



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 04:15 AM UTC

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

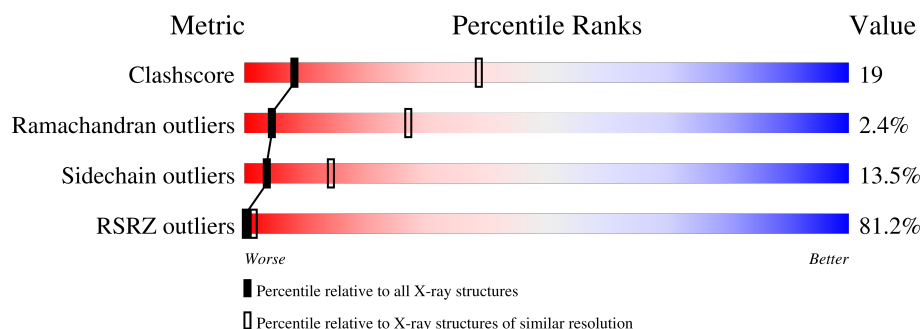
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	1007 (9.70-4.04)
Ramachandran outliers	187476	1054 (10.00-4.00)
Sidechain outliers	187428	1017 (10.00-4.00)
RSRZ outliers	180081	1161 (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	83% 53% 30% 12% 6%
1	B	284	86% 60% 26% 11% •
1	C	284	76% 53% 29% 14% 5%
1	D	284	80% 54% 26% 15% •

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.

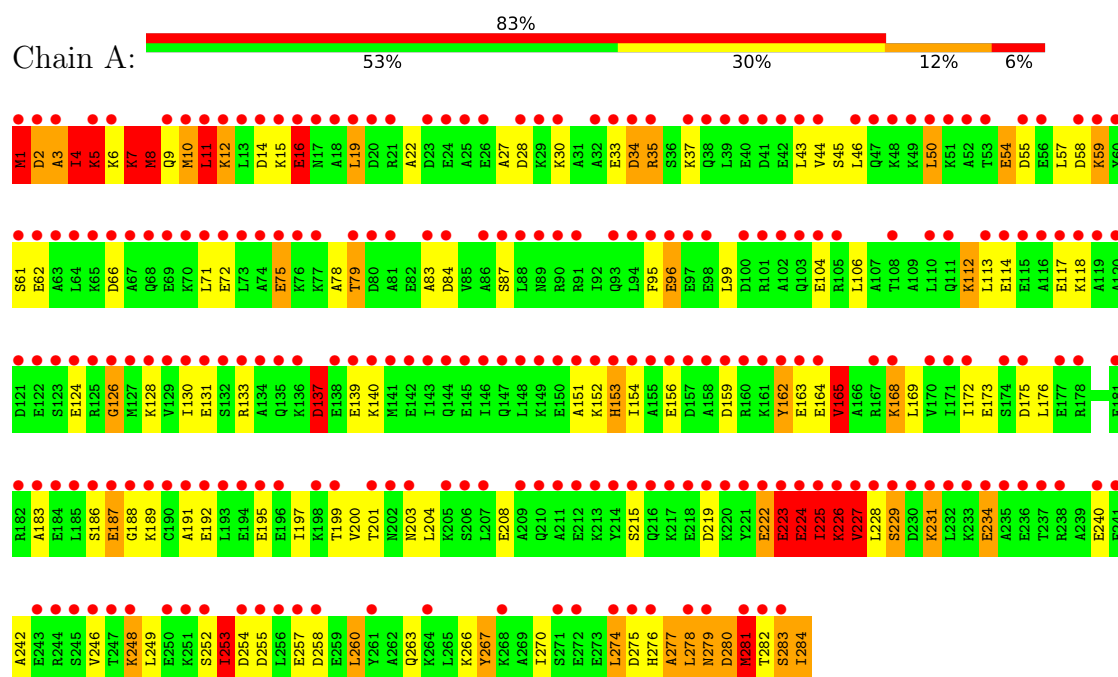
- Molecule 1 is a protein called TROPOMYOSIN.

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			

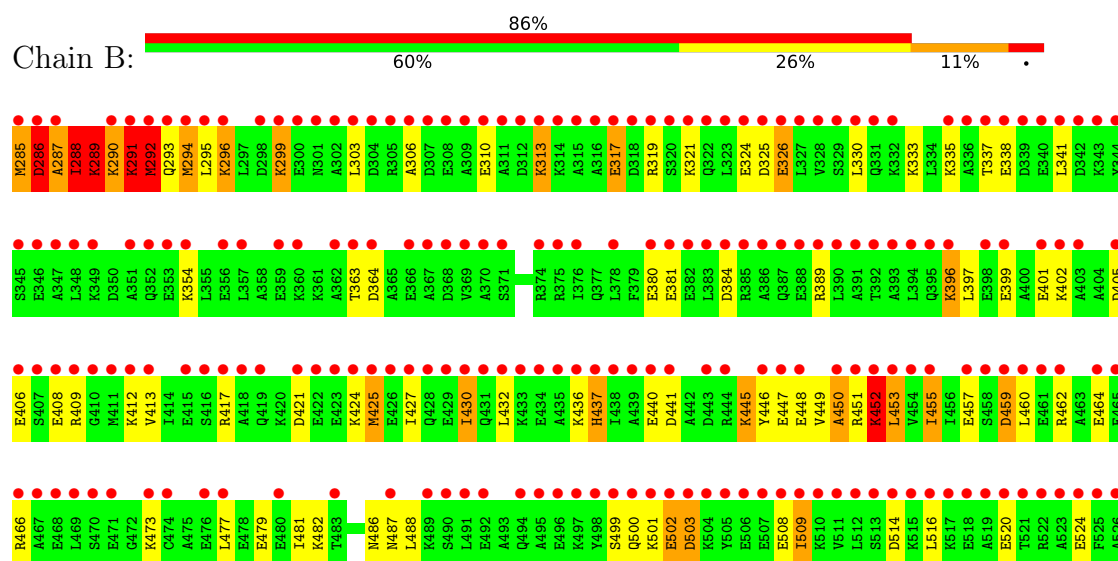
3 Residue-property plots

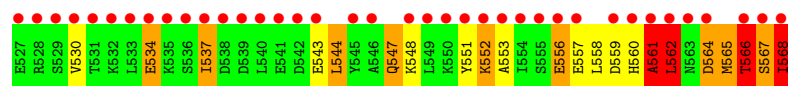
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

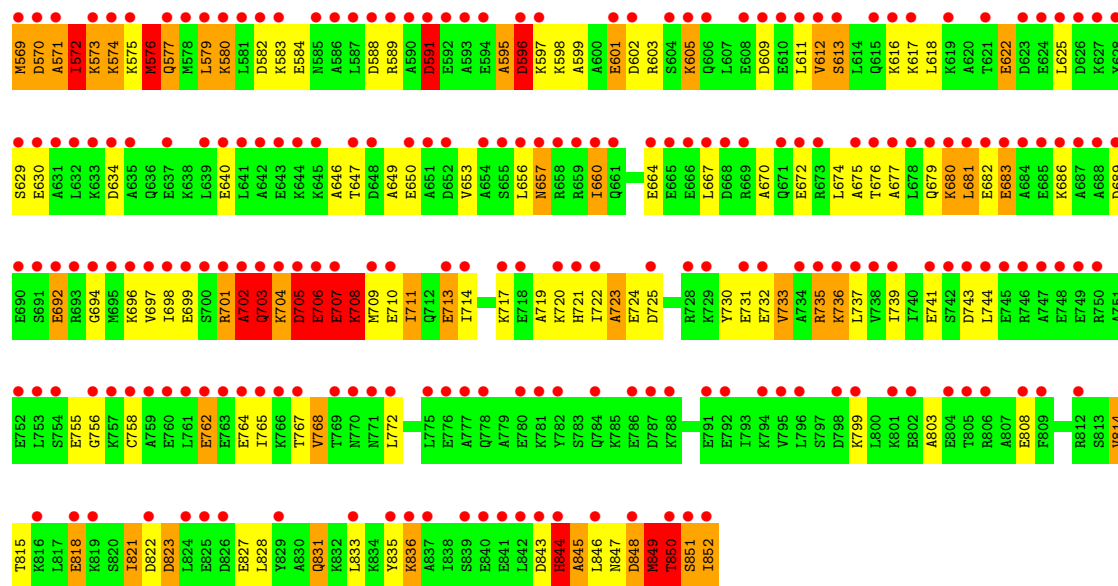
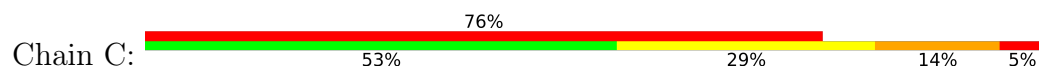


• Molecule 1: TROPOMYOSIN

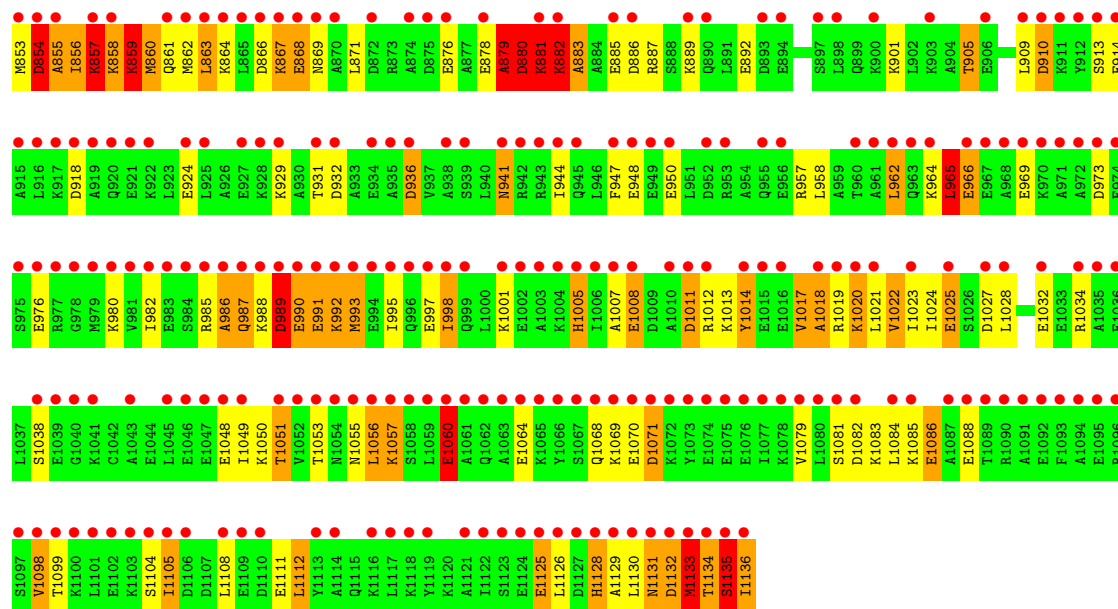
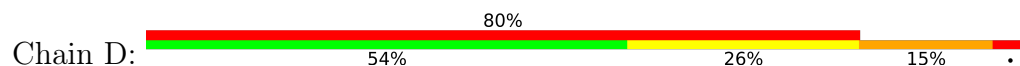




● Molecule 1: TROPOMYOSIN



● 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	40
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%)	4	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%)	6	20
1	C	245/245 (100%)	213 (87%)	32 (13%)	4	15
1	D	245/245 (100%)	212 (86%)	33 (14%)	4	14
All	All	980/980 (100%)	848 (86%)	132 (14%)	4	14

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%)	6.51	236 (83%) 0 1	174, 174, 174, 174	0
1	B	284/284 (100%)	6.81	245 (86%) 0 1	174, 174, 174, 174	0
1	C	284/284 (100%)	5.53	215 (75%) 0 2	174, 174, 174, 174	0
1	D	284/284 (100%)	6.34	226 (79%) 0 1	174, 174, 174, 174	0
All	All	1136/1136 (100%)	6.30	922 (81%) 0 1	174, 174, 174, 174	0

All (922) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	223	GLU	42.9
1	D	1134	THR	40.9
1	C	682	GLU	38.3
1	A	2	ASP	32.8
1	B	395	GLN	30.3
1	A	216	GLN	30.2
1	B	560	HIS	30.2
1	A	219	ASP	29.6
1	B	353	GLU	29.0
1	B	541	GLU	28.3
1	D	910	ASP	28.2
1	D	922	LYS	26.5
1	D	913	SER	26.0
1	C	585	ASN	25.3
1	A	220	LYS	25.0
1	C	791	GLU	25.0
1	A	20	ASP	24.9
1	D	1019	ARG	24.9
1	C	763	GLU	24.4
1	A	9	GLN	24.3
1	B	374	ARG	24.2

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Mol	Chain	Res	Type	RSRZ
1	D	1047	GLU	24.2
1	C	578	MET	23.5
1	A	215	SER	23.1
1	D	1016	GLU	22.8
1	B	451	ARG	22.6
1	C	784	GLN	22.5
1	D	921	GLU	22.4
1	B	563	ASN	22.4
1	A	16	GLU	22.1
1	C	701	ARG	21.6
1	A	198	LYS	21.5
1	A	56	GLU	21.0
1	A	222	GLU	20.6
1	C	693	ARG	20.4
1	D	861	GLN	20.3
1	A	12	LYS	20.3
1	A	5	LYS	20.1
1	C	582	ASP	20.1
1	D	854	ASP	20.0
1	D	1064	GLU	19.6
1	B	437	HIS	19.6
1	C	750	ARG	19.5
1	A	90	ARG	19.5
1	B	557	GLU	19.5
1	D	977	ARG	19.4
1	D	893	ASP	19.4
1	C	752	GLU	19.4
1	D	858	LYS	19.2
1	B	556	GLU	19.1
1	B	454	VAL	19.0
1	D	889	LYS	18.9
1	B	545	TYR	18.8
1	D	917	LYS	18.8
1	A	202	ASN	18.8
1	B	498	TYR	18.7
1	C	812	ARG	18.6
1	B	367	ALA	18.6
1	A	181	GLU	18.5
1	C	697	VAL	18.3
1	A	79	THR	18.1
1	B	494	GLN	18.0
1	C	571	ALA	17.9

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Mol	Chain	Res	Type	RSRZ
1	D	945	GLN	17.9
1	C	570	ASP	17.6
1	B	552	LYS	17.5
1	B	487	ASN	17.2
1	A	136	LYS	17.2
1	B	462	ARG	17.1
1	C	686	LYS	17.1
1	A	282	THR	17.1
1	B	549	LEU	17.0
1	B	567	SER	16.9
1	B	360	LYS	16.9
1	B	444	ARG	16.8
1	A	185	LEU	16.5
1	A	218	GLU	16.4
1	B	564	ASP	16.3
1	C	658	ARG	16.3
1	D	1110	ASP	16.2
1	D	885	GLU	16.0
1	B	559	ASP	15.8
1	A	69	GLU	15.7
1	B	429	GLU	15.6
1	B	294	MET	15.6
1	C	671	GLN	15.6
1	B	548	LYS	15.6
1	B	399	GLU	15.6
1	D	865	LEU	15.5
1	D	939	SER	15.5
1	C	710	GLU	15.4
1	D	1011	ASP	15.2
1	D	974	GLU	15.2
1	A	132	SER	14.9
1	B	398	GLU	14.9
1	B	394	LEU	14.9
1	D	928	LYS	14.9
1	C	589	ARG	14.8
1	B	461	GLU	14.8
1	A	152	LYS	14.8
1	C	575	LYS	14.8
1	D	943	ARG	14.7
1	B	287	ALA	14.7
1	A	13	LEU	14.7
1	B	546	ALA	14.7

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Mol	Chain	Res	Type	RSRZ
1	C	728	ARG	14.7
1	A	194	GLU	14.6
1	C	746	ARG	14.4
1	A	48	LYS	14.4
1	B	307	ASP	14.2
1	D	970	LYS	14.2
1	A	68	GLN	14.2
1	D	935	ALA	14.1
1	A	76	LYS	14.1
1	A	149	LYS	14.1
1	D	924	GLU	14.0
1	C	806	ARG	14.0
1	C	735	ARG	14.0
1	C	714	ILE	13.9
1	D	1068	GLN	13.9
1	A	145	GLU	13.8
1	D	1054	ASN	13.8
1	D	1106	ASP	13.7
1	B	468	GLU	13.6
1	B	356	GLU	13.6
1	C	721	HIS	13.5
1	B	419	GLN	13.4
1	A	189	LYS	13.4
1	A	168	LYS	13.3
1	A	164	GLU	13.3
1	A	192	GLU	13.2
1	A	139	GLU	13.2
1	D	997	GLU	13.2
1	D	1130	LEU	13.2
1	C	799	LYS	13.1
1	D	994	GLU	12.9
1	B	371	SER	12.9
1	D	1023	ILE	12.9
1	B	408	GLU	12.8
1	C	679	GLN	12.8
1	B	433	LYS	12.8
1	D	1001	LYS	12.8
1	B	469	LEU	12.7
1	C	617	LYS	12.7
1	B	364	ASP	12.6
1	D	966	GLU	12.6
1	A	178	ARG	12.5

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Mol	Chain	Res	Type	RSRZ
1	A	133	ARG	12.5
1	A	142	GLU	12.4
1	B	525	PHE	12.4
1	A	226	LYS	12.3
1	B	473	LYS	12.3
1	B	384	ASP	12.3
1	A	224	GLU	12.1
1	C	795	VAL	12.1
1	B	491	LEU	12.1
1	A	72	GLU	12.1
1	D	990	GLU	12.1
1	D	1032	GLU	12.0
1	A	91	ARG	12.0
1	D	914	GLU	12.0
1	B	458	SER	11.9
1	D	949	GLU	11.9
1	B	300	GLU	11.8
1	D	878	GLU	11.8
1	D	1051	THR	11.7
1	B	566	THR	11.7
1	B	426	GLU	11.7
1	D	882	LYS	11.7
1	B	450	ALA	11.6
1	B	290	LYS	11.6
1	C	802	GLU	11.6
1	B	542	ASP	11.5
1	B	387	GLN	11.5
1	D	915	ALA	11.4
1	A	87	SER	11.4
1	B	518	GLU	11.4
1	D	1057	LYS	11.3
1	C	732	GLU	11.3
1	A	26	GLU	11.3
1	D	862	MET	11.1
1	A	167	ARG	11.1
1	C	704	LYS	11.0
1	B	314	LYS	11.0
1	D	925	LEU	11.0
1	B	380	GLU	11.0
1	A	258	ASP	10.9
1	D	985	ARG	10.9
1	D	1012	ARG	10.9

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Mol	Chain	Res	Type	RSRZ
1	B	528	ARG	10.9
1	A	80	ASP	10.8
1	C	748	GLU	10.8
1	A	217	LYS	10.7
1	A	150	GLU	10.7
1	C	767	THR	10.7
1	B	291	LYS	10.6
1	C	672	GLU	10.5
1	C	588	ASP	10.5
1	A	153	HIS	10.5
1	C	780	GLU	10.4
1	A	125	ARG	10.4
1	B	457	GLU	10.4
1	B	535	LYS	10.3
1	C	581	LEU	10.3
1	A	6	LYS	10.3
1	C	788	LYS	10.2
1	A	135	GLN	10.2
1	C	616	LYS	10.2
1	B	470	SER	10.2
1	C	628	TYR	10.1
1	D	948	GLU	10.0
1	B	423	GLU	10.0
1	D	876	GLU	9.9
1	B	388	GLU	9.8
1	C	833	LEU	9.8
1	C	739	ILE	9.8
1	D	1020	LYS	9.8
1	D	1053	THR	9.7
1	D	981	VAL	9.7
1	B	460	LEU	9.7
1	A	23	ASP	9.7
1	C	683	GLU	9.6
1	D	1005	HIS	9.6
1	C	664	GLU	9.6
1	B	305	ARG	9.5
1	C	826	ASP	9.5
1	B	349	LYS	9.4
1	B	500	GLN	9.4
1	C	612	VAL	9.4
1	A	161	LYS	9.4
1	A	115	GLU	9.3

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Mol	Chain	Res	Type	RSRZ
1	B	453	LEU	9.3
1	A	97	GLU	9.3
1	A	227	VAL	9.3
1	C	840	GLU	9.3
1	D	881	LYS	9.3
1	B	507	GLU	9.2
1	D	952	ASP	9.2
1	A	159	ASP	9.2
1	D	919	ALA	9.1
1	A	182	ARG	9.1
1	B	318	ASP	9.1
1	D	956	GLU	9.1
1	B	311	ALA	9.0
1	B	406	GLU	9.0
1	C	637	GLU	9.0
1	B	402	LYS	9.0
1	B	443	ASP	9.0
1	B	508	GLU	9.0
1	C	592	GLU	9.0
1	A	211	ALA	8.8
1	B	363	THR	8.8
1	C	606	GLN	8.8
1	A	212	GLU	8.8
1	D	976	GLU	8.8
1	D	920	GLN	8.8
1	A	73	LEU	8.7
1	C	757	LYS	8.7
1	C	808	GLU	8.7
1	B	308	GLU	8.7
1	D	1062	GLN	8.7
1	D	1103	LYS	8.7
1	D	909	LEU	8.6
1	C	731	GLU	8.6
1	B	446	TYR	8.6
1	D	991	GLU	8.6
1	B	474	CYS	8.5
1	C	690	GLU	8.5
1	A	44	VAL	8.5
1	A	83	ALA	8.5
1	B	532	LYS	8.5
1	A	114	GLU	8.5
1	B	496	GLU	8.5

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Mol	Chain	Res	Type	RSRZ
1	B	352	GLN	8.5
1	B	310	GLU	8.5
1	B	465	GLU	8.5
1	D	1027	ASP	8.5
1	D	1085	LYS	8.4
1	A	146	ILE	8.4
1	A	157	ASP	8.4
1	C	706	GLU	8.4
1	C	736	LYS	8.4
1	D	886	ASP	8.4
1	D	869	ASN	8.3
1	B	431	GLN	8.3
1	D	1025	GLU	8.3
1	C	829	TYR	8.3
1	D	1089	THR	8.3
1	C	743	ASP	8.2
1	C	668	ASP	8.2
1	A	60	TYR	8.2
1	B	346	GLU	8.2
1	D	964	LYS	8.2
1	B	522	ARG	8.2
1	D	963	GLN	8.1
1	A	279	ASN	8.1
1	D	1058	SER	8.1
1	D	1066	TYR	8.1
1	B	391	ALA	8.1
1	B	524	GLU	8.1
1	B	529	SER	8.1
1	A	128	LYS	8.1
1	A	94	LEU	8.1
1	A	254	ASP	8.0
1	A	51	LYS	8.0
1	D	967	GLU	8.0
1	A	55	ASP	8.0
1	B	298	ASP	8.0
1	C	753	LEU	7.9
1	C	675	ALA	7.9
1	B	343	LYS	7.9
1	D	868	GLU	7.9
1	B	539	ASP	7.9
1	C	801	LYS	7.9
1	B	490	SER	7.9

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Mol	Chain	Res	Type	RSRZ
1	D	1127	ASP	7.9
1	C	624	GLU	7.9
1	C	781	LYS	7.8
1	D	872	ASP	7.8
1	A	247	THR	7.8
1	A	37	LYS	7.8
1	D	916	LEU	7.8
1	C	692	GLU	7.7
1	D	1039	GLU	7.7
1	B	447	GLU	7.7
1	D	929	LYS	7.7
1	B	553	ALA	7.7
1	D	1128	HIS	7.7
1	D	1008	GLU	7.6
1	D	1065	LYS	7.6
1	D	1092	GLU	7.6
1	D	1061	ALA	7.6
1	D	1082	ASP	7.5
1	A	122	GLU	7.5
1	D	1088	GLU	7.5
1	B	385	ARG	7.5
1	B	551	TYR	7.5
1	A	104	GLU	7.4
1	D	988	LYS	7.4
1	A	160	ARG	7.4
1	A	65	LYS	7.4
1	C	678	LEU	7.4
1	A	24	GLU	7.4
1	A	213	LYS	7.3
1	A	171	ILE	7.3
1	B	304	ASP	7.3
1	C	705	ASP	7.3
1	D	1078	LYS	7.3
1	A	119	ALA	7.3
1	D	1124	GLU	7.2
1	A	77	LYS	7.2
1	D	1014	TYR	7.2
1	B	412	LYS	7.1
1	C	673	ARG	7.1
1	C	650	GLU	7.1
1	A	233	LYS	7.1
1	B	440	GLU	7.1

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Mol	Chain	Res	Type	RSRZ
1	A	84	ASP	7.1
1	D	897	SER	7.1
1	A	190	CYS	7.1
1	D	1055	ASN	7.1
1	D	983	GLU	7.1
1	A	93	GLN	7.0
1	D	1091	ALA	6.9
1	A	184	GLU	6.9
1	C	574	LYS	6.9
1	B	466	ARG	6.9
1	C	707	GLU	6.9
1	B	329	SER	6.9
1	D	1028	LEU	6.9
1	C	694	GLY	6.8
1	B	520	GLU	6.8
1	B	438	ILE	6.8
1	B	375	ARG	6.8
1	C	619	LYS	6.8
1	D	993	MET	6.8
1	B	296	LYS	6.8
1	C	844	HIS	6.8
1	B	325	ASP	6.7
1	C	762	GLU	6.7
1	D	1133	MET	6.7
1	B	521	THR	6.7
1	A	205	LYS	6.6
1	A	236	GLU	6.6
1	D	979	MET	6.6
1	B	340	GLU	6.5
1	A	1	MET	6.5
1	C	689	ASP	6.5
1	B	550	LYS	6.5
1	C	766	LYS	6.4
1	D	931	THR	6.4
1	D	1075	GLU	6.4
1	A	275	ASP	6.4
1	D	857	LYS	6.4
1	C	648	ASP	6.4
1	B	415	GLU	6.4
1	D	1015	GLU	6.4
1	A	272	GLU	6.3
1	C	699	GLU	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	268	LYS	6.3
1	B	322	GLN	6.3
1	B	344	TYR	6.3
1	A	147	GLN	6.2
1	A	210	GLN	6.2
1	A	154	ILE	6.2
1	D	1081	SER	6.2
1	C	577	GLN	6.2
1	A	214	TYR	6.2
1	B	504	LYS	6.2
1	C	792	GLU	6.1
1	B	339	ASP	6.1
1	B	471	GLU	6.1
1	D	864	LYS	6.1
1	B	555	SER	6.1
1	A	117	GLU	6.1
1	B	538	ASP	6.1
1	C	809	PHE	6.1
1	C	798	ASP	6.1
1	C	695	MET	6.0
1	A	75	GLU	6.0
1	C	665	GLU	6.0
1	D	1117	LEU	6.0
1	A	203	ASN	6.0
1	D	1118	LYS	6.0
1	B	464	GLU	5.9
1	A	129	VAL	5.9
1	A	156	GLU	5.9
1	D	1074	GLU	5.9
1	B	505	TYR	5.9
1	D	1041	LYS	5.9
1	A	148	LEU	5.9
1	B	370	ALA	5.9
1	C	626	ASP	5.9
1	A	188	GLY	5.9
1	D	998	ILE	5.8
1	A	95	PHE	5.8
1	D	942	ARG	5.8
1	B	501	LYS	5.7
1	D	960	THR	5.7
1	B	401	GLU	5.7
1	C	630	GLU	5.7

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Mol	Chain	Res	Type	RSRZ
1	B	321	LYS	5.7
1	B	537	ILE	5.7
1	D	1131	ASN	5.6
1	B	523	ALA	5.6
1	C	669	ARG	5.6
1	A	66	ASP	5.6
1	D	984	SER	5.6
1	D	955	GLN	5.6
1	B	381	GLU	5.6
1	D	853	MET	5.6
1	A	98	GLU	5.6
1	D	975	SER	5.5
1	C	787	ASP	5.5
1	B	378	LEU	5.5
1	D	1071	ASP	5.5
1	D	982	ILE	5.5
1	C	741	GLU	5.5
1	A	231	LYS	5.5
1	B	502	GLU	5.5
1	D	1125	GLU	5.5
1	A	59	LYS	5.5
1	B	366	GLU	5.5
1	C	700	SER	5.4
1	A	143	ILE	5.4
1	C	691	SER	5.4
1	C	777	ALA	5.4
1	B	455	ILE	5.4
1	B	331	GLN	5.4
1	A	230	ASP	5.4
1	A	195	GLU	5.4
1	C	756	GLY	5.4
1	D	1094	ALA	5.4
1	A	118	LYS	5.4
1	A	70	LYS	5.3
1	B	534	GLU	5.3
1	D	1084	LEU	5.3
1	D	947	PHE	5.3
1	D	950	GLU	5.3
1	B	303	LEU	5.3
1	D	918	ASP	5.3
1	A	121	ASP	5.3
1	C	688	ALA	5.3

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Mol	Chain	Res	Type	RSRZ
1	C	759	ALA	5.3
1	B	434	GLU	5.3
1	A	193	LEU	5.3
1	B	435	ALA	5.2
1	B	357	LEU	5.2
1	B	536	SER	5.2
1	C	722	ILE	5.2
1	B	531	THR	5.2
1	C	836	LYS	5.2
1	C	778	GLN	5.2
1	B	320	SER	5.2
1	A	111	GLN	5.2
1	A	250	GLU	5.1
1	C	685	GLU	5.1
1	A	120	ALA	5.1
1	B	418	ALA	5.1
1	C	591	ASP	5.1
1	D	1096	ARG	5.1
1	D	900	LYS	5.1
1	D	986	ALA	5.0
1	A	261	TYR	5.0
1	A	174	SER	5.0
1	D	1097	SER	5.0
1	C	794	LYS	5.0
1	C	764	GLU	4.9
1	D	1123	SER	4.9
1	D	1087	ALA	4.9
1	A	86	ALA	4.9
1	A	196	GLU	4.9
1	C	725	ASP	4.9
1	A	19	LEU	4.9
1	B	511	VAL	4.9
1	C	610	GLU	4.9
1	A	209	ALA	4.8
1	C	608	GLU	4.8
1	D	1067	SER	4.8
1	B	337	THR	4.8
1	B	516	LEU	4.8
1	C	816	LYS	4.8
1	B	492	GLU	4.8
1	B	436	LYS	4.8
1	D	1021	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	698	ILE	4.8
1	A	34	ASP	4.8
1	A	110	LEU	4.8
1	D	969	GLU	4.7
1	C	684	ALA	4.7
1	D	1095	GLU	4.7
1	B	467	ALA	4.7
1	A	238	ARG	4.7
1	C	822	ASP	4.7
1	A	140	LYS	4.7
1	B	306	ALA	4.7
1	D	972	ALA	4.7
1	A	17	ASN	4.6
1	A	162	TYR	4.6
1	D	978	GLY	4.6
1	B	292	MET	4.6
1	C	696	LYS	4.6
1	A	257	GLU	4.6
1	A	271	SER	4.6
1	A	237	THR	4.6
1	D	1072	LYS	4.6
1	B	422	GLU	4.6
1	B	483	THR	4.5
1	B	332	LYS	4.5
1	D	941	ASN	4.5
1	A	33	GLU	4.5
1	B	459	ASP	4.5
1	B	405	ASP	4.5
1	B	417	ARG	4.5
1	B	527	GLU	4.5
1	C	713	GLU	4.5
1	B	309	ALA	4.5
1	A	228	LEU	4.5
1	D	1046	GLU	4.5
1	A	251	LYS	4.4
1	D	1063	ALA	4.4
1	D	1077	ILE	4.4
1	A	58	ASP	4.4
1	B	368	ASP	4.4
1	A	177	GLU	4.4
1	D	1135	SER	4.4
1	A	116	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	855	ALA	4.4
1	B	497	LYS	4.4
1	A	126	GLY	4.4
1	C	825	GLU	4.4
1	D	927	GLU	4.4
1	D	968	ALA	4.3
1	C	718	GLU	4.3
1	D	1099	THR	4.3
1	D	1122	ILE	4.3
1	A	41	ASP	4.3
1	A	240	GLU	4.3
1	C	661	GLN	4.3
1	A	241	PHE	4.3
1	B	315	ALA	4.3
1	B	409	ARG	4.3
1	D	1018	ALA	4.3
1	C	573	LYS	4.3
1	A	21	ARG	4.2
1	B	335	LYS	4.2
1	A	64	LEU	4.2
1	D	1036	GLU	4.2
1	B	519	ALA	4.2
1	B	359	GLU	4.2
1	D	973	ASP	4.2
1	C	703	GLN	4.2
1	B	568	ILE	4.2
1	C	677	ALA	4.2
1	D	906	GLU	4.2
1	D	867	LYS	4.2
1	D	932	ASP	4.2
1	C	841	GLU	4.1
1	A	278	LEU	4.1
1	B	416	SER	4.1
1	A	155	ALA	4.1
1	C	631	ALA	4.1
1	C	596	ASP	4.1
1	C	623	ASP	4.1
1	C	643	GLU	4.1
1	B	448	GLU	4.1
1	A	113	LEU	4.1
1	D	1043	ALA	4.1
1	B	428	GLN	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	123	SER	4.1
1	B	319	ARG	4.1
1	D	938	ALA	4.0
1	C	776	GLU	4.0
1	B	509	ILE	4.0
1	C	852	ILE	4.0
1	A	151	ALA	4.0
1	D	1121	ALA	4.0
1	D	1002	GLU	4.0
1	B	293	GLN	4.0
1	A	264	LYS	4.0
1	A	206	SER	4.0
1	B	513	SER	4.0
1	D	1052	VAL	4.0
1	A	191	ALA	4.0
1	D	1048	GLU	3.9
1	D	1060	GLU	3.9
1	A	47	GLN	3.9
1	A	100	ASP	3.9
1	D	1070	GLU	3.9
1	A	29	LYS	3.9
1	C	656	LEU	3.9
1	A	175	ASP	3.9
1	D	1006	ILE	3.9
1	B	495	ALA	3.8
1	D	1049	ILE	3.8
1	A	235	ALA	3.8
1	C	586	ALA	3.8
1	C	702	ALA	3.8
1	C	837	ALA	3.8
1	D	995	ILE	3.8
1	C	657	ASN	3.8
1	A	244	ARG	3.8
1	B	313	LYS	3.8
1	C	613	SER	3.8
1	C	641	LEU	3.8
1	A	101	ARG	3.8
1	D	1004	LYS	3.8
1	C	579	LEU	3.8
1	B	430	ILE	3.8
1	C	765	ILE	3.8
1	B	480	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	804	GLU	3.8
1	A	225	ILE	3.7
1	A	276	HIS	3.7
1	B	421	ASP	3.7
1	A	30	LYS	3.7
1	A	144	GLN	3.7
1	A	187	GLU	3.7
1	A	89	ASN	3.7
1	C	659	ARG	3.7
1	D	1093	PHE	3.7
1	B	396	LYS	3.7
1	D	980	LYS	3.7
1	C	805	THR	3.7
1	C	771	ASN	3.6
1	C	605	LYS	3.6
1	A	138	GLU	3.6
1	B	324	GLU	3.6
1	D	1035	ALA	3.6
1	B	503	ASP	3.6
1	A	46	LEU	3.6
1	A	81	ALA	3.6
1	B	392	THR	3.6
1	A	62	GLU	3.6
1	D	1102	GLU	3.6
1	C	645	LYS	3.6
1	A	74	ALA	3.6
1	C	850	THR	3.6
1	B	390	LEU	3.6
1	B	411	MET	3.6
1	C	629	SER	3.6
1	C	639	LEU	3.5
1	D	989	ASP	3.5
1	A	163	GLU	3.5
1	B	499	SER	3.5
1	A	201	THR	3.5
1	C	769	THR	3.5
1	B	382	GLU	3.5
1	D	1003	ALA	3.5
1	A	28	ASP	3.4
1	A	40	GLU	3.4
1	A	53	THR	3.4
1	B	427	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	842	LEU	3.4
1	C	717	LYS	3.4
1	C	709	MET	3.4
1	C	642	ALA	3.4
1	C	627	LYS	3.4
1	D	1090	ARG	3.4
1	B	425	MET	3.4
1	B	326	GLU	3.3
1	B	543	GLU	3.3
1	A	14	ASP	3.3
1	D	1007	ALA	3.3
1	A	10	MET	3.3
1	B	348	LEU	3.3
1	D	1059	LEU	3.3
1	A	124	GLU	3.3
1	A	63	ALA	3.3
1	A	105	ARG	3.3
1	D	1079	VAL	3.3
1	A	172	ILE	3.3
1	C	818	GLU	3.3
1	A	18	ALA	3.3
1	B	439	ALA	3.3
1	D	953	ARG	3.3
1	A	61	SER	3.3
1	D	1105	ILE	3.3
1	A	67	ALA	3.2
1	C	651	ALA	3.2
1	C	734	ALA	3.2
1	B	533	LEU	3.2
1	A	283	SER	3.2
1	C	621	THR	3.2
1	C	655	SER	3.2
1	D	934	GLU	3.2
1	D	1040	GLY	3.2
1	A	52	ALA	3.2
1	D	1101	LEU	3.2
1	A	15	LYS	3.2
1	A	248	LYS	3.2
1	D	1136	ILE	3.2
1	D	999	GLN	3.1
1	D	912	TYR	3.1
1	D	971	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	330	LEU	3.1
1	D	1056	LEU	3.1
1	B	386	ALA	3.1
1	B	327	LEU	3.1
1	B	341	LEU	3.1
1	C	601	GLU	3.1
1	C	770	ASN	3.1
1	B	362	ALA	3.1
1	A	71	LEU	3.1
1	A	141	MET	3.1
1	C	819	LYS	3.1
1	C	681	LEU	3.1
1	A	35	ARG	3.1
1	B	338	GLU	3.1
1	C	609	ASP	3.1
1	A	49	LYS	3.1
1	D	987	GLN	3.0
1	A	274	LEU	3.0
1	B	295	LEU	3.0
1	C	654	ALA	3.0
1	C	737	LEU	3.0
1	A	255	ASP	3.0
1	C	633	LYS	3.0
1	B	489	LYS	3.0
1	C	660	ILE	3.0
1	D	1114	ALA	3.0
1	A	186	SER	3.0
1	B	389	ARG	3.0
1	C	647	THR	3.0
1	B	336	ALA	3.0
1	C	580	LYS	3.0
1	B	317	GLU	3.0
1	B	506	GLU	3.0
1	D	890	GLN	3.0
1	B	512	LEU	3.0
1	B	301	ASN	3.0
1	B	354	LYS	3.0
1	D	1126	LEU	2.9
1	B	345	SER	2.9
1	C	604	SER	2.9
1	D	1010	ALA	2.9
1	A	246	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	745	GLU	2.9
1	C	851	SER	2.9
1	C	786	GLU	2.9
1	C	644	LYS	2.9
1	A	43	LEU	2.9
1	B	302	ALA	2.9
1	C	583	LYS	2.9
1	A	25	ALA	2.9
1	C	720	LYS	2.9
1	C	652	ASP	2.9
1	D	944	ILE	2.8
1	B	393	ALA	2.8
1	A	229	SER	2.8
1	A	130	ILE	2.8
1	B	515	LYS	2.8
1	B	383	LEU	2.8
1	C	687	ALA	2.8
1	B	452	LYS	2.8
1	A	103	GLN	2.8
1	B	316	ALA	2.8
1	C	729	LYS	2.7
1	C	640	GLU	2.7
1	C	754	SER	2.7
1	A	281	MET	2.7
1	C	625	LEU	2.7
1	A	183	ALA	2.7
1	B	514	ASP	2.7
1	D	863	LEU	2.7
1	C	632	LEU	2.7
1	A	245	SER	2.7
1	C	761	LEU	2.7
1	B	526	ALA	2.6
1	D	1073	TYR	2.6
1	B	376	ILE	2.6
1	C	680	LYS	2.6
1	D	1080	LEU	2.6
1	A	3	ALA	2.6
1	C	758	CYS	2.6
1	C	666	GLU	2.6
1	D	1045	LEU	2.6
1	C	597	LYS	2.6
1	D	870	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	1034	ARG	2.6
1	D	1038	SER	2.6
1	C	615	GLN	2.6
1	A	170	VAL	2.6
1	C	590	ALA	2.6
1	B	299	LYS	2.5
1	A	108	THR	2.5
1	A	88	LEU	2.5
1	B	323	LEU	2.5
1	C	835	TYR	2.5
1	D	992	LYS	2.5
1	D	1104	SER	2.5
1	B	286	ASP	2.5
1	B	517	LYS	2.5
1	D	1098	VAL	2.5
1	A	32	ALA	2.5
1	C	635	ALA	2.5
1	C	839	SER	2.5
1	D	874	ALA	2.5
1	D	961	ALA	2.5
1	D	996	GLN	2.5
1	B	312	ASP	2.5
1	C	782	TYR	2.5
1	B	540	LEU	2.5
1	A	102	ALA	2.5
1	B	561	ALA	2.5
1	A	131	GLU	2.5
1	C	749	GLU	2.5
1	D	911	LYS	2.5
1	A	134	ALA	2.5
1	B	347	ALA	2.5
1	D	1100	LYS	2.5
1	A	232	LEU	2.5
1	B	413	VAL	2.5
1	C	772	LEU	2.4
1	C	775	LEU	2.4
1	B	407	SER	2.4
1	B	441	ASP	2.4
1	B	530	VAL	2.4
1	B	351	ALA	2.4
1	A	199	THR	2.4
1	D	1108	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	846	LEU	2.4
1	A	221	TYR	2.4
1	C	569	MET	2.4
1	D	962	LEU	2.4
1	D	1069	LYS	2.4
1	D	1129	ALA	2.3
1	A	243	GLU	2.3
1	C	760	GLU	2.3
1	B	369	VAL	2.3
1	A	39	LEU	2.3
1	A	207	LEU	2.3
1	A	158	ALA	2.3
1	D	1116	LYS	2.3
1	C	848	ASP	2.3
1	C	738	VAL	2.3
1	D	903	LYS	2.3
1	C	587	LEU	2.3
1	A	256	LEU	2.3
1	C	594	GLU	2.3
1	C	744	LEU	2.3
1	B	410	GLY	2.3
1	B	403	ALA	2.3
1	A	234	GLU	2.3
1	B	562	LEU	2.3
1	D	1132	ASP	2.3
1	B	328	VAL	2.2
1	C	611	LEU	2.2
1	A	38	GLN	2.2
1	A	42	GLU	2.2
1	B	476	GLU	2.2
1	B	554	ILE	2.2
1	B	342	ASP	2.2
1	D	1113	TYR	2.2
1	A	96	GLU	2.2
1	B	510	LYS	2.2
1	C	843	ASP	2.2
1	C	676	THR	2.2
1	B	432	LEU	2.2
1	C	667	LEU	2.2
1	D	866	ASP	2.2
1	A	127	MET	2.2
1	D	936	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	1076	GLU	2.2
1	C	796	LEU	2.1
1	D	898	LEU	2.1
1	C	742	SER	2.1
1	C	593	ALA	2.1
1	C	824	LEU	2.1
1	D	894	GLU	2.1
1	A	11	LEU	2.1
1	C	634	ASP	2.1
1	B	424	LYS	2.1
1	C	747	ALA	2.1
1	A	252	SER	2.1
1	C	602	ASP	2.1
1	D	875	ASP	2.1
1	B	477	LEU	2.1
1	A	50	LEU	2.0
1	B	285	MET	2.0
1	D	1119	TYR	2.0
1	D	1109	GLU	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 oligosaccharides 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.