2.00	0.44
1:D:864:LYS:NZ	1:D:868:GLU:OE2	2.51	0.44
1:C:583:LYS:NZ	1:D:866:ASP:CG	2.76	0.44
1:C:848:ASP:HA	1:C:851:SER:N	2.30	0.44
1:A:8:MET:CE	1:B:295:LEU:HB2	2.48	0.44
1:B:534:GLU:O	1:B:537:ILE:HG22	2.17	0.44
1:D:857:LYS:C	1:D:858:LYS:O	2.61	0.43
1:A:169:LEU:O	1:A:172:ILE:HG22	2.18	0.43
1:C:744:LEU:HD11	1:D:1027:ASP:HB3	2.00	0.43
1:C:762:GLU:O	1:C:765:ILE:HG22	2.18	0.43
1:D:1108:LEU:O	1:D:1112:LEU:HD13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:704:LYS:NZ	1:C:705:ASP:OD2	2.52	0.43
1:A:168:LYS:NZ	1:B:457:GLU:OE2	2.52	0.43
1:C:649:ALA:O	1:C:653:VAL:HG23	2.19	0.43
1:C:702:ALA:C	1:C:708:LYS:CD	2.91	0.43
1:C:704:LYS:O	1:C:708:LYS:CB	2.67	0.43
1:A:35:ARG:NH1	1:B:324:GLU:OE2	2.51	0.43
1:C:698:ILE:HG21	1:D:982:ILE:HG23	2.01	0.43
1:D:1008:GLU:HB3	1:D:1012:ARG:HH11	1.83	0.43
1:D:1011:ASP:O	1:D:1014:TYR:HB3	2.19	0.43
1:D:1068:GLN:HA	1:D:1071:ASP:OD1	2.18	0.43
1:D:1083:LYS:NZ	1:D:1086:GLU:OE1	2.51	0.43
1:D:1126:LEU:O	1:D:1130:LEU:HD13	2.18	0.43
1:B:292:MET:HG2	1:B:293:GLN:N	2.33	0.43
1:B:516:LEU:O	1:B:520:GLU:HB2	2.19	0.43
1:C:682:GLU:OE1	1:C:686:LYS:NZ	2.51	0.43
1:C:852:ILE:C	1:C:852:ILE:HG22	2.43	0.43
1:D:988:LYS:O	1:D:992:LYS:HD2	2.18	0.43
1:A:54:GLU:OE1	1:B:333:LYS:NZ	2.51	0.43
1:A:96:GLU:O	1:A:99:LEU:HB2	2.19	0.43
1:A:151:ALA:O	1:A:154:ILE:HG22	2.19	0.43
1:A:4:ILE:O	1:A:7:LYS:HG3	2.18	0.43
1:C:701:ARG:O	1:C:708:LYS:HD2	2.18	0.43
1:D:997:GLU:HG2	1:D:1001:LYS:HZ2	1.83	0.43
1:B:562:LEU:O	1:B:566:THR:HB	2.19	0.42
1:C:704:LYS:C	1:C:708:LYS:CB	2.92	0.42
1:B:313:LYS:NZ	1:B:317:GLU:HG3	2.33	0.42
1:C:736:LYS:HA	1:C:739:ILE:HG22	2.01	0.42
1:A:11:LEU:HD23	1:B:295:LEU:O	2.19	0.42
1:A:12:LYS:NZ	1:A:16:GLU:OE1	2.52	0.42
1:C:580:LYS:NZ	1:C:584:GLU:OE2	2.52	0.42
1:C:698:ILE:HD11	1:D:986:ALA:HB3	2.01	0.42
1:B:565:MET:HA	1:B:568:ILE:CG2	2.48	0.42
1:C:719:ALA:O	1:C:722:ILE:HG22	2.18	0.42
1:C:833:LEU:O	1:C:836:LYS:HB2	2.19	0.42
1:D:879:ALA:O	1:D:880:ASP:CB	2.63	0.42
1:C:591:ASP:O	1:C:595:ALA:HB2	2.18	0.42
1:C:736:LYS:NZ	1:D:1025:GLU:OE1	2.53	0.42
1:A:152:LYS:HZ2	1:A:156:GLU:CD	2.27	0.42
1:C:580:LYS:NZ	1:C:584:GLU:CD	2.77	0.42
1:A:14:ASP:CG	1:B:299:LYS:HZ3	2.26	0.42
1:B:285:MET:HA	1:B:288:ILE:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:854:ASP:CG	1:D:858:LYS:NZ	2.78	0.42
1:B:559:ASP:O	1:B:562:LEU:HB3	2.20	0.42
1:C:755:GLU:O	1:C:758:CYS:HB2	2.20	0.42
1:D:1053:THR:O	1:D:1057:LYS:HD2	2.20	0.42
1:C:702:ALA:O	1:C:708:LYS:CG	2.66	0.42
1:C:707:GLU:N	1:C:708:LYS:CG	2.79	0.42
1:D:879:ALA:O	1:D:880:ASP:HB2	2.19	0.42
1:D:991:GLU:OE1	1:D:992:LYS:NZ	2.52	0.42
1:D:965:LEU:O	1:D:969:GLU:HG3	2.19	0.42
1:B:565:MET:HA	1:B:568:ILE:HG22	2.01	0.41
1:C:713:GLU:CD	1:C:717:LYS:NZ	2.78	0.41
1:D:1020:LYS:O	1:D:1023:ILE:HG22	2.20	0.41
1:A:279:ASN:HA	1:A:282:THR:OG1	2.20	0.41
1:A:231:LYS:NZ	1:A:234:GLU:CD	2.78	0.41
1:A:7:LYS:O	1:A:10:MET:N	2.54	0.41
1:A:114:GLU:HG2	1:A:118:LYS:HZ1	1.85	0.41
1:C:583:LYS:HZ1	1:D:866:ASP:CG	2.27	0.41
1:C:705:ASP:N	1:C:708:LYS:CG	2.83	0.41
1:A:12:LYS:NZ	1:A:16:GLU:OE2	2.53	0.41
1:D:855:ALA:C	1:D:857:LYS:N	2.76	0.41
1:A:46:LEU:O	1:A:50:LEU:HB2	2.20	0.41
1:A:50:LEU:HD21	1:B:333:LYS:HB3	2.02	0.41
1:A:187:GLU:CD	1:B:466:ARG:HH11	2.29	0.41
1:C:682:GLU:HG2	1:C:686:LYS:NZ	2.36	0.41
1:C:692:GLU:OE2	1:C:696:LYS:NZ	2.53	0.41
1:D:976:GLU:OE1	1:D:980:LYS:NZ	2.53	0.41
1:C:612:VAL:O	1:C:616:LYS:NZ	2.54	0.41
1:D:910:ASP:O	1:D:913:SER:HB3	2.21	0.41
1:D:1125:GLU:O	1:D:1129:ALA:HB2	2.20	0.41
1:D:905:THR:O	1:D:909:LEU:HB2	2.21	0.40
1:D:1057:LYS:HZ2	1:D:1060:GLU:CD	2.25	0.40
1:A:280:ASP:C	1:A:282:THR:N	2.76	0.40
1:B:335:LYS:NZ	1:B:338:GLU:OE2	2.53	0.40
1:C:755:GLU:CD	1:D:1034:ARG:HH11	2.28	0.40
1:A:126:GLY:O	1:A:130:ILE:HG22	2.21	0.40
1:C:599:ALA:O	1:C:603:ARG:HB2	2.22	0.40
1:C:720:LYS:O	1:C:723:ALA:HB3	2.21	0.40
1:D:1081:SER:O	1:D:1085:LYS:NZ	2.54	0.40
1:A:223:GLU:O	1:A:224:GLU:CB	2.69	0.40
1:A:224:GLU:CD	1:A:226:LYS:HB2	2.46	0.40
1:C:613:SER:O	1:C:617:LYS:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:LYS:O	1:A:172:ILE:HB	2.22	0.40
1:C:572:ILE:O	1:C:573:LYS:C	2.65	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:851:SER:O	1:D:857:LYS:O[3_364]	2.14	0.06
1:C:848:ASP:O	1:D:856:ILE:O[3_364]	2.16	0.04
1:C:852:ILE:N	1:D:860:MET:N[3_364]	2.17	0.03

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	282/284 (99%)	241 (86%)	32 (11%)	9 (3%)	3	21
1	B	282/284 (99%)	250 (89%)	28 (10%)	4 (1%)	9	41
1	C	282/284 (99%)	246 (87%)	30 (11%)	6 (2%)	5	30
1	D	282/284 (99%)	246 (87%)	28 (10%)	8 (3%)	4	24
All	All	1128/1136 (99%)	983 (87%)	118 (10%)	27 (2%)	5	27

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	570	ASP
1	C	845	ALA
1	D	854	ASP
1	D	880	ASP
1	D	1133	MET
1	A	4	ILE

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Mol	Chain	Res	Type
1	A	59	LYS
1	A	66	ASP
1	A	72	GLU
1	B	288	ILE
1	C	640	GLU
1	C	708	LYS
1	D	1079	VAL
1	D	1099	THR
1	A	7	LYS
1	C	844	HIS
1	D	879	ALA
1	D	986	ALA
1	A	71	LEU
1	A	224	GLU
1	B	286	ASP
1	B	553	ALA
1	A	58	ASP
1	A	113	LEU
1	B	561	ALA
1	C	634	ASP
1	D	1098	VAL

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	245/245 (100%)	205 (84%)	40 (16%)	2	10
1	B	245/245 (100%)	218 (89%)	27 (11%)	5	18
1	C	245/245 (100%)	213 (87%)	32 (13%)	3	14
1	D	245/245 (100%)	212 (86%)	33 (14%)	3	13
All	All	980/980 (100%)	848 (86%)	132 (14%)	3	13

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	4	ILE
1	A	5	LYS
1	A	7	LYS
1	A	8	MET
1	A	11	LEU
1	A	15	LYS
1	A	16	GLU
1	A	28	ASP
1	A	30	LYS
1	A	33	GLU
1	A	34	ASP
1	A	44	VAL
1	A	50	LEU
1	A	54	GLU
1	A	79	THR
1	A	84	ASP
1	A	87	SER
1	A	112	LYS
1	A	137	ASP
1	A	153	HIS
1	A	159	ASP
1	A	165	VAL
1	A	175	ASP
1	A	197	ILE
1	A	199	THR
1	A	200	VAL
1	A	201	THR
1	A	224	GLU
1	A	225	ILE
1	A	226	LYS
1	A	227	VAL
1	A	229	SER
1	A	231	LYS
1	A	234	GLU
1	A	248	LYS
1	A	253	ILE
1	A	274	LEU
1	A	278	LEU
1	A	281	MET
1	B	285	MET
1	B	288	ILE
1	B	289	LYS

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Mol	Chain	Res	Type
1	B	291	LYS
1	B	292	MET
1	B	313	LYS
1	B	317	GLU
1	B	326	GLU
1	B	341	LEU
1	B	396	LYS
1	B	413	VAL
1	B	430	ILE
1	B	432	LEU
1	B	437	HIS
1	B	452	LYS
1	B	455	ILE
1	B	459	ASP
1	B	479	GLU
1	B	509	ILE
1	B	524	GLU
1	B	537	ILE
1	B	544	LEU
1	B	552	LYS
1	B	556	GLU
1	B	562	LEU
1	B	566	THR
1	B	568	ILE
1	C	572	ILE
1	C	576	MET
1	C	579	LEU
1	C	591	ASP
1	C	596	ASP
1	C	611	LEU
1	C	612	VAL
1	C	618	LEU
1	C	647	THR
1	C	657	ASN
1	C	660	ILE
1	C	676	THR
1	C	680	LYS
1	C	692	GLU
1	C	705	ASP
1	C	706	GLU
1	C	708	LYS
1	C	711	ILE

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Mol	Chain	Res	Type
1	C	713	GLU
1	C	735	ARG
1	C	736	LYS
1	C	743	ASP
1	C	767	THR
1	C	799	LYS
1	C	808	GLU
1	C	814	VAL
1	C	815	THR
1	C	821	ILE
1	C	823	ASP
1	C	836	LYS
1	C	849	MET
1	C	850	THR
1	D	857	LYS
1	D	881	LYS
1	D	882	LYS
1	D	892	GLU
1	D	905	THR
1	D	910	ASP
1	D	924	GLU
1	D	931	THR
1	D	936	ASP
1	D	947	PHE
1	D	964	LYS
1	D	965	LEU
1	D	966	GLU
1	D	989	ASP
1	D	992	LYS
1	D	1005	HIS
1	D	1017	VAL
1	D	1020	LYS
1	D	1022	VAL
1	D	1025	GLU
1	D	1038	SER
1	D	1049	ILE
1	D	1051	THR
1	D	1057	LYS
1	D	1060	GLU
1	D	1086	GLU
1	D	1104	SER
1	D	1105	ILE

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Mol	Chain	Res	Type
1	D	1112	LEU
1	D	1125	GLU
1	D	1128	HIS
1	D	1134	THR
1	D	1136	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	135	GLN
1	A	203	ASN
1	A	263	GLN
1	B	322	GLN
1	B	373	ASN
1	B	428	GLN
1	B	487	ASN
1	B	547	GLN
1	C	585	ASN
1	C	771	ASN
1	C	831	GLN
1	D	945	GLN
1	D	996	GLN
1	D	1054	ASN
1	D	1055	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	851:SER	C	852:ILE	N	1.70

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	284/284 (100%)	5.82	226 (79%) 0 1	174, 174, 174, 174	0
1	B	284/284 (100%)	6.11	233 (82%) 0 1	174, 174, 174, 174	0
1	C	284/284 (100%)	4.93	200 (70%) 0 1	174, 174, 174, 174	0
1	D	284/284 (100%)	5.67	213 (75%) 0 1	174, 174, 174, 174	0
All	All	1136/1136 (100%)	5.63	872 (76%) 0 1	174, 174, 174, 174	0

All (872) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	223	GLU	39.3
1	D	1134	THR	37.3
1	C	682	GLU	35.0
1	A	2	ASP	29.4
1	B	560	HIS	27.5
1	B	395	GLN	27.4
1	A	216	GLN	27.3
1	A	219	ASP	26.6
1	B	353	GLU	26.5
1	B	541	GLU	25.8
1	D	910	ASP	25.3
1	D	913	SER	24.2
1	D	922	LYS	23.8
1	C	585	ASN	23.7
1	C	791	GLU	22.8
1	A	220	LYS	22.5
1	A	20	ASP	22.3
1	C	763	GLU	22.3
1	C	578	MET	22.2
1	D	1019	ARG	22.1
1	D	1047	GLU	22.1

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Mol	Chain	Res	Type	RSRZ
1	A	9	GLN	21.9
1	A	215	SER	21.5
1	B	374	ARG	21.5
1	B	563	ASN	21.0
1	D	1016	GLU	20.8
1	D	921	GLU	20.5
1	C	784	GLN	20.3
1	A	16	GLU	20.2
1	B	451	ARG	20.1
1	A	198	LYS	19.2
1	A	56	GLU	19.2
1	C	701	ARG	19.1
1	A	222	GLU	18.8
1	D	861	GLN	18.3
1	A	12	LYS	18.2
1	C	693	ARG	18.1
1	A	5	LYS	18.0
1	C	582	ASP	18.0
1	D	854	ASP	17.9
1	D	1064	GLU	17.9
1	B	557	GLU	17.8
1	B	437	HIS	17.7
1	C	752	GLU	17.7
1	A	202	ASN	17.6
1	B	545	TYR	17.5
1	B	556	GLU	17.4
1	B	454	VAL	17.4
1	D	893	ASP	17.4
1	B	498	TYR	17.3
1	C	750	ARG	17.3
1	A	90	ARG	17.3
1	D	977	ARG	17.2
1	D	858	LYS	17.2
1	D	889	LYS	16.9
1	A	181	GLU	16.9
1	B	367	ALA	16.8
1	D	917	LYS	16.8
1	C	697	VAL	16.7
1	C	812	ARG	16.4
1	A	79	THR	16.4
1	B	494	GLN	16.3
1	C	571	ALA	16.2

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Mol	Chain	Res	Type	RSRZ
1	B	487	ASN	16.2
1	D	945	GLN	16.1
1	B	549	LEU	15.8
1	C	570	ASP	15.8
1	B	567	SER	15.7
1	B	552	LYS	15.6
1	A	282	THR	15.5
1	A	136	LYS	15.4
1	A	185	LEU	15.3
1	C	686	LYS	15.3
1	B	462	ARG	15.1
1	B	360	LYS	15.1
1	A	218	GLU	15.0
1	B	444	ARG	14.9
1	B	294	MET	14.6
1	B	564	ASP	14.6
1	D	885	GLU	14.5
1	D	1110	ASP	14.5
1	C	658	ARG	14.4
1	D	939	SER	14.3
1	D	865	LEU	14.3
1	A	69	GLU	14.3
1	B	429	GLU	14.2
1	B	399	GLU	14.2
1	B	559	ASP	14.1
1	C	710	GLU	14.0
1	C	671	GLN	14.0
1	B	548	LYS	13.9
1	A	132	SER	13.8
1	D	974	GLU	13.8
1	B	394	LEU	13.8
1	D	1011	ASP	13.6
1	B	398	GLU	13.6
1	A	13	LEU	13.6
1	B	461	GLU	13.5
1	A	194	GLU	13.3
1	D	928	LYS	13.3
1	B	287	ALA	13.3
1	B	546	ALA	13.3
1	A	152	LYS	13.2
1	C	575	LYS	13.2
1	C	589	ARG	13.1

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Mol	Chain	Res	Type	RSRZ
1	D	943	ARG	13.0
1	C	728	ARG	12.9
1	D	1054	ASN	12.9
1	A	48	LYS	12.9
1	C	714	ILE	12.8
1	D	935	ALA	12.8
1	A	68	GLN	12.7
1	C	746	ARG	12.7
1	D	924	GLU	12.7
1	B	307	ASP	12.7
1	D	970	LYS	12.7
1	A	76	LYS	12.6
1	A	149	LYS	12.6
1	A	145	GLU	12.5
1	D	1068	GLN	12.5
1	B	468	GLU	12.4
1	B	356	GLU	12.4
1	C	806	ARG	12.4
1	C	735	ARG	12.3
1	D	1106	ASP	12.2
1	C	721	HIS	12.2
1	D	1130	LEU	12.2
1	A	164	GLU	12.1
1	A	192	GLU	12.0
1	A	139	GLU	12.0
1	D	997	GLU	12.0
1	B	419	GLN	12.0
1	A	189	LYS	11.9
1	B	371	SER	11.9
1	A	168	LYS	11.9
1	D	1023	ILE	11.9
1	B	469	LEU	11.7
1	D	994	GLU	11.7
1	C	799	LYS	11.7
1	B	525	PHE	11.7
1	B	408	GLU	11.7
1	C	679	GLN	11.5
1	D	966	GLU	11.4
1	B	433	LYS	11.4
1	D	1001	LYS	11.4
1	A	142	GLU	11.3
1	C	617	LYS	11.3

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Mol	Chain	Res	Type	RSRZ
1	B	364	ASP	11.3
1	B	491	LEU	11.2
1	A	178	ARG	11.0
1	C	795	VAL	11.0
1	A	133	ARG	11.0
1	A	224	GLU	11.0
1	B	458	SER	11.0
1	A	72	GLU	11.0
1	D	990	GLU	11.0
1	D	1032	GLU	10.9
1	B	384	ASP	10.9
1	A	226	LYS	10.9
1	B	473	LYS	10.9
1	D	914	GLU	10.9
1	D	949	GLU	10.8
1	B	300	GLU	10.7
1	D	878	GLU	10.7
1	B	426	GLU	10.6
1	D	1051	THR	10.6
1	A	91	ARG	10.6
1	B	566	THR	10.6
1	A	87	SER	10.5
1	C	802	GLU	10.5
1	B	450	ALA	10.5
1	D	862	MET	10.5
1	D	882	LYS	10.4
1	B	518	GLU	10.3
1	B	290	LYS	10.3
1	D	915	ALA	10.3
1	B	387	GLN	10.3
1	C	732	GLU	10.3
1	B	542	ASP	10.3
1	A	26	GLU	10.2
1	D	925	LEU	10.1
1	D	1057	LYS	10.1
1	B	380	GLU	9.9
1	C	704	LYS	9.8
1	A	167	ARG	9.8
1	B	314	LYS	9.8
1	C	748	GLU	9.8
1	A	258	ASP	9.7
1	A	150	GLU	9.7

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Mol	Chain	Res	Type	RSRZ
1	A	80	ASP	9.6
1	C	767	THR	9.6
1	D	985	ARG	9.6
1	D	1012	ARG	9.6
1	B	528	ARG	9.5
1	C	672	GLU	9.5
1	A	217	LYS	9.5
1	C	780	GLU	9.5
1	C	581	LEU	9.4
1	A	153	HIS	9.4
1	B	457	GLU	9.4
1	B	291	LYS	9.4
1	B	470	SER	9.4
1	C	588	ASP	9.3
1	C	628	TYR	9.3
1	B	535	LYS	9.2
1	A	125	ARG	9.2
1	A	6	LYS	9.1
1	A	135	GLN	9.1
1	D	948	GLU	9.1
1	C	788	LYS	9.1
1	C	616	LYS	9.0
1	B	423	GLU	9.0
1	D	876	GLU	9.0
1	C	833	LEU	9.0
1	C	739	ILE	9.0
1	B	460	LEU	8.9
1	B	388	GLU	8.9
1	D	981	VAL	8.8
1	D	1053	THR	8.8
1	C	683	GLU	8.7
1	C	664	GLU	8.7
1	D	1020	LYS	8.7
1	D	1005	HIS	8.6
1	A	23	ASP	8.6
1	C	612	VAL	8.5
1	B	453	LEU	8.5
1	B	500	GLN	8.4
1	A	115	GLU	8.4
1	A	227	VAL	8.4
1	A	97	GLU	8.4
1	C	840	GLU	8.4

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Mol	Chain	Res	Type	RSRZ
1	C	826	ASP	8.4
1	B	349	LYS	8.4
1	B	507	GLU	8.4
1	B	305	ARG	8.3
1	A	161	LYS	8.3
1	D	919	ALA	8.2
1	D	881	LYS	8.2
1	D	956	GLU	8.2
1	D	952	ASP	8.2
1	B	474	CYS	8.2
1	A	159	ASP	8.2
1	B	406	GLU	8.2
1	C	637	GLU	8.2
1	B	311	ALA	8.1
1	B	508	GLU	8.1
1	C	592	GLU	8.1
1	B	318	ASP	8.1
1	A	73	LEU	8.0
1	A	182	ARG	8.0
1	B	443	ASP	8.0
1	B	402	LYS	8.0
1	A	212	GLU	7.9
1	D	976	GLU	7.9
1	A	211	ALA	7.9
1	B	363	THR	7.9
1	D	909	LEU	7.9
1	B	446	TYR	7.9
1	C	808	GLU	7.9
1	B	308	GLU	7.9
1	C	606	GLN	7.9
1	D	920	GLN	7.8
1	C	731	GLU	7.8
1	D	1062	GLN	7.7
1	C	757	LYS	7.7
1	D	991	GLU	7.7
1	A	44	VAL	7.7
1	C	690	GLU	7.7
1	D	869	ASN	7.7
1	A	146	ILE	7.7
1	A	114	GLU	7.7
1	B	496	GLU	7.7
1	A	83	ALA	7.7

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Mol	Chain	Res	Type	RSRZ
1	B	310	GLU	7.7
1	B	465	GLU	7.7
1	D	1103	LYS	7.7
1	C	829	TYR	7.6
1	C	706	GLU	7.6
1	B	352	GLN	7.6
1	A	279	ASN	7.6
1	B	532	LYS	7.5
1	A	60	TYR	7.5
1	D	1027	ASP	7.5
1	D	1058	SER	7.5
1	D	1025	GLU	7.5
1	D	1066	TYR	7.5
1	A	157	ASP	7.4
1	D	1085	LYS	7.4
1	B	529	SER	7.4
1	D	1089	THR	7.4
1	D	886	ASP	7.4
1	C	736	LYS	7.4
1	A	94	LEU	7.4
1	B	431	GLN	7.4
1	B	346	GLU	7.4
1	B	524	GLU	7.3
1	C	743	ASP	7.3
1	B	391	ALA	7.3
1	C	753	LEU	7.3
1	B	490	SER	7.3
1	C	668	ASP	7.3
1	D	963	GLN	7.3
1	D	967	GLU	7.2
1	D	964	LYS	7.2
1	D	868	GLU	7.1
1	B	522	ARG	7.1
1	A	128	LYS	7.1
1	A	254	ASP	7.1
1	C	675	ALA	7.1
1	C	624	GLU	7.1
1	D	916	LEU	7.1
1	A	51	LYS	7.1
1	A	55	ASP	7.0
1	B	298	ASP	7.0
1	A	247	THR	7.0

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Mol	Chain	Res	Type	RSRZ
1	B	343	LYS	7.0
1	B	539	ASP	7.0
1	C	692	GLU	7.0
1	D	1127	ASP	7.0
1	C	801	LYS	7.0
1	D	1039	GLU	7.0
1	B	447	GLU	6.9
1	D	872	ASP	6.9
1	C	781	LYS	6.9
1	B	553	ALA	6.9
1	D	1128	HIS	6.9
1	D	1008	GLU	6.9
1	A	37	LYS	6.9
1	B	551	TYR	6.8
1	D	1092	GLU	6.8
1	D	929	LYS	6.8
1	D	1061	ALA	6.8
1	A	122	GLU	6.8
1	A	190	CYS	6.8
1	C	678	LEU	6.8
1	D	1088	GLU	6.7
1	A	104	GLU	6.7
1	D	1065	LYS	6.7
1	A	171	ILE	6.7
1	A	24	GLU	6.7
1	D	1082	ASP	6.7
1	D	1014	TYR	6.6
1	D	1055	ASN	6.6
1	D	988	LYS	6.5
1	D	1124	GLU	6.5
1	D	897	SER	6.5
1	A	65	LYS	6.5
1	B	385	ARG	6.5
1	A	119	ALA	6.5
1	A	160	ARG	6.5
1	B	304	ASP	6.4
1	C	705	ASP	6.4
1	C	650	GLU	6.4
1	A	213	LYS	6.4
1	B	440	GLU	6.4
1	D	1078	LYS	6.4
1	A	77	LYS	6.4

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Mol	Chain	Res	Type	RSRZ
1	D	983	GLU	6.4
1	D	993	MET	6.3
1	B	329	SER	6.3
1	B	412	LYS	6.3
1	A	233	LYS	6.3
1	A	84	ASP	6.3
1	D	1028	LEU	6.3
1	D	1133	MET	6.3
1	A	184	GLU	6.2
1	B	438	ILE	6.2
1	C	673	ARG	6.2
1	D	1091	ALA	6.2
1	C	707	GLU	6.2
1	A	93	GLN	6.2
1	C	694	GLY	6.2
1	B	520	GLU	6.2
1	D	979	MET	6.1
1	C	574	LYS	6.1
1	C	762	GLU	6.1
1	C	844	HIS	6.1
1	B	466	ARG	6.0
1	A	1	MET	6.0
1	B	521	THR	6.0
1	C	619	LYS	6.0
1	B	296	LYS	6.0
1	B	325	ASP	6.0
1	B	375	ARG	5.9
1	A	236	GLU	5.9
1	B	340	GLU	5.9
1	A	205	LYS	5.8
1	D	1075	GLU	5.8
1	D	931	THR	5.8
1	B	344	TYR	5.7
1	B	415	GLU	5.7
1	D	1015	GLU	5.7
1	C	689	ASP	5.7
1	D	1081	SER	5.7
1	A	154	ILE	5.7
1	A	272	GLU	5.7
1	B	550	LYS	5.7
1	C	699	GLU	5.7
1	C	766	LYS	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	214	TYR	5.7
1	C	809	PHE	5.6
1	A	275	ASP	5.6
1	C	648	ASP	5.6
1	D	857	LYS	5.6
1	C	695	MET	5.6
1	B	555	SER	5.6
1	B	322	GLN	5.6
1	A	147	GLN	5.5
1	A	210	GLN	5.5
1	A	268	LYS	5.5
1	C	792	GLU	5.5
1	A	203	ASN	5.5
1	C	577	GLN	5.5
1	B	471	GLU	5.5
1	A	117	GLU	5.5
1	D	1117	LEU	5.4
1	B	504	LYS	5.4
1	B	505	TYR	5.4
1	A	75	GLU	5.4
1	B	339	ASP	5.4
1	C	665	GLU	5.4
1	A	148	LEU	5.4
1	A	95	PHE	5.4
1	B	538	ASP	5.3
1	D	864	LYS	5.3
1	B	464	GLU	5.3
1	C	798	ASP	5.3
1	A	129	VAL	5.3
1	A	156	GLU	5.3
1	D	1074	GLU	5.3
1	D	998	ILE	5.3
1	A	188	GLY	5.3
1	B	370	ALA	5.3
1	D	1118	LYS	5.2
1	D	1131	ASN	5.2
1	D	1041	LYS	5.2
1	C	626	ASP	5.2
1	D	853	MET	5.2
1	B	537	ILE	5.1
1	B	401	GLU	5.1
1	D	960	THR	5.1

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Mol	Chain	Res	Type	RSRZ
1	C	630	GLU	5.1
1	D	984	SER	5.1
1	D	975	SER	5.1
1	B	501	LYS	5.0
1	B	523	ALA	5.0
1	B	378	LEU	5.0
1	D	982	ILE	5.0
1	B	381	GLU	5.0
1	D	942	ARG	5.0
1	C	700	SER	5.0
1	A	98	GLU	5.0
1	B	321	LYS	5.0
1	C	691	SER	5.0
1	A	143	ILE	4.9
1	D	947	PHE	4.9
1	D	955	GLN	4.9
1	B	455	ILE	4.9
1	C	741	GLU	4.9
1	A	66	ASP	4.9
1	B	502	GLU	4.9
1	D	1125	GLU	4.9
1	B	366	GLU	4.9
1	C	669	ARG	4.9
1	C	787	ASP	4.8
1	D	1084	LEU	4.8
1	D	1071	ASP	4.8
1	C	756	GLY	4.8
1	C	777	ALA	4.8
1	A	195	GLU	4.8
1	B	303	LEU	4.8
1	A	231	LYS	4.8
1	B	536	SER	4.8
1	B	534	GLU	4.8
1	D	1094	ALA	4.8
1	A	59	LYS	4.8
1	A	193	LEU	4.8
1	B	331	GLN	4.8
1	B	357	LEU	4.8
1	C	722	ILE	4.8
1	B	320	SER	4.8
1	D	950	GLU	4.7
1	A	230	ASP	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	434	GLU	4.7
1	A	118	LYS	4.7
1	C	688	ALA	4.7
1	C	759	ALA	4.7
1	A	70	LYS	4.7
1	B	435	ALA	4.7
1	B	531	THR	4.7
1	D	918	ASP	4.6
1	A	121	ASP	4.6
1	A	250	GLU	4.6
1	C	685	GLU	4.6
1	C	778	GLN	4.6
1	A	111	GLN	4.6
1	A	120	ALA	4.6
1	B	418	ALA	4.6
1	C	836	LYS	4.6
1	A	261	TYR	4.6
1	A	174	SER	4.5
1	D	1097	SER	4.5
1	D	1123	SER	4.5
1	D	986	ALA	4.5
1	C	591	ASP	4.5
1	A	19	LEU	4.4
1	C	764	GLU	4.4
1	D	900	LYS	4.4
1	D	1067	SER	4.4
1	D	1096	ARG	4.4
1	B	516	LEU	4.4
1	A	196	GLU	4.4
1	D	1087	ALA	4.4
1	B	511	VAL	4.4
1	A	86	ALA	4.4
1	C	610	GLU	4.4
1	C	608	GLU	4.3
1	C	698	ILE	4.3
1	D	1021	LEU	4.3
1	A	110	LEU	4.3
1	C	794	LYS	4.3
1	A	209	ALA	4.3
1	B	337	THR	4.3
1	C	725	ASP	4.3
1	B	492	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	17	ASN	4.3
1	B	292	MET	4.3
1	D	969	GLU	4.2
1	D	1095	GLU	4.2
1	A	162	TYR	4.2
1	C	684	ALA	4.2
1	C	816	LYS	4.2
1	A	34	ASP	4.2
1	B	436	LYS	4.2
1	B	467	ALA	4.2
1	D	941	ASN	4.2
1	A	271	SER	4.2
1	D	978	GLY	4.1
1	B	306	ALA	4.1
1	D	972	ALA	4.1
1	C	822	ASP	4.1
1	A	257	GLU	4.1
1	A	140	LYS	4.1
1	B	422	GLU	4.1
1	A	237	THR	4.0
1	A	238	ARG	4.0
1	A	228	LEU	4.0
1	B	483	THR	4.0
1	D	1135	SER	4.0
1	A	33	GLU	4.0
1	D	1077	ILE	4.0
1	C	696	LYS	4.0
1	B	527	GLU	4.0
1	C	713	GLU	4.0
1	D	1046	GLU	4.0
1	D	1072	LYS	4.0
1	B	309	ALA	4.0
1	B	332	LYS	3.9
1	A	241	PHE	3.9
1	A	177	GLU	3.9
1	D	1063	ALA	3.9
1	B	459	ASP	3.9
1	A	126	GLY	3.9
1	B	405	ASP	3.9
1	C	825	GLU	3.9
1	A	116	ALA	3.9
1	D	855	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	1122	ILE	3.9
1	D	927	GLU	3.9
1	A	58	ASP	3.9
1	B	368	ASP	3.9
1	A	251	LYS	3.9
1	B	417	ARG	3.8
1	D	968	ALA	3.8
1	C	718	GLU	3.8
1	B	497	LYS	3.8
1	A	64	LEU	3.8
1	D	1099	THR	3.8
1	A	240	GLU	3.8
1	B	568	ILE	3.8
1	B	315	ALA	3.8
1	D	1018	ALA	3.8
1	D	1036	GLU	3.8
1	B	359	GLU	3.7
1	B	416	SER	3.7
1	A	41	ASP	3.7
1	C	661	GLN	3.7
1	B	519	ALA	3.7
1	A	278	LEU	3.7
1	D	906	GLU	3.7
1	C	573	LYS	3.7
1	C	841	GLU	3.7
1	C	677	ALA	3.7
1	A	123	SER	3.7
1	B	335	LYS	3.7
1	C	703	GLN	3.7
1	D	973	ASP	3.7
1	A	113	LEU	3.7
1	B	409	ARG	3.7
1	A	21	ARG	3.6
1	B	509	ILE	3.6
1	C	852	ILE	3.6
1	A	155	ALA	3.6
1	C	631	ALA	3.6
1	C	643	GLU	3.6
1	D	932	ASP	3.6
1	B	448	GLU	3.6
1	A	206	SER	3.6
1	B	513	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	867	LYS	3.6
1	D	1043	ALA	3.6
1	C	776	GLU	3.6
1	C	596	ASP	3.6
1	D	938	ALA	3.6
1	C	623	ASP	3.6
1	B	428	GLN	3.5
1	A	151	ALA	3.5
1	D	1121	ALA	3.5
1	D	1002	GLU	3.5
1	D	1052	VAL	3.5
1	D	1048	GLU	3.5
1	D	1060	GLU	3.5
1	C	656	LEU	3.5
1	D	1070	GLU	3.5
1	A	191	ALA	3.5
1	B	293	GLN	3.5
1	B	319	ARG	3.5
1	D	1006	ILE	3.5
1	C	657	ASN	3.5
1	D	1049	ILE	3.5
1	A	47	GLN	3.4
1	D	995	ILE	3.4
1	A	264	LYS	3.4
1	A	100	ASP	3.4
1	C	613	SER	3.4
1	C	641	LEU	3.4
1	A	29	LYS	3.4
1	D	1093	PHE	3.4
1	B	495	ALA	3.4
1	C	579	LEU	3.4
1	A	235	ALA	3.4
1	B	430	ILE	3.4
1	C	586	ALA	3.4
1	C	702	ALA	3.4
1	C	765	ILE	3.4
1	C	837	ALA	3.4
1	A	89	ASN	3.4
1	A	175	ASP	3.4
1	A	225	ILE	3.4
1	B	480	GLU	3.3
1	C	804	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	771	ASN	3.3
1	A	276	HIS	3.3
1	A	187	GLU	3.3
1	B	411	MET	3.3
1	B	313	LYS	3.3
1	D	1004	LYS	3.3
1	B	421	ASP	3.2
1	A	46	LEU	3.2
1	A	144	GLN	3.2
1	A	244	ARG	3.2
1	A	101	ARG	3.2
1	A	30	LYS	3.2
1	C	629	SER	3.2
1	C	805	THR	3.2
1	A	138	GLU	3.2
1	B	324	GLU	3.2
1	B	390	LEU	3.2
1	D	1035	ALA	3.2
1	A	62	GLU	3.2
1	D	1102	GLU	3.2
1	A	81	ALA	3.2
1	B	396	LYS	3.2
1	C	639	LEU	3.2
1	D	980	LYS	3.2
1	B	392	THR	3.2
1	B	499	SER	3.2
1	C	659	ARG	3.1
1	A	74	ALA	3.1
1	C	850	THR	3.1
1	B	503	ASP	3.1
1	C	605	LYS	3.1
1	C	709	MET	3.1
1	A	163	GLU	3.1
1	C	645	LYS	3.1
1	B	425	MET	3.1
1	B	427	ILE	3.1
1	A	201	THR	3.1
1	C	769	THR	3.1
1	C	842	LEU	3.1
1	B	382	GLU	3.1
1	A	10	MET	3.0
1	A	40	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	1003	ALA	3.0
1	D	989	ASP	3.0
1	A	53	THR	3.0
1	A	28	ASP	3.0
1	C	642	ALA	3.0
1	B	348	LEU	3.0
1	D	1059	LEU	3.0
1	B	326	GLU	2.9
1	B	543	GLU	2.9
1	A	61	SER	2.9
1	C	717	LYS	2.9
1	A	172	ILE	2.9
1	D	1007	ALA	2.9
1	D	1105	ILE	2.9
1	C	627	LYS	2.9
1	A	283	SER	2.9
1	A	124	GLU	2.9
1	A	14	ASP	2.9
1	C	655	SER	2.9
1	D	1079	VAL	2.9
1	B	533	LEU	2.9
1	C	818	GLU	2.9
1	A	63	ALA	2.9
1	A	18	ALA	2.8
1	B	439	ALA	2.8
1	D	1090	ARG	2.8
1	A	67	ALA	2.8
1	C	651	ALA	2.8
1	C	734	ALA	2.8
1	D	1101	LEU	2.8
1	D	1040	GLY	2.8
1	D	1136	ILE	2.8
1	D	934	GLU	2.8
1	C	621	THR	2.8
1	A	141	MET	2.8
1	C	770	ASN	2.8
1	D	912	TYR	2.8
1	A	52	ALA	2.8
1	B	330	LEU	2.8
1	D	1056	LEU	2.8
1	A	105	ARG	2.8
1	B	327	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	341	LEU	2.8
1	D	953	ARG	2.8
1	A	71	LEU	2.7
1	C	681	LEU	2.7
1	D	971	ALA	2.7
1	C	601	GLU	2.7
1	D	999	GLN	2.7
1	A	274	LEU	2.7
1	B	295	LEU	2.7
1	B	386	ALA	2.7
1	A	15	LYS	2.7
1	A	248	LYS	2.7
1	B	362	ALA	2.7
1	C	737	LEU	2.7
1	B	338	GLU	2.7
1	A	186	SER	2.7
1	C	660	ILE	2.7
1	B	301	ASN	2.7
1	C	654	ALA	2.7
1	B	345	SER	2.6
1	C	604	SER	2.6
1	C	609	ASP	2.6
1	B	512	LEU	2.6
1	D	987	GLN	2.6
1	C	819	LYS	2.6
1	D	1126	LEU	2.6
1	D	1114	ALA	2.6
1	C	851	SER	2.6
1	C	647	THR	2.6
1	A	255	ASP	2.6
1	B	317	GLU	2.6
1	B	506	GLU	2.6
1	A	49	LYS	2.6
1	B	336	ALA	2.6
1	A	35	ARG	2.6
1	C	633	LYS	2.6
1	A	246	VAL	2.6
1	C	745	GLU	2.6
1	A	43	LEU	2.6
1	B	489	LYS	2.6
1	D	890	GLN	2.6
1	D	1010	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	229	SER	2.5
1	C	786	GLU	2.5
1	C	580	LYS	2.5
1	D	944	ILE	2.5
1	B	389	ARG	2.5
1	A	130	ILE	2.5
1	B	302	ALA	2.5
1	B	354	LYS	2.5
1	A	25	ALA	2.5
1	B	383	LEU	2.5
1	B	393	ALA	2.5
1	C	644	LYS	2.5
1	A	281	MET	2.4
1	C	652	ASP	2.4
1	C	583	LYS	2.4
1	C	720	LYS	2.4
1	C	687	ALA	2.4
1	C	758	CYS	2.4
1	C	754	SER	2.4
1	B	515	LYS	2.4
1	B	316	ALA	2.4
1	C	625	LEU	2.4
1	A	245	SER	2.4
1	A	103	GLN	2.4
1	D	863	LEU	2.4
1	C	640	GLU	2.4
1	C	632	LEU	2.4
1	B	452	LYS	2.4
1	C	761	LEU	2.3
1	D	1073	TYR	2.3
1	A	183	ALA	2.3
1	B	376	ILE	2.3
1	C	729	LYS	2.3
1	D	1080	LEU	2.3
1	D	1038	SER	2.3
1	D	1045	LEU	2.3
1	B	526	ALA	2.3
1	B	514	ASP	2.3
1	C	666	GLU	2.3
1	A	3	ALA	2.3
1	D	1104	SER	2.2
1	A	170	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	870	ALA	2.2
1	A	88	LEU	2.2
1	B	323	LEU	2.2
1	C	835	TYR	2.2
1	C	590	ALA	2.2
1	C	839	SER	2.2
1	C	680	LYS	2.2
1	C	615	GLN	2.2
1	C	782	TYR	2.2
1	B	540	LEU	2.2
1	A	108	THR	2.2
1	C	597	LYS	2.2
1	B	407	SER	2.2
1	D	1098	VAL	2.2
1	A	232	LEU	2.2
1	D	1034	ARG	2.2
1	A	32	ALA	2.2
1	C	635	ALA	2.2
1	D	874	ALA	2.2
1	D	961	ALA	2.2
1	C	772	LEU	2.2
1	C	775	LEU	2.2
1	A	131	GLU	2.2
1	C	749	GLU	2.2
1	B	299	LYS	2.1
1	A	102	ALA	2.1
1	B	561	ALA	2.1
1	B	286	ASP	2.1
1	B	413	VAL	2.1
1	C	569	MET	2.1
1	D	996	GLN	2.1
1	A	134	ALA	2.1
1	B	347	ALA	2.1
1	B	312	ASP	2.1
1	D	992	LYS	2.1
1	B	517	LYS	2.1
1	D	1108	LEU	2.1
1	B	530	VAL	2.1
1	C	846	LEU	2.1
1	A	221	TYR	2.1
1	D	911	LYS	2.1
1	D	962	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	351	ALA	2.1
1	D	1100	LYS	2.1
1	A	199	THR	2.1
1	B	441	ASP	2.1
1	A	39	LEU	2.0
1	A	207	LEU	2.0
1	A	243	GLU	2.0
1	C	760	GLU	2.0
1	D	1129	ALA	2.0
1	B	369	VAL	2.0
1	C	587	LEU	2.0

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 monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.