Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 06:41 PM GMT

PDB ID	:	1C1G
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

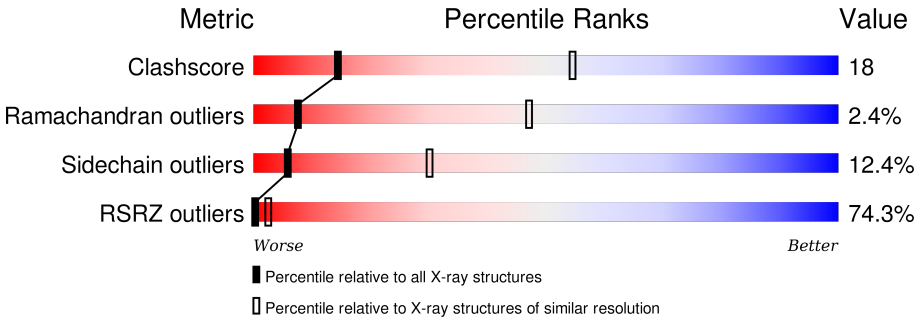
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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	102246	1063 (10.00-3.70)
Ramachandran outliers	100387	1035 (9.50-3.66)
Sidechain outliers	100360	1005 (9.50-3.66)
RSRZ outliers	91569	1013 (9.50-3.66)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	73% 64% 24% 8% •
1	B	284	86% 68% 22% 8% •
1	C	284	71% 62% 26% 8% •
1	D	284	67% 60% 28% 8% •

2 Entry composition (i)

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.

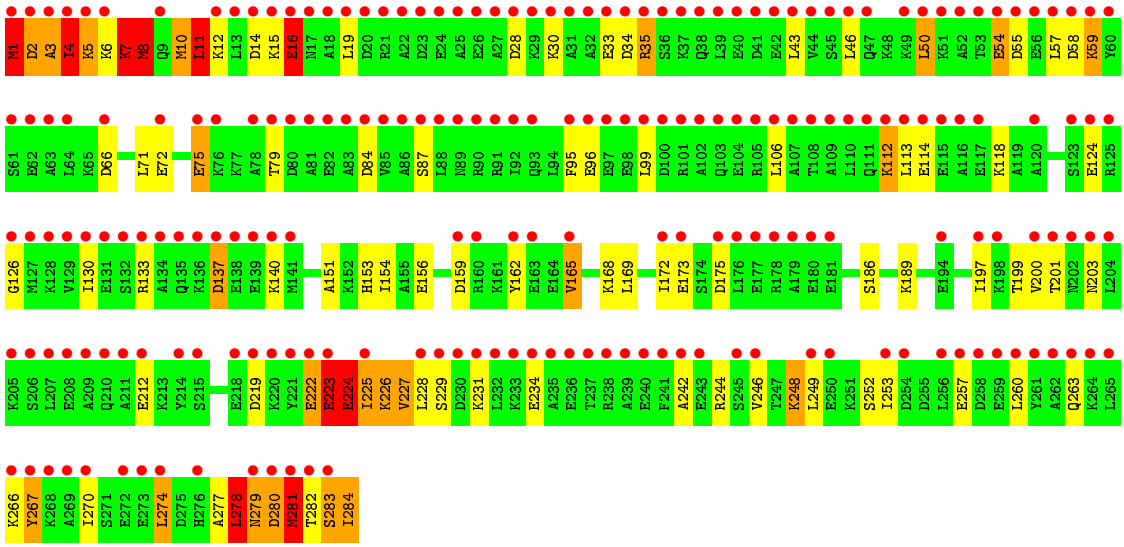
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	0	0
			2290	1402	387	494	7			
1	B	284	Total	C	N	O	S	0	0	0
			2290	1402	387	494	7			
1	C	284	Total	C	N	O	S	0	0	0
			2290	1402	387	494	7			
1	D	284	Total	C	N	O	S	0	0	0
			2290	1402	387	494	7			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

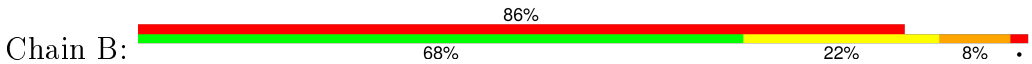
- Molecule 1: TROPOMYOSIN

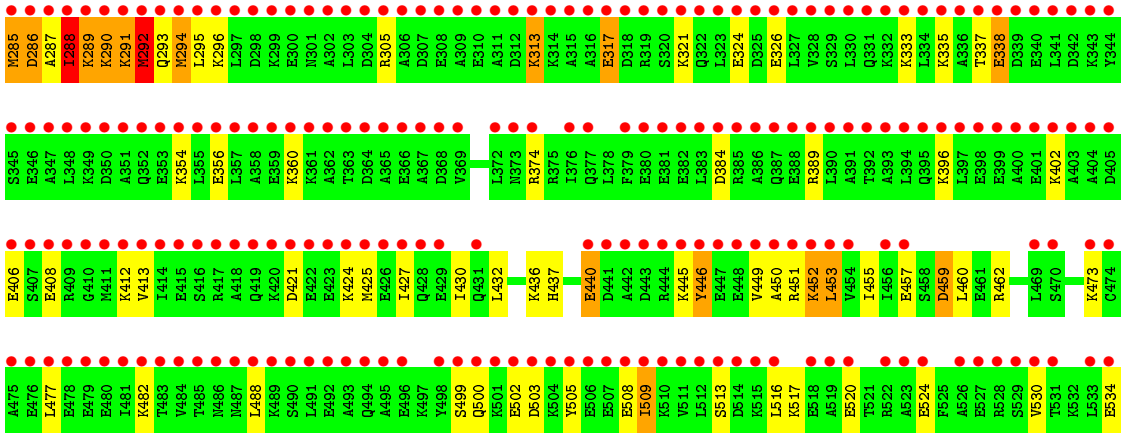
Chain A:

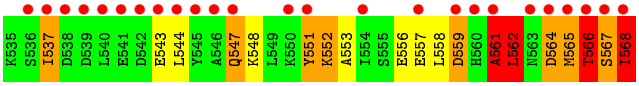


- Molecule 1: TROPOMYOSIN

Chain B:

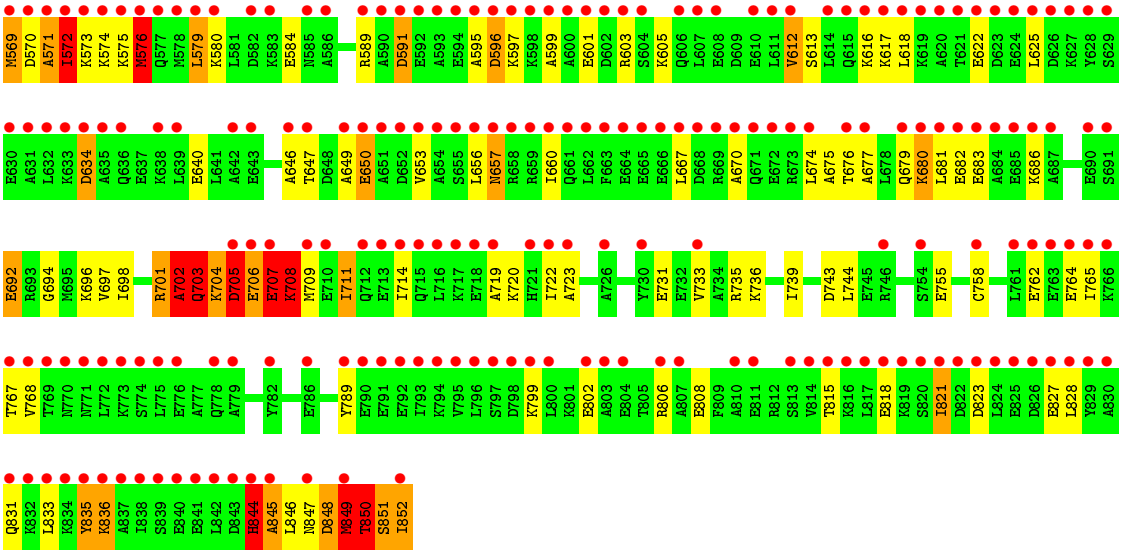






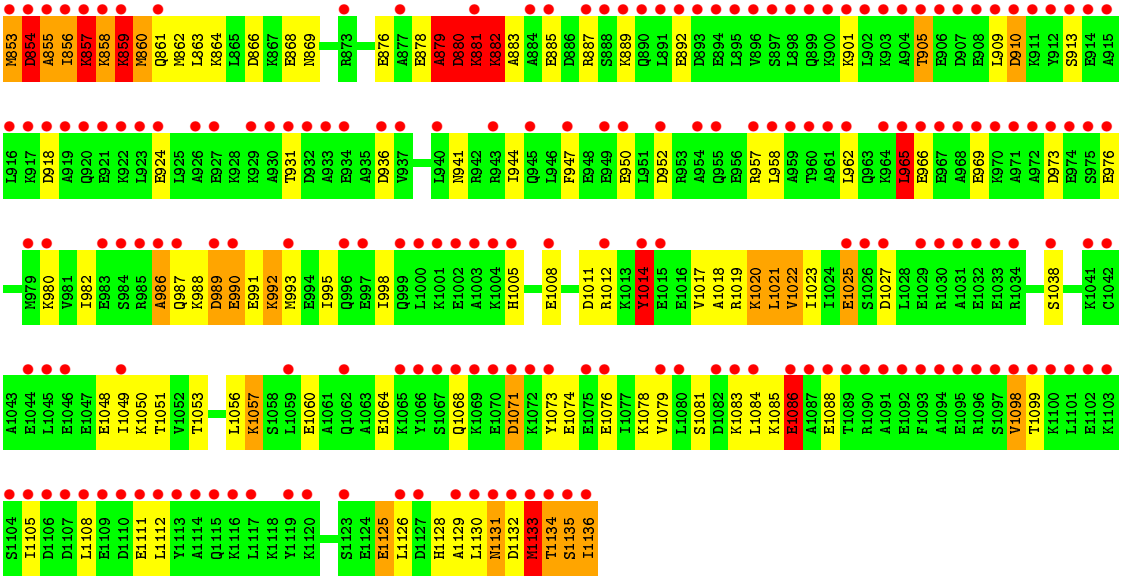
- Molecule 1: TROPOMYOSIN

Chain C:



- Molecule 1: TROPOMYOSIN

Chain D:



4 Data and refinement statistics (i)

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 99.89 – 7.00	Depositor EDS
% Data completeness (in resolution range)	96.4 (100.00-7.00) 96.4 (99.89-7.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.35 (at 6.73Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.404 , (Not available) 0.413 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	210.9	Xtriage
Anisotropy	1.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.54 , 457.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.34$, $< L^2 > = 0.17$	Xtriage
Outliers	4 of 3118 reflections (0.128%)	Xtriage
F_o,F_c correlation	0.67	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.86	3/2299 (0.1%)	1.79	56/3062 (1.8%)
1	B	0.80	2/2299 (0.1%)	1.63	41/3062 (1.3%)
1	C	1.28	11/2299 (0.5%)	1.86	59/3062 (1.9%)
1	D	0.91	8/2299 (0.3%)	1.82	67/3062 (2.2%)
All	All	0.98	24/9196 (0.3%)	1.78	223/12248 (1.8%)

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 (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	852	ILE	N-CA	30.96	2.08	1.46
1	C	852	ILE	CA-CB	21.53	2.04	1.54
1	C	851	SER	C-N	15.91	1.70	1.34
1	C	572	ILE	CA-CB	11.53	1.81	1.54
1	D	859	LYS	N-CA	10.74	1.67	1.46
1	C	705	ASP	N-CA	9.29	1.65	1.46
1	C	705	ASP	CA-C	9.07	1.76	1.52
1	D	860	MET	N-CA	8.86	1.64	1.46
1	C	705	ASP	C-N	8.60	1.53	1.34
1	A	224	GLU	CA-CB	8.43	1.72	1.53
1	D	858	LYS	C-N	8.01	1.52	1.34
1	C	851	SER	CA-C	7.28	1.71	1.52
1	D	858	LYS	C-O	6.26	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	859	LYS	CA-C	5.96	1.68	1.52
1	C	708	LYS	CB-CG	5.90	1.68	1.52
1	A	223	GLU	N-CA	5.76	1.57	1.46
1	C	708	LYS	CG-CD	5.56	1.71	1.52
1	B	568	ILE	CB-CG2	-5.52	1.35	1.52
1	A	224	GLU	CB-CG	5.34	1.62	1.52
1	D	860	MET	C-N	5.25	1.46	1.34
1	D	860	MET	CA-C	5.17	1.66	1.52
1	D	879	ALA	N-CA	5.14	1.56	1.46
1	B	565	MET	N-CA	5.06	1.56	1.46
1	C	704	LYS	C-N	5.03	1.45	1.34

All (223) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	4	ILE	CA-CB-CG2	-21.88	67.14	110.90
1	C	572	ILE	N-CA-CB	-21.77	60.73	110.80
1	B	568	ILE	N-CA-CB	-21.05	62.38	110.80
1	C	852	ILE	CB-CA-C	-18.23	75.14	111.60
1	A	223	GLU	CA-C-N	-17.61	78.46	117.20
1	C	708	LYS	CA-CB-CG	15.88	148.34	113.40
1	D	879	ALA	CA-C-N	-15.44	83.22	117.20
1	D	856	ILE	CB-CA-C	15.44	142.47	111.60
1	B	565	MET	CG-SD-CE	14.66	123.65	100.20
1	A	224	GLU	CA-CB-CG	14.30	144.85	113.40
1	D	880	ASP	N-CA-C	14.07	148.99	111.00
1	D	858	LYS	CA-C-O	-13.89	90.92	120.10
1	A	224	GLU	CA-C-N	-13.69	87.09	117.20
1	C	572	ILE	N-CA-C	-13.41	74.79	111.00
1	C	851	SER	CA-C-O	-13.23	92.32	120.10
1	D	856	ILE	N-CA-CB	-13.04	80.82	110.80
1	D	861	GLN	C-N-CA	-12.63	90.13	121.70
1	B	568	ILE	N-CA-C	-12.51	77.23	111.00
1	A	4	ILE	CA-CB-CG1	12.32	134.42	111.00
1	C	572	ILE	CA-CB-CG2	12.15	135.20	110.90
1	C	852	ILE	CG1-CB-CG2	-12.01	84.97	111.40
1	D	862	MET	CA-C-N	12.01	143.62	117.20
1	D	856	ILE	N-CA-C	-11.73	79.32	111.00
1	B	565	MET	CA-CB-CG	11.59	133.01	113.30
1	C	851	SER	CA-C-N	11.56	142.64	117.20
1	C	847	ASN	C-N-CA	-11.39	93.22	121.70
1	C	572	ILE	CG1-CB-CG2	-11.35	86.43	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	708	LYS	CG-CD-CE	11.17	145.40	111.90
1	C	851	SER	N-CA-C	11.11	141.00	111.00
1	D	880	ASP	CA-CB-CG	11.08	137.77	113.40
1	A	226	LYS	CA-C-N	11.07	141.55	117.20
1	A	7	LYS	CA-CB-CG	11.04	137.68	113.40
1	C	851	SER	C-N-CA	10.70	148.44	121.70
1	C	851	SER	N-CA-CB	-10.64	94.53	110.50
1	D	1014	TYR	CB-CG-CD2	-10.40	114.76	121.00
1	C	702	ALA	CA-C-N	-10.26	94.62	117.20
1	B	551	TYR	CB-CG-CD2	-10.25	114.85	121.00
1	A	224	GLU	N-CA-C	10.14	138.38	111.00
1	C	852	ILE	N-CA-CB	10.05	133.91	110.80
1	D	856	ILE	CA-C-N	9.97	139.13	117.20
1	D	859	LYS	O-C-N	-9.80	107.02	122.70
1	A	281	MET	CB-CA-C	-9.75	90.89	110.40
1	A	223	GLU	CA-C-O	9.67	140.41	120.10
1	C	708	LYS	CB-CG-CD	9.65	136.70	111.60
1	C	708	LYS	N-CA-CB	-9.59	93.34	110.60
1	D	882	LYS	CA-C-N	9.59	138.30	117.20
1	B	288	ILE	CA-CB-CG2	-9.56	91.78	110.90
1	D	880	ASP	CA-C-N	-9.51	96.29	117.20
1	C	852	ILE	N-CA-C	9.46	136.53	111.00
1	D	856	ILE	CG1-CB-CG2	-9.37	90.79	111.40
1	C	571	ALA	C-N-CA	9.30	144.96	121.70
1	C	589	ARG	NE-CZ-NH1	-9.07	115.77	120.30
1	A	281	MET	O-C-N	-9.03	108.26	122.70
1	A	35	ARG	NE-CZ-NH1	-8.91	115.84	120.30
1	D	861	GLN	N-CA-C	-8.88	87.03	111.00
1	A	1	MET	N-CA-C	-8.81	87.21	111.00
1	B	446	TYR	CB-CG-CD2	-8.80	115.72	121.00
1	A	281	MET	N-CA-CB	8.65	126.17	110.60
1	A	5	LYS	CA-CB-CG	8.61	132.35	113.40
1	B	564	ASP	CA-C-N	8.61	136.14	117.20
1	D	860	MET	CA-CB-CG	8.52	127.78	113.30
1	B	294	MET	CA-C-N	8.51	135.93	117.20
1	B	564	ASP	N-CA-CB	-8.47	95.36	110.60
1	B	565	MET	N-CA-CB	8.42	125.75	110.60
1	A	284	ILE	CG1-CB-CG2	-8.38	92.97	111.40
1	B	564	ASP	CA-CB-CG	8.32	131.69	113.40
1	A	284	ILE	CA-CB-CG2	-8.25	94.39	110.90
1	B	561	ALA	CA-C-N	-8.23	99.09	117.20
1	D	858	LYS	CA-C-N	8.23	135.31	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	280	ASP	N-CA-CB	-8.19	95.86	110.60
1	B	453	LEU	CA-CB-CG	8.19	134.13	115.30
1	D	858	LYS	C-N-CA	8.19	142.16	121.70
1	B	568	ILE	CB-CA-C	8.15	127.90	111.60
1	A	4	ILE	CG1-CB-CG2	-8.13	93.50	111.40
1	D	878	GLU	O-C-N	8.13	135.70	122.70
1	A	8	MET	CA-CB-CG	8.10	127.07	113.30
1	C	852	ILE	CA-CB-CG2	7.98	126.85	110.90
1	D	859	LYS	N-CA-C	7.94	132.43	111.00
1	D	878	GLU	C-N-CA	7.92	141.49	121.70
1	C	572	ILE	CB-CA-C	7.88	127.36	111.60
1	A	283	SER	CA-C-N	7.80	134.36	117.20
1	C	849	MET	N-CA-CB	7.75	124.55	110.60
1	D	857	LYS	CA-C-N	-7.75	100.15	117.20
1	D	879	ALA	CA-C-O	7.68	136.24	120.10
1	D	1014	TYR	CA-CB-CG	7.67	127.97	113.40
1	B	565	MET	CB-CA-C	-7.64	95.12	110.40
1	C	572	ILE	CA-C-N	7.58	133.88	117.20
1	A	284	ILE	CA-CB-CG1	7.58	125.41	111.00
1	A	7	LYS	C-N-CA	-7.58	102.76	121.70
1	B	446	TYR	CA-CB-CG	7.58	127.80	113.40
1	C	848	ASP	N-CA-CB	-7.58	96.97	110.60
1	C	705	ASP	CA-C-N	7.57	133.86	117.20
1	B	292	MET	CA-CB-CG	7.55	126.13	113.30
1	C	850	THR	CA-CB-CG2	7.53	122.94	112.40
1	A	222	GLU	O-C-N	7.50	134.70	122.70
1	A	3	ALA	CA-C-N	7.43	133.56	117.20
1	D	880	ASP	CB-CG-OD1	7.37	124.93	118.30
1	C	706	GLU	CA-C-N	7.33	133.31	117.20
1	D	1021	LEU	CA-CB-CG	7.22	131.91	115.30
1	D	862	MET	O-C-N	-7.21	111.16	122.70
1	C	708	LYS	N-CA-C	7.18	130.39	111.00
1	A	226	LYS	CA-C-O	-7.18	105.03	120.10
1	D	862	MET	CA-C-O	-7.15	105.09	120.10
1	B	564	ASP	CB-CA-C	7.13	124.67	110.40
1	A	225	ILE	N-CA-C	-7.11	91.80	111.00
1	A	5	LYS	CB-CA-C	-7.03	96.33	110.40
1	C	576	MET	N-CA-CB	7.00	123.20	110.60
1	C	576	MET	CB-CA-C	-6.95	96.50	110.40
1	D	853	MET	O-C-N	-6.94	111.59	122.70
1	C	702	ALA	O-C-N	6.94	133.80	122.70
1	B	288	ILE	CA-CB-CG1	6.91	124.13	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	858	LYS	N-CA-C	-6.90	92.36	111.00
1	B	551	TYR	CB-CG-CD1	6.90	125.14	121.00
1	A	244	ARG	NE-CZ-NH1	-6.88	116.86	120.30
1	A	224	GLU	O-C-N	6.86	133.68	122.70
1	B	338	GLU	OE1-CD-OE2	-6.82	115.11	123.30
1	D	1133	MET	CA-CB-CG	6.80	124.87	113.30
1	C	573	LYS	CA-CB-CG	6.80	128.37	113.40
1	B	505	TYR	CB-CG-CD2	-6.79	116.93	121.00
1	A	280	ASP	CB-CA-C	6.76	123.91	110.40
1	D	860	MET	O-C-N	-6.76	111.89	122.70
1	D	854	ASP	N-CA-C	6.70	129.10	111.00
1	C	701	ARG	O-C-N	6.70	133.42	122.70
1	C	789	TYR	CB-CG-CD2	-6.68	116.99	121.00
1	B	566	THR	O-C-N	-6.65	112.06	122.70
1	A	173	GLU	CA-CB-CG	6.63	127.98	113.40
1	D	1014	TYR	CB-CG-CD1	6.60	124.96	121.00
1	A	7	LYS	N-CA-CB	6.60	122.48	110.60
1	C	705	ASP	N-CA-C	6.56	128.71	111.00
1	C	705	ASP	O-C-N	-6.52	112.27	122.70
1	B	374	ARG	NE-CZ-NH2	6.44	123.52	120.30
1	D	862	MET	CA-CB-CG	6.42	124.21	113.30
1	D	858	LYS	O-C-N	6.40	132.94	122.70
1	D	887	ARG	NE-CZ-NH1	-6.40	117.10	120.30
1	C	848	ASP	N-CA-C	6.38	128.23	111.00
1	C	847	ASN	CA-C-N	-6.37	103.19	117.20
1	C	849	MET	CB-CA-C	-6.33	97.75	110.40
1	A	280	ASP	CB-CG-OD1	6.32	123.99	118.30
1	B	446	TYR	CB-CG-CD1	6.30	124.78	121.00
1	C	569	MET	O-C-N	-6.28	112.66	122.70
1	D	860	MET	N-CA-C	6.28	127.94	111.00
1	A	279	ASN	CA-C-N	-6.24	103.47	117.20
1	D	857	LYS	N-CA-C	6.22	127.78	111.00
1	A	212	GLU	OE1-CD-OE2	-6.21	115.85	123.30
1	D	1073	TYR	CB-CG-CD2	-6.18	117.29	121.00
1	A	4	ILE	CA-C-N	-6.15	103.66	117.20
1	C	704	LYS	CA-C-O	-6.15	107.19	120.10
1	D	856	ILE	CA-C-O	-6.13	107.23	120.10
1	D	1132	ASP	CA-C-N	-6.12	103.75	117.20
1	B	294	MET	O-C-N	-6.07	112.99	122.70
1	D	882	LYS	CA-C-O	-6.04	107.42	120.10
1	A	223	GLU	N-CA-C	6.01	127.23	111.00
1	D	880	ASP	O-C-N	6.01	132.32	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2	ASP	CA-C-N	-6.01	103.98	117.20
1	D	965	LEU	CA-CB-CG	6.00	129.09	115.30
1	D	854	ASP	O-C-N	-5.99	113.11	122.70
1	C	849	MET	CA-CB-CG	5.98	123.46	113.30
1	B	564	ASP	CA-C-O	-5.95	107.60	120.10
1	A	283	SER	CA-C-O	-5.95	107.61	120.10
1	A	278	LEU	CA-CB-CG	5.93	128.95	115.30
1	B	305	ARG	NE-CZ-NH2	5.91	123.25	120.30
1	D	990	GLU	N-CA-C	-5.91	95.05	111.00
1	D	855	ALA	O-C-N	-5.90	113.26	122.70
1	A	226	LYS	O-C-N	-5.89	113.27	122.70
1	A	222	GLU	C-N-CA	5.83	136.28	121.70
1	D	857	LYS	CB-CA-C	-5.82	98.76	110.40
1	A	267	TYR	CB-CG-CD1	-5.82	117.51	121.00
1	C	569	MET	CA-C-N	5.79	129.94	117.20
1	B	561	ALA	O-C-N	5.78	131.95	122.70
1	D	879	ALA	N-CA-C	5.78	126.60	111.00
1	B	482	LYS	CA-CB-CG	5.78	126.11	113.40
1	C	848	ASP	O-C-N	-5.78	113.45	122.70
1	C	572	ILE	CA-C-O	-5.76	108.00	120.10
1	D	881	LYS	CA-CB-CG	5.75	126.06	113.40
1	B	440	GLU	OE1-CD-OE2	-5.75	116.41	123.30
1	C	806	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	A	35	ARG	NE-CZ-NH2	5.71	123.16	120.30
1	C	701	ARG	C-N-CA	5.69	135.92	121.70
1	C	802	GLU	OE1-CD-OE2	-5.68	116.49	123.30
1	D	856	ILE	O-C-N	-5.67	113.62	122.70
1	A	11	LEU	CA-CB-CG	-5.64	102.33	115.30
1	D	858	LYS	CB-CA-C	5.63	121.67	110.40
1	D	1131	ASN	CA-C-N	5.59	129.50	117.20
1	C	703	GLN	CA-C-O	-5.58	108.38	120.10
1	B	566	THR	CA-CB-CG2	5.56	120.18	112.40
1	B	562	LEU	CA-CB-CG	5.54	128.04	115.30
1	C	650	GLU	OE1-CD-OE2	-5.54	116.65	123.30
1	C	835	TYR	CB-CG-CD2	-5.53	117.68	121.00
1	A	75	GLU	CA-CB-CG	-5.53	101.24	113.40
1	D	853	MET	N-CA-C	5.51	125.87	111.00
1	D	882	LYS	O-C-N	-5.51	113.89	122.70
1	C	848	ASP	CB-CA-C	5.50	121.39	110.40
1	B	289	LYS	CA-CB-CG	5.49	125.47	113.40
1	D	854	ASP	CA-C-N	5.47	129.24	117.20
1	D	887	ARG	NE-CZ-NH2	5.44	123.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	10	MET	CA-C-N	5.44	129.16	117.20
1	D	860	MET	N-CA-CB	-5.42	100.85	110.60
1	A	3	ALA	CA-C-O	-5.41	108.74	120.10
1	C	849	MET	N-CA-C	-5.38	96.47	111.00
1	C	572	ILE	CA-CB-CG1	-5.36	100.81	111.00
1	B	290	LYS	C-N-CA	-5.36	108.31	121.70
1	D	853	MET	CA-CB-CG	5.35	122.40	113.30
1	D	1098	VAL	N-CA-C	-5.35	96.55	111.00
1	A	156	GLU	OE1-CD-OE2	-5.34	116.89	123.30
1	B	567	SER	C-N-CA	5.31	134.98	121.70
1	D	860	MET	CA-C-N	5.28	128.82	117.20
1	A	2	ASP	CA-C-O	5.26	131.15	120.10
1	B	565	MET	N-CA-C	-5.23	96.87	111.00
1	D	1086	GLU	OE1-CD-OE2	-5.18	117.08	123.30
1	B	566	THR	CA-C-N	5.18	128.59	117.20
1	A	14	ASP	CB-CG-OD1	5.17	122.96	118.30
1	D	880	ASP	CA-C-O	5.17	130.95	120.10
1	C	707	GLU	C-N-CA	-5.16	108.80	121.70
1	A	16	GLU	CA-C-N	5.14	128.51	117.20
1	C	703	GLN	C-N-CA	5.11	134.47	121.70
1	A	225	ILE	C-N-CA	-5.11	108.94	121.70
1	C	706	GLU	O-C-N	-5.10	114.54	122.70
1	B	292	MET	CB-CA-C	-5.08	100.25	110.40
1	D	856	ILE	CA-CB-CG2	5.07	121.03	110.90
1	D	1076	GLU	OE1-CD-OE2	-5.05	117.24	123.30
1	A	224	GLU	CA-C-O	5.03	130.67	120.10
1	B	547	GLN	CA-CB-CG	-5.03	102.34	113.40
1	A	1	MET	CA-CB-CG	5.02	121.83	113.30

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

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Mol	Chain	Res	Type	Group
1	D	879	ALA	Mainchain,Peptide

5.2 Too-close contacts (i)

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	96	0
1	B	2290	0	2292	87	0
1	C	2290	0	2291	120	3
1	D	2290	0	2292	84	3
All	All	9160	0	9170	330	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 18.

All (330) 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:CA	1:C:572:ILE:CB	1.81	1.58
1:D:859:LYS:CA	1:D:859:LYS:N	1.67	1.51
1:C:705:ASP:C	1:C:705:ASP:CA	1.76	1.50
1:C:572:ILE:CB	1:C:572:ILE:N	1.71	1.46
1:C:851:SER:C	1:C:852:ILE:N	1.70	1.44
1:C:852:ILE:CA	1:C:852:ILE:CB	2.04	1.35
1:C:572:ILE:HB	1:C:572:ILE:N	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:C	1:C:852:ILE:CB	2.27	1.03
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:HA	1:C:852:ILE:N	1.79	0.97
1:C:572:ILE:HB	1:C:572:ILE:H	1.28	0.95
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:703:GLN:C	1:C:708:LYS:HG2	1.92	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:571:ALA:C	1:C:572:ILE:HB	1.96	0.85
1:A:224:GLU:HB2	1:A:227:VAL:H	1.44	0.82
1:C:572:ILE:CG1	1:C:572:ILE:CA	2.57	0.81
1:A:223:GLU:HA	1:A:224:GLU:HG2	1.64	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:569:MET:C	1:C:572:ILE:HG22	2.05	0.76
1:C:571:ALA:C	1:C:572:ILE:CB	2.53	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:A:8:MET:HE1	1:B:296:LYS:N	2.04	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:B:449:VAL:HA	1:B:452:LYS:HB2	1.72	0.71
1:A:1:MET:H2	1:A:4:ILE:H	1.38	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:D:859:LYS:HA	1:D:859:LYS:N	1.95	0.69
1:A:43:LEU:HD11	1:B:326:GLU:HB3	1.76	0.68
1:C:705:ASP:CB	1:C:705:ASP:C	2.60	0.68
1:A:224:GLU:HB2	1:A:226:LYS:C	2.14	0.67
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:A:8:MET:SD	1:B:292:MET:CA	2.84	0.65
1:A:2:ASP:O	1:A:5:LYS:HB3	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:706:GLU:C	1:C:708:LYS:HB2	2.18	0.64
1:C:706:GLU:N	1:C:708:LYS:CG	2.60	0.64
1:C:852:ILE:HB	1:C:852:ILE:CA	2.21	0.64
1:D:860:MET:HA	1:D:863:LEU:N	2.09	0.64
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:C:704:LYS:N	1:C:708:LYS:HG2	2.13	0.63
1:B:286:ASP:O	1:B:289:LYS:HB3	1.97	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: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:CB	1:D:859:LYS:N	2.58	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:C:705:ASP:O	1:C:709:MET:HB2	2.00	0.61
1:A:224:GLU:HB3	1:A:226:LYS:H	1.66	0.61
1:A:4:ILE:HD11	1:B:288:ILE:HD12	1.83	0.60
1:C:702:ALA:C	1:C:708:LYS:HD3	2.22	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:D:880:ASP:HB3	1:D:882:LYS:H	1.66	0.59
1:B:421:ASP:O	1:B:425:MET:HB2	2.03	0.59
1:B:285:MET:C	1:B:288:ILE:HG13	2.23	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:8:MET:HE1	1:B:295:LEU:C	2.23	0.58
1:A:186:SER:HA	1:A:189:LYS:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:N	1:A:4:ILE:HG12	2.19	0.57
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: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: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:D:986:ALA:HA	1:D:989:ASP:OD1	2.05	0.57
1:B:408:GLU:O	1:B:412:LYS:HG3	2.05	0.57
1:A:278:LEU:O	1:A:281:MET:HB3	2.04	0.57
1:A:224:GLU:CB	1:A:227:VAL:H	2.17	0.56
1:C:852:ILE:C	1:C:852:ILE:CG2	2.73	0.56
1:A:224:GLU:HB3	1:A:226:LYS:N	2.20	0.56
1:D:1133:MET:HG2	1:D:1134:THR:N	2.19	0.56
1:C:706:GLU:N	1:C:708:LYS:HE3	2.21	0.56
1:D:1084:LEU:O	1:D:1088:GLU:HB2	2.05	0.56
1:D:1019:ARG:HA	1:D:1022:VAL:HG12	1.87	0.56
1:A:7:LYS:HD2	1:A:8:MET:HG2	1.88	0.55
1:C:705:ASP:C	1:C:708:LYS:HB3	2.26	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:C:569:MET:O	1:C:572:ILE:HG22	2.07	0.55
1:C:572:ILE:HG13	1:C:572:ILE:CA	2.37	0.55
1:B:445:LYS:O	1:B:449:VAL:HG12	2.07	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:B:500:GLN:HA	1:B:503:ASP:OD1	2.09	0.53
1:A:225:ILE:HD11	1:B:508:GLU:HB3	1.89	0.53
1:C:677:ALA:O	1:C:681:LEU:HB2	2.08	0.53
1:D:880:ASP:CG	1:D:882:LYS:HB2	2.29	0.53
1:A:8:MET:CG	1:B:292:MET:HA	2.38	0.53
1:C:701:ARG:O	1:C:708:LYS:CD	2.56	0.53
1:A:137:ASP:CG	1:A:140:LYS:HZ1	2.11	0.53
1:C:625:LEU:HD22	1:D:905:THR:HG22	1.90	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:C:705:ASP:C	1:C:708:LYS:CB	2.78	0.52
1:A:223:GLU:HA	1:A:224:GLU:CG	2.36	0.52
1:B:565:MET:CA	1:B:568:ILE:HG22	2.40	0.52
1:B:548:LYS:O	1:B:552:LYS:HD2	2.10	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:C:702:ALA:CA	1:C:708:LYS:HD3	2.41	0.51
1:C:848:ASP:C	1:C:850:THR:N	2.62	0.51
1:D:995:ILE:O	1:D:998:ILE:HG22	2.10	0.51
1:A:283:SER:O	1:A:284:ILE:HD13	2.10	0.51
1:A:55:ASP:O	1:A:59:LYS:HG2	2.11	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:D:876:GLU:O	1:D:879:ALA:HB3	2.11	0.50
1:A:4:ILE:HG13	1:B:288:ILE:HG21	1.94	0.50
1:B:291:LYS:HE2	1:B:294:MET:HB3	1.93	0.50
1:A:263:GLN:HE22	1:B:544:LEU:HG	1.75	0.50
1:D:1050:LYS:HA	1:D:1053:THR:OG1	2.11	0.50
1:D:880:ASP:CB	1:D:883:ALA:N	2.70	0.50
1:C:764:GLU:O	1:C:768:VAL:HG12	2.11	0.50
1:A:242:ALA:O	1:A:246:VAL:HG23	2.12	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:114:GLU:HG2	1:A:118:LYS:NZ	2.27	0.49
1:C:705:ASP:HA	1:C:708:LYS:HB3	1.94	0.49
1:C:656:LEU:O	1:C:660:ILE:HD13	2.12	0.49
1:B:402:LYS:O	1:B:406:GLU:HG3	2.11	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:A:114:GLU:HG2	1:A:118:LYS:HZ2	1.78	0.49
1:C:680:LYS:HA	1:C:683:GLU:HB2	1.94	0.49
1:C:667:LEU:HD11	1:D:950:GLU:HB3	1.95	0.49
1:B:558:LEU:O	1:B:562:LEU:HB2	2.12	0.48
1:B:317:GLU:O	1:B:321:LYS:HG3	2.13	0.48
1:C:596:ASP:CG	1:D:881:LYS:HZ3	2.17	0.48
1:A:280:ASP:HB3	1:B:565:MET:CE	2.43	0.48
1:A:7:LYS:HG3	1:A:8:MET:H	1.79	0.48
1:A:8:MET:HE2	1:B:295:LEU:HB2	1.95	0.48
1:C:702:ALA:O	1:C:708:LYS:CD	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:597:LYS:NZ	1:C:601:GLU:OE2	2.47	0.48
1:C:702:ALA:HA	1:C:708:LYS:CE	2.34	0.48
1:B:451:ARG:O	1:B:455:ILE:HB	2.14	0.48
1:D:987:GLN:HA	1:D:990:GLU:HB2	1.95	0.48
1:D:854:ASP:C	1:D:857:LYS:HB3	2.33	0.48
1:D:1064:GLU:O	1:D:1068:GLN:HG3	2.14	0.47
1:D:1126:LEU:O	1:D:1129:ALA:HB3	2.14	0.47
1:D:941:ASN:O	1:D:944:ILE:HG22	2.14	0.47
1:C:705:ASP:O	1:C:705:ASP:CA	2.51	0.47
1:C:576:MET:HG3	1:D:859:LYS:HG3	1.95	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:A:133:ARG:O	1:A:137:ASP:HB2	2.14	0.47
1:D:856:ILE:HA	1:D:859:LYS:CB	2.44	0.47
1:B:543:GLU:HG3	1:B:547:GLN:HE21	1.80	0.47
1:A:225:ILE:HD12	1:B:509:ILE:HG13	1.95	0.47
1:C:703:GLN:O	1:C:708:LYS:N	2.48	0.47
1:D:879:ALA:O	1:D:880:ASP:CB	2.63	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:280:ASP:C	1:A:282:THR:H	2.18	0.46
1:C:701:ARG:O	1:C:708:LYS:HD3	2.16	0.46
1:B:564:ASP:C	1:B:566:THR:N	2.69	0.46
1:A:203:ASN:HB3	1:B:488:LEU:HD11	1.98	0.46
1:C:601:GLU:O	1:C:605:LYS:HG3	2.15	0.46
1:A:106:LEU:HD21	1:B:389:ARG:HD3	1.96	0.46
1:B:473:LYS:HZ3	1:B:477:LEU:HD11	1.81	0.46
1:C:818:GLU:O	1:C:821:ILE:HG22	2.16	0.46
1:D:880:ASP:HB3	1:D:882:LYS:CA	2.45	0.46
1:C:579:LEU:HG	1:D:860:MET:HG3	1.96	0.46
1:C:705:ASP:CA	1:C:708:LYS:HD2	2.45	0.46
1:C:674:LEU:HD21	1:D:957:ARG:HD3	1.97	0.46
1:D:1014:TYR:O	1:D:1018:ALA:HB2	2.15	0.46
1:C:694:GLY:O	1:C:697:VAL:HG12	2.16	0.46
1:B:436:LYS:HZ3	1:B:440:GLU:CD	2.19	0.46
1:C:612:VAL:HG22	1:C:616:LYS:NZ	2.31	0.46
1:A:4:ILE:CG1	1:B:288:ILE:HG21	2.45	0.45
1:B:292:MET:HG2	1:B:293:GLN:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:GLU:O	1:A:19:LEU:HB2	2.16	0.45
1:A:224:GLU:HB2	1:A:226:LYS:CA	2.47	0.45
1:A:7:LYS:NZ	1:B:292:MET:HB2	2.31	0.45
1:B:290:LYS:O	1:B:293:GLN:HB2	2.15	0.45
1:C:653:VAL:O	1:C:657:ASN:HB2	2.16	0.45
1:A:75:GLU:CD	1:B:354:LYS:HZ3	2.20	0.45
1:B:450:ALA:O	1:B:453:LEU:HG	2.17	0.45
1:B:356:GLU:OE2	1:B:360:LYS:NZ	2.49	0.45
1:D:880:ASP:CB	1:D:883:ALA:H	2.23	0.45
1:A:95:PHE:O	1:A:99:LEU:HD13	2.16	0.45
1:D:958:LEU:O	1:D:962:LEU:HB2	2.16	0.45
1:C:622:GLU:OE1	1:D:901:LYS:NZ	2.50	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:D:859:LYS:H	1:D:859:LYS:CA	2.07	0.45
1:B:285:MET:N	1:B:288:ILE:HD11	2.32	0.45
1:A:112:LYS:HB2	1:A:112:LYS:NZ	2.32	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:C:704:LYS:O	1:C:708:LYS:CA	2.65	0.44
1:B:424:LYS:HA	1:B:427:ILE:HB	1.99	0.44
1:D:856:ILE:HG21	1:D:856:ILE:HD13	1.62	0.44
1:A:7:LYS:HD3	1:A:8:MET:HG2	1.99	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:D:864:LYS:NZ	1:D:868:GLU:OE2	2.51	0.44
1:C:848:ASP:HA	1:C:851:SER:N	2.30	0.44
1:C:844:HIS:O	1:C:845:ALA:C	2.56	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:A:169:LEU:O	1:A:172:ILE:HG22	2.18	0.43
1:D:1108:LEU:O	1:D:1112:LEU:HD13	2.18	0.43
1:C:762:GLU:O	1:C:765:ILE:HG22	2.18	0.43
1:C:744:LEU:HD11	1:D:1027:ASP:HB3	2.00	0.43
1:C:704:LYS:NZ	1:C:705:ASP:OD2	2.52	0.43
1:C:704:LYS:O	1:C:708:LYS:CB	2.67	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:B:513:SER:O	1:B:517:LYS:NZ	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:698:ILE:HG21	1:D:982:ILE:HG23	2.01	0.43
1:D:1126:LEU:O	1:D:1130:LEU:HD13	2.18	0.43
1:D:1068:GLN:HA	1:D:1071:ASP:OD1	2.18	0.43
1:D:1011:ASP:O	1:D:1014:TYR:HB3	2.19	0.43
1:D:1008:GLU:HB3	1:D:1012:ARG:HH11	1.83	0.43
1:A:35:ARG:NH1	1:B:324:GLU:OE2	2.51	0.43
1:D:1083:LYS:NZ	1:D:1086:GLU:OE1	2.51	0.43
1:B:292:MET:HG2	1:B:293:GLN:N	2.33	0.43
1:D:988:LYS:O	1:D:992:LYS:HD2	2.18	0.43
1:C:682:GLU:OE1	1:C:686:LYS:NZ	2.51	0.43
1:B:516:LEU:O	1:B:520:GLU:HB2	2.19	0.43
1:A:3:ALA:O	1:A:4:ILE:C	2.57	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:54:GLU:OE1	1:B:333:LYS:NZ	2.51	0.43
1:C:701:ARG:O	1:C:708:LYS:HD2	2.18	0.43
1:C:848:ASP:C	1:C:851:SER:N	2.72	0.43
1:A:4:ILE:O	1:A:7:LYS:HG3	2.18	0.43
1:B:562:LEU:O	1:B:566:THR:HB	2.19	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:C:698:ILE:HD11	1:D:986:ALA:HB3	2.01	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: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:C:736:LYS:NZ	1:D:1025:GLU:OE1	2.53	0.42
1:C:591:ASP:O	1:C:595:ALA:HB2	2.18	0.42
1:B:285:MET:HA	1:B:288:ILE:CD1	2.50	0.42
1:D:1074:GLU:OE2	1:D:1078:LYS:NZ	2.49	0.42
1:B:559:ASP:O	1:B:562:LEU:HB3	2.20	0.42
1:D:1053:THR:O	1:D:1057:LYS:HD2	2.20	0.42
1:C:755:GLU:O	1:C:758:CYS:HB2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:705:ASP:N	1:C:708:LYS:CG	2.83	0.41
1:A:7:LYS:O	1:A:10:MET:N	2.54	0.41
1:A:12:LYS:NZ	1:A:16:GLU:OE2	2.53	0.41
1:C:682:GLU:HG2	1:C:686:LYS:NZ	2.36	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:C:704:LYS:C	1:C:708:LYS:CG	2.89	0.41
1:A:1:MET:H2	1:A:4:ILE:HG12	1.83	0.41
1:D:976:GLU:OE1	1:D:980:LYS:NZ	2.53	0.41
1:C:692:GLU:OE2	1:C:696:LYS:NZ	2.53	0.41
1:D:1125:GLU:O	1:D:1129:ALA:HB2	2.20	0.41
1:D:910:ASP:O	1:D:913:SER:HB3	2.21	0.41
1:D:905:THR:O	1:D:909:LEU:HB2	2.21	0.40
1:B:335:LYS:NZ	1:B:338:GLU:OE2	2.53	0.40
1:C:720:LYS:O	1:C:723:ALA:HB3	2.21	0.40
1:A:126:GLY:O	1:A:130:ILE:HG22	2.21	0.40
1:D:1081:SER:O	1:D:1085:LYS:NZ	2.54	0.40
1:C:599:ALA:O	1:C:603:ARG:HB2	2.22	0.40
1:A:223:GLU:O	1:A:224:GLU:CB	2.69	0.40
1:C:613:SER:O	1:C:617:LYS:HG2	2.21	0.40
1:A:168:LYS:O	1:A:172:ILE:HB	2.22	0.40
1:C:680:LYS:HZ3	1:D:965:LEU:HA	1.87	0.40
1:C:612:VAL:HG22	1:C:616:LYS:HZ2	1.86	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%)	5 41
1	B	282/284 (99%)	250 (89%)	28 (10%)	4 (1%)	14 58
1	C	282/284 (99%)	246 (87%)	30 (11%)	6 (2%)	9 50
1	D	282/284 (99%)	246 (87%)	28 (10%)	8 (3%)	6 44
All	All	1128/1136 (99%)	983 (87%)	118 (10%)	27 (2%)	7 47

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
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 (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	245/245 (100%)	209 (85%)	36 (15%)	4	24
1	B	245/245 (100%)	220 (90%)	25 (10%)	9	37
1	C	245/245 (100%)	217 (89%)	28 (11%)	7	32
1	D	245/245 (100%)	212 (86%)	33 (14%)	5	27
All	All	980/980 (100%)	858 (88%)	122 (12%)	6	30

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	4	ILE
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	50	LEU
1	A	54	GLU
1	A	79	THR
1	A	84	ASP
1	A	87	SER
1	A	112	LYS
1	A	124	GLU
1	A	137	ASP
1	A	153	HIS
1	A	159	ASP
1	A	165	VAL
1	A	175	ASP
1	A	197	ILE

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Mol	Chain	Res	Type
1	A	199	THR
1	A	200	VAL
1	A	201	THR
1	A	224	GLU
1	A	227	VAL
1	A	229	SER
1	A	231	LYS
1	A	234	GLU
1	A	248	LYS
1	A	274	LEU
1	A	278	LEU
1	A	281	MET
1	B	285	MET
1	B	288	ILE
1	B	291	LYS
1	B	292	MET
1	B	313	LYS
1	B	317	GLU
1	B	384	ASP
1	B	396	LYS
1	B	413	VAL
1	B	430	ILE
1	B	432	LEU
1	B	437	HIS
1	B	446	TYR
1	B	452	LYS
1	B	459	ASP
1	B	509	ILE
1	B	524	GLU
1	B	537	ILE
1	B	551	TYR
1	B	552	LYS
1	B	556	GLU
1	B	559	ASP
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

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Mol	Chain	Res	Type
1	C	612	VAL
1	C	618	LEU
1	C	634	ASP
1	C	647	THR
1	C	657	ASN
1	C	676	THR
1	C	680	LYS
1	C	692	GLU
1	C	705	ASP
1	C	708	LYS
1	C	711	ILE
1	C	743	ASP
1	C	767	THR
1	C	799	LYS
1	C	808	GLU
1	C	815	THR
1	C	821	ILE
1	C	823	ASP
1	C	835	TYR
1	C	836	LYS
1	C	844	HIS
1	C	849	MET
1	C	850	THR
1	D	853	MET
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	918	ASP
1	D	924	GLU
1	D	931	THR
1	D	936	ASP
1	D	947	PHE
1	D	952	ASP
1	D	965	LEU
1	D	966	GLU
1	D	973	ASP
1	D	989	ASP
1	D	992	LYS
1	D	1005	HIS

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Mol	Chain	Res	Type
1	D	1014	TYR
1	D	1020	LYS
1	D	1022	VAL
1	D	1025	GLU
1	D	1038	SER
1	D	1049	ILE
1	D	1057	LYS
1	D	1071	ASP
1	D	1086	GLU
1	D	1105	ILE
1	D	1125	GLU
1	D	1128	HIS
1	D	1134	THR
1	D	1136	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	ASN
1	B	431	GLN
1	D	1055	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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, 95^{th} 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%)	3.44	207 (72%)	0	2	174, 174, 174, 174	0
1	B	284/284 (100%)	3.91	243 (85%)	0	2	174, 174, 174, 174	0
1	C	284/284 (100%)	3.61	203 (71%)	0	3	174, 174, 174, 174	0
1	D	284/284 (100%)	3.13	191 (67%)	0	3	174, 174, 174, 174	0
All	All	1136/1136 (100%)	3.52	844 (74%)	0	2	174, 174, 174, 174	0

All (844) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ASP	15.2
1	C	657	ASN	15.0
1	C	596	ASP	13.1
1	A	36	SER	12.0
1	D	905	THR	11.8
1	C	660	ILE	11.7
1	C	658	ARG	11.7
1	C	653	VAL	11.2
1	A	33	GLU	10.8
1	A	30	LYS	10.8
1	B	483	THR	10.6
1	A	40	GLU	10.5
1	A	34	ASP	10.3
1	D	898	LEU	10.2
1	D	901	LYS	9.8
1	C	599	ALA	9.7
1	C	604	SER	9.7
1	A	25	ALA	9.7
1	A	32	ALA	9.7
1	C	654	ALA	9.6
1	A	137	ASP	9.5

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Mol	Chain	Res	Type	RSRZ
1	B	380	GLU	9.3
1	B	479	GLU	9.2
1	C	600	ALA	9.2
1	C	831	GLN	9.2
1	C	655	SER	9.2
1	B	346	GLU	9.1
1	D	1134	THR	9.1
1	C	661	GLN	9.0
1	C	825	GLU	9.0
1	B	480	GLU	9.0
1	C	826	ASP	9.0
1	B	484	VAL	9.0
1	B	342	ASP	8.9
1	A	39	LEU	8.9
1	B	286	ASP	8.9
1	D	858	LYS	8.8
1	A	29	LYS	8.7
1	D	894	GLU	8.5
1	A	28	ASP	8.5
1	C	659	ARG	8.4
1	A	35	ARG	8.4
1	A	22	ALA	8.3
1	C	656	LEU	8.3
1	A	20	ASP	8.1
1	D	892	GLU	8.1
1	C	840	GLU	8.0
1	B	350	ASP	8.0
1	A	38	GLN	8.0
1	D	912	TYR	7.9
1	D	899	GLN	7.9
1	B	541	GLU	7.9
1	C	603	ARG	7.8
1	C	839	SER	7.8
1	D	888	SER	7.8
1	B	343	LYS	7.7
1	C	827	GLU	7.6
1	C	629	SER	7.6
1	C	824	LEU	7.6
1	C	821	ILE	7.6
1	A	24	GLU	7.6
1	C	822	ASP	7.5
1	C	594	GLU	7.5

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Mol	Chain	Res	Type	RSRZ
1	C	828	LEU	7.5
1	B	487	ASN	7.5
1	C	593	ALA	7.4
1	D	907	ASP	7.4
1	D	908	GLU	7.3
1	A	21	ARG	7.3
1	A	3	ALA	7.3
1	B	407	SER	7.2
1	A	26	GLU	7.2
1	B	485	THR	7.2
1	A	95	PHE	7.2
1	C	829	TYR	7.2
1	B	488	LEU	7.1
1	D	902	LEU	7.1
1	A	84	ASP	7.1
1	B	353	GLU	7.1
1	B	491	LEU	7.1
1	C	832	LYS	7.1
1	D	1104	SER	7.0
1	B	486	ASN	7.0
1	D	895	LEU	7.0
1	A	92	ILE	7.0
1	A	1	MET	6.9
1	C	837	ALA	6.9
1	B	564	ASP	6.9
1	B	363	THR	6.9
1	C	820	SER	6.9
1	D	911	LYS	6.9
1	D	855	ALA	6.9
1	A	31	ALA	6.8
1	B	379	PHE	6.8
1	D	904	ALA	6.8
1	A	205	LYS	6.8
1	B	396	LYS	6.8
1	B	494	GLN	6.8
1	C	823	ASP	6.8
1	C	771	ASN	6.7
1	C	836	LYS	6.7
1	C	664	GLU	6.7
1	A	5	LYS	6.7
1	B	383	LEU	6.7
1	D	906	GLU	6.7

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Mol	Chain	Res	Type	RSRZ
1	D	910	ASP	6.7
1	D	1069	LYS	6.7
1	C	595	ALA	6.7
1	A	263	GLN	6.7
1	C	607	LEU	6.7
1	C	571	ALA	6.6
1	B	482	LYS	6.6
1	D	854	ASP	6.6
1	A	99	LEU	6.5
1	B	400	ALA	6.5
1	C	597	LYS	6.5
1	B	323	LEU	6.5
1	C	590	ALA	6.4
1	A	80	ASP	6.4
1	B	492	GLU	6.4
1	C	833	LEU	6.4
1	A	111	GLN	6.4
1	B	543	GLU	6.4
1	D	909	LEU	6.4
1	A	56	GLU	6.3
1	B	384	ASP	6.3
1	D	1116	LYS	6.3
1	B	408	GLU	6.3
1	C	628	TYR	6.3
1	B	409	ARG	6.3
1	D	897	SER	6.3
1	C	838	ILE	6.3
1	D	885	GLU	6.3
1	D	933	ALA	6.3
1	B	393	ALA	6.2
1	B	481	ILE	6.2
1	B	540	LEU	6.2
1	D	1101	LEU	6.2
1	D	914	GLU	6.2
1	A	81	ALA	6.2
1	C	818	GLU	6.1
1	D	965	LEU	6.1
1	D	1133	MET	6.1
1	B	537	ILE	6.1
1	A	37	LYS	6.1
1	B	421	ASP	6.1
1	B	338	GLU	6.1

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Mol	Chain	Res	Type	RSRZ
1	D	891	LEU	6.1
1	A	53	THR	6.0
1	B	362	ALA	6.0
1	A	239	ALA	6.0
1	C	841	GLU	6.0
1	A	204	LEU	6.0
1	D	968	ALA	6.0
1	B	337	THR	5.9
1	A	235	ALA	5.9
1	B	418	ALA	5.9
1	A	60	TYR	5.9
1	D	913	SER	5.9
1	B	386	ALA	5.9
1	A	96	GLU	5.9
1	D	1135	SER	5.9
1	B	387	GLN	5.8
1	C	817	LEU	5.8
1	B	356	GLU	5.8
1	B	347	ALA	5.8
1	B	538	ASP	5.8
1	C	663	PHE	5.8
1	C	577	GLN	5.8
1	B	392	THR	5.8
1	D	1066	TYR	5.7
1	D	903	LYS	5.7
1	C	622	GLU	5.7
1	C	670	ALA	5.7
1	C	666	GLU	5.7
1	D	1112	LEU	5.7
1	C	662	LEU	5.7
1	B	354	LYS	5.6
1	B	542	ASP	5.6
1	A	82	GLU	5.6
1	A	130	ILE	5.6
1	A	23	ASP	5.6
1	B	339	ASP	5.6
1	A	127	MET	5.6
1	A	103	GLN	5.6
1	C	650	GLU	5.6
1	C	652	ASP	5.6
1	A	42	GLU	5.5
1	A	112	LYS	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	267	TYR	5.5
1	D	1097	SER	5.5
1	C	625	LEU	5.5
1	B	415	GLU	5.5
1	D	900	LYS	5.5
1	D	974	GLU	5.5
1	D	1108	LEU	5.4
1	C	778	GLN	5.4
1	A	208	GLU	5.4
1	B	376	ILE	5.4
1	A	43	LEU	5.4
1	B	344	TYR	5.4
1	A	16	GLU	5.4
1	B	319	ARG	5.4
1	B	358	ALA	5.4
1	A	202	ASN	5.4
1	A	201	THR	5.4
1	B	345	SER	5.4
1	A	237	THR	5.4
1	D	915	ALA	5.4
1	D	1131	ASN	5.3
1	A	88	LEU	5.3
1	C	790	GLU	5.3
1	A	236	GLU	5.3
1	B	406	GLU	5.3
1	C	574	LYS	5.3
1	A	27	ALA	5.3
1	A	109	ALA	5.3
1	C	602	ASP	5.3
1	C	621	THR	5.3
1	B	411	MET	5.3
1	B	567	SER	5.2
1	B	359	GLU	5.2
1	C	835	TYR	5.2
1	C	768	VAL	5.2
1	B	414	ILE	5.2
1	D	964	LYS	5.2
1	A	55	ASP	5.2
1	D	1073	TYR	5.2
1	B	405	ASP	5.1
1	B	330	LEU	5.1
1	B	498	TYR	5.1

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Mol	Chain	Res	Type	RSRZ
1	C	635	ALA	5.1
1	D	1030	ARG	5.1
1	B	499	SER	5.1
1	B	478	GLU	5.1
1	B	326	GLU	5.1
1	B	349	LYS	5.1
1	B	526	ALA	5.1
1	B	360	LYS	5.1
1	C	592	GLU	5.1
1	C	667	LEU	5.1
1	B	377	GLN	5.1
1	B	287	ALA	5.0
1	B	361	LYS	5.0
1	D	1096	ARG	5.0
1	C	570	ASP	5.0
1	C	769	THR	5.0
1	C	774	SER	5.0
1	A	116	ALA	5.0
1	C	634	ASP	5.0
1	B	404	ALA	5.0
1	B	495	ALA	4.9
1	D	934	GLU	4.9
1	B	320	SER	4.9
1	D	936	ASP	4.9
1	B	490	SER	4.9
1	A	85	VAL	4.9
1	B	331	GLN	4.9
1	B	298	ASP	4.9
1	C	810	ALA	4.9
1	C	611	LEU	4.9
1	D	1115	GLN	4.9
1	D	1029	GLU	4.9
1	B	302	ALA	4.8
1	B	388	GLU	4.8
1	B	324	GLU	4.8
1	C	767	THR	4.8
1	A	138	GLU	4.8
1	C	610	GLU	4.8
1	A	206	SER	4.8
1	D	969	GLU	4.8
1	B	533	LEU	4.8
1	A	57	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	340	GLU	4.8
1	B	329	SER	4.8
1	B	382	GLU	4.8
1	C	713	GLU	4.8
1	C	631	ALA	4.8
1	B	515	LYS	4.8
1	C	726	ALA	4.7
1	D	1094	ALA	4.7
1	A	79	THR	4.7
1	B	403	ALA	4.7
1	C	770	ASN	4.7
1	D	893	ASP	4.7
1	B	530	VAL	4.7
1	B	373	ASN	4.6
1	B	390	LEU	4.6
1	A	234	GLU	4.6
1	A	113	LEU	4.6
1	B	285	MET	4.6
1	D	972	ALA	4.6
1	B	341	LEU	4.6
1	B	316	ALA	4.6
1	B	506	GLU	4.6
1	C	830	ALA	4.6
1	A	9	GLN	4.6
1	B	511	VAL	4.6
1	C	575	LYS	4.6
1	A	115	GLU	4.6
1	A	253	ILE	4.6
1	B	397	LEU	4.6
1	A	6	LYS	4.6
1	A	108	THR	4.6
1	D	889	LYS	4.6
1	B	327	LEU	4.6
1	D	1136	ILE	4.6
1	B	325	ASP	4.6
1	C	766	LYS	4.6
1	D	1130	LEU	4.6
1	C	813	SER	4.5
1	D	996	GLN	4.5
1	C	814	VAL	4.5
1	B	381	GLU	4.5
1	C	582	ASP	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	598	LYS	4.5
1	D	1132	ASP	4.5
1	C	792	GLU	4.5
1	A	102	ALA	4.5
1	B	514	ASP	4.5
1	A	134	ALA	4.5
1	B	519	ALA	4.5
1	C	807	ALA	4.5
1	B	293	GLN	4.5
1	D	975	SER	4.5
1	A	242	ALA	4.5
1	A	52	ALA	4.5
1	B	534	GLU	4.5
1	C	601	GLU	4.5
1	D	1000	LEU	4.5
1	C	705	ASP	4.5
1	B	401	GLU	4.4
1	A	83	ALA	4.4
1	A	54	GLU	4.4
1	B	510	LYS	4.4
1	B	389	ARG	4.4
1	B	410	GLY	4.4
1	D	1062	GLN	4.4
1	B	352	GLN	4.4
1	D	1087	ALA	4.4
1	D	1076	GLU	4.4
1	A	45	SER	4.4
1	C	793	ILE	4.4
1	A	87	SER	4.4
1	A	46	LEU	4.4
1	B	372	LEU	4.4
1	B	334	LEU	4.3
1	D	1111	GLU	4.3
1	A	133	ARG	4.3
1	B	512	LEU	4.3
1	B	355	LEU	4.3
1	A	257	GLU	4.3
1	C	626	ASP	4.3
1	A	15	LYS	4.3
1	D	1100	LYS	4.3
1	C	834	LYS	4.3
1	A	18	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	300	GLU	4.2
1	C	591	ASP	4.2
1	B	307	ASP	4.2
1	B	301	ASN	4.2
1	B	333	LYS	4.2
1	C	706	GLU	4.2
1	D	1113	TYR	4.2
1	B	477	LEU	4.2
1	B	364	ASP	4.2
1	A	17	ASN	4.2
1	A	106	LEU	4.2
1	C	638	LYS	4.2
1	C	677	ALA	4.2
1	A	232	LEU	4.2
1	B	322	GLN	4.2
1	C	578	MET	4.2
1	D	1123	SER	4.2
1	A	61	SER	4.2
1	B	539	ASP	4.1
1	C	796	LEU	4.1
1	B	398	GLU	4.1
1	B	365	ALA	4.1
1	A	107	ALA	4.1
1	C	775	LEU	4.1
1	C	716	LEU	4.1
1	A	238	ARG	4.1
1	C	719	ALA	4.1
1	C	651	ALA	4.1
1	D	1072	LYS	4.1
1	B	290	LYS	4.1
1	B	423	GLU	4.1
1	C	754	SER	4.1
1	B	412	LYS	4.1
1	D	896	VAL	4.1
1	A	207	LEU	4.1
1	C	673	ARG	4.1
1	D	971	ALA	4.0
1	B	557	GLU	4.0
1	A	233	LYS	4.0
1	B	391	ALA	4.0
1	D	1099	THR	4.0
1	B	568	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	619	LYS	4.0
1	B	318	ASP	4.0
1	D	1065	LYS	4.0
1	C	680	LYS	4.0
1	D	881	LYS	4.0
1	B	536	SER	4.0
1	D	1070	GLU	4.0
1	C	682	GLU	4.0
1	A	98	GLU	4.0
1	A	124	GLU	4.0
1	B	351	ALA	3.9
1	A	136	LYS	3.9
1	D	922	LYS	3.9
1	C	615	GLN	3.9
1	D	1105	ILE	3.9
1	D	966	GLU	3.9
1	D	1109	GLU	3.9
1	A	89	ASN	3.9
1	A	203	ASN	3.9
1	B	291	LYS	3.9
1	B	357	LEU	3.9
1	C	786	GLU	3.9
1	B	399	GLU	3.9
1	C	589	ARG	3.9
1	C	811	GLU	3.9
1	C	819	LYS	3.9
1	B	425	MET	3.9
1	A	175	ASP	3.9
1	B	416	SER	3.9
1	A	91	ARG	3.9
1	C	715	GLN	3.9
1	B	446	TYR	3.9
1	D	1080	LEU	3.9
1	A	243	GLU	3.8
1	D	1120	LYS	3.8
1	A	269	ALA	3.8
1	D	930	ALA	3.8
1	A	49	LYS	3.8
1	A	59	LYS	3.8
1	D	967	GLU	3.8
1	D	989	ASP	3.8
1	A	176	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	449	VAL	3.8
1	B	505	TYR	3.8
1	A	19	LEU	3.8
1	A	266	LYS	3.8
1	C	632	LEU	3.8
1	C	800	LEU	3.8
1	A	209	ALA	3.8
1	B	547	GLN	3.8
1	A	240	GLU	3.8
1	B	424	LYS	3.8
1	D	1127	ASP	3.8
1	C	803	ALA	3.8
1	B	503	ASP	3.8
1	D	884	ALA	3.8
1	D	1095	GLU	3.8
1	C	797	SER	3.8
1	C	816	LYS	3.8
1	B	473	LYS	3.8
1	B	306	ALA	3.8
1	A	180	GLU	3.8
1	B	518	GLU	3.8
1	C	618	LEU	3.7
1	C	789	TYR	3.7
1	D	1092	GLU	3.7
1	D	1098	VAL	3.7
1	D	1129	ALA	3.7
1	C	712	GLN	3.7
1	D	1093	PHE	3.7
1	C	649	ALA	3.7
1	A	223	GLU	3.7
1	D	1110	ASP	3.7
1	B	289	LYS	3.7
1	C	671	GLN	3.7
1	B	476	GLU	3.7
1	D	916	LEU	3.7
1	B	312	ASP	3.7
1	D	926	ALA	3.7
1	B	566	THR	3.7
1	B	507	GLU	3.7
1	A	100	ASP	3.6
1	D	973	ASP	3.6
1	B	310	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	110	LEU	3.6
1	A	282	THR	3.6
1	B	313	LYS	3.6
1	A	250	GLU	3.6
1	D	1083	LYS	3.6
1	C	606	GLN	3.6
1	D	1102	GLU	3.6
1	C	844	HIS	3.6
1	D	958	LEU	3.6
1	B	335	LYS	3.6
1	C	614	LEU	3.6
1	B	502	GLU	3.6
1	B	444	ARG	3.6
1	C	665	GLU	3.6
1	B	522	ARG	3.6
1	D	1086	GLU	3.6
1	B	561	ALA	3.6
1	D	1090	ARG	3.5
1	C	630	GLU	3.5
1	C	576	MET	3.5
1	C	691	SER	3.5
1	A	123	SER	3.5
1	A	172	ILE	3.5
1	B	493	ALA	3.5
1	D	919	ALA	3.5
1	C	624	GLU	3.5
1	C	764	GLU	3.5
1	D	1119	TYR	3.5
1	C	608	GLU	3.5
1	B	328	VAL	3.5
1	D	961	ALA	3.5
1	A	131	GLU	3.5
1	B	544	LEU	3.5
1	C	765	ILE	3.4
1	D	955	GLN	3.4
1	A	58	ASP	3.4
1	C	782	TYR	3.4
1	D	1091	ALA	3.4
1	D	1014	TYR	3.4
1	A	140	LYS	3.4
1	D	923	LEU	3.4
1	D	937	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	984	SER	3.4
1	D	997	GLU	3.4
1	A	78	ALA	3.4
1	C	799	LYS	3.4
1	A	75	GLU	3.4
1	C	573	LYS	3.4
1	B	470	SER	3.4
1	C	773	LYS	3.4
1	D	1107	ASP	3.4
1	B	452	LYS	3.4
1	D	1103	LYS	3.4
1	D	970	LYS	3.4
1	A	93	GLN	3.4
1	D	993	MET	3.3
1	B	336	ALA	3.3
1	B	450	ALA	3.3
1	A	273	GLU	3.3
1	B	443	ASP	3.3
1	A	241	PHE	3.3
1	B	420	LYS	3.3
1	C	686	LYS	3.3
1	A	12	LYS	3.3
1	A	249	LEU	3.3
1	B	426	GLU	3.3
1	A	222	GLU	3.3
1	B	317	GLU	3.2
1	B	305	ARG	3.2
1	A	50	LEU	3.2
1	D	890	GLN	3.2
1	D	979	MET	3.2
1	D	1026	SER	3.2
1	A	128	LYS	3.2
1	D	1008	GLU	3.2
1	B	332	LYS	3.2
1	B	417	ARG	3.2
1	B	453	LEU	3.2
1	A	13	LEU	3.2
1	C	795	VAL	3.2
1	D	983	GLU	3.2
1	A	41	ASP	3.2
1	B	441	ASP	3.2
1	C	772	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	86	ALA	3.2
1	C	684	ALA	3.2
1	D	918	ASP	3.2
1	D	986	ALA	3.2
1	B	422	GLU	3.2
1	C	845	ALA	3.2
1	D	1003	ALA	3.2
1	B	489	LYS	3.2
1	B	429	GLU	3.2
1	D	949	GLU	3.2
1	B	563	ASN	3.2
1	D	1084	LEU	3.1
1	C	623	ASP	3.1
1	C	646	ALA	3.1
1	A	105	ARG	3.1
1	B	560	HIS	3.1
1	B	523	ALA	3.1
1	B	554	ILE	3.1
1	A	231	LYS	3.1
1	B	501	LYS	3.1
1	A	259	GLU	3.1
1	D	952	ASP	3.1
1	C	683	GLU	3.1
1	C	722	ILE	3.1
1	D	1068	GLN	3.1
1	D	962	LEU	3.1
1	C	733	VAL	3.1
1	A	177	GLU	3.1
1	C	585	ASN	3.1
1	D	859	LYS	3.1
1	A	160	ARG	3.1
1	B	294	MET	3.1
1	A	139	GLU	3.1
1	C	668	ASP	3.1
1	C	758	CYS	3.1
1	C	642	ALA	3.1
1	D	980	LYS	3.0
1	C	676	THR	3.0
1	A	64	LEU	3.0
1	B	469	LEU	3.0
1	B	296	LYS	3.0
1	B	529	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	268	LYS	3.0
1	C	761	LEU	3.0
1	C	794	LYS	3.0
1	B	297	LEU	3.0
1	C	779	ALA	3.0
1	A	126	GLY	3.0
1	A	72	GLU	3.0
1	A	179	ALA	3.0
1	D	929	LYS	3.0
1	B	309	ALA	2.9
1	B	368	ASP	2.9
1	A	246	VAL	2.9
1	D	1126	LEU	2.9
1	A	212	GLU	2.9
1	B	428	GLN	2.9
1	A	120	ALA	2.9
1	D	1106	ASP	2.9
1	C	627	LYS	2.9
1	A	254	ASP	2.9
1	C	709	MET	2.9
1	D	940	LEU	2.9
1	B	440	GLU	2.9
1	A	4	ILE	2.9
1	C	843	ASP	2.9
1	D	987	GLN	2.9
1	A	256	LEU	2.9
1	D	1005	HIS	2.9
1	A	261	TYR	2.9
1	C	798	ASP	2.9
1	C	572	ILE	2.9
1	D	1004	LYS	2.9
1	C	804	GLU	2.9
1	C	616	LYS	2.9
1	C	669	ARG	2.9
1	D	857	LYS	2.9
1	A	272	GLU	2.9
1	B	527	GLU	2.9
1	D	947	PHE	2.8
1	D	1042	CYS	2.8
1	B	292	MET	2.8
1	C	674	LEU	2.8
1	D	853	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	114	GLU	2.8
1	A	211	ALA	2.8
1	C	776	GLU	2.8
1	B	395	GLN	2.8
1	D	1015	GLU	2.8
1	A	104	GLU	2.8
1	B	448	GLU	2.8
1	D	887	ARG	2.8
1	B	394	LEU	2.8
1	B	550	LYS	2.8
1	A	218	GLU	2.8
1	A	47	GLN	2.8
1	A	135	GLN	2.8
1	D	1117	LEU	2.8
1	B	385	ARG	2.8
1	B	427	ILE	2.8
1	B	442	ALA	2.8
1	D	1089	THR	2.8
1	A	258	ASP	2.8
1	B	295	LEU	2.8
1	D	1079	VAL	2.8
1	A	229	SER	2.8
1	C	681	LEU	2.8
1	B	565	MET	2.8
1	A	51	LYS	2.7
1	C	806	ARG	2.7
1	C	710	GLU	2.7
1	B	496	GLU	2.7
1	B	509	ILE	2.7
1	B	419	GLN	2.7
1	D	1033	GLU	2.7
1	B	369	VAL	2.7
1	B	402	LYS	2.7
1	B	508	GLU	2.7
1	C	679	GLN	2.7
1	B	348	LEU	2.7
1	D	873	ARG	2.7
1	B	321	LYS	2.7
1	D	1044	GLU	2.7
1	B	367	ALA	2.7
1	A	97	GLU	2.7
1	D	1031	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	1012	ARG	2.7
1	A	181	GLU	2.7
1	A	245	SER	2.7
1	A	141	MET	2.7
1	A	260	LEU	2.7
1	C	746	ARG	2.6
1	B	315	ALA	2.6
1	A	283	SER	2.6
1	B	545	TYR	2.6
1	B	413	VAL	2.6
1	D	1034	ARG	2.6
1	C	714	ILE	2.6
1	A	279	ASN	2.6
1	B	304	ASP	2.6
1	D	920	GLN	2.6
1	B	311	ALA	2.6
1	D	959	ALA	2.6
1	A	63	ALA	2.6
1	B	445	LYS	2.6
1	D	999	GLN	2.6
1	D	1088	GLU	2.6
1	A	270	ILE	2.6
1	D	1045	LEU	2.6
1	B	308	GLU	2.6
1	C	730	TYR	2.6
1	C	802	GLU	2.6
1	A	214	TYR	2.6
1	B	447	GLU	2.5
1	C	586	ALA	2.5
1	D	1025	GLU	2.5
1	C	763	GLU	2.5
1	D	1075	GLU	2.5
1	C	633	LYS	2.5
1	B	314	LYS	2.5
1	B	431	GLN	2.5
1	A	76	LYS	2.5
1	C	672	GLU	2.5
1	C	685	GLU	2.5
1	B	299	LYS	2.5
1	A	210	GLN	2.5
1	C	815	THR	2.5
1	B	516	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	931	THR	2.5
1	C	690	GLU	2.5
1	C	569	MET	2.5
1	C	791	GLU	2.5
1	A	262	ALA	2.5
1	D	1059	LEU	2.5
1	C	617	LYS	2.4
1	D	877	ALA	2.4
1	A	132	SER	2.4
1	A	276	HIS	2.4
1	D	954	ALA	2.4
1	D	1041	LYS	2.4
1	D	1001	LYS	2.4
1	B	366	GLU	2.4
1	A	230	ASP	2.4
1	B	374	ARG	2.4
1	D	917	LYS	2.4
1	D	1067	SER	2.4
1	D	976	GLU	2.4
1	D	1114	ALA	2.4
1	A	198	LYS	2.4
1	B	451	ARG	2.4
1	C	717	LYS	2.4
1	D	960	THR	2.4
1	B	456	ILE	2.4
1	D	1046	GLU	2.4
1	A	219	ASP	2.4
1	A	178	ARG	2.3
1	D	1082	ASP	2.3
1	A	162	TYR	2.3
1	A	221	TYR	2.3
1	D	1049	ILE	2.3
1	A	200	VAL	2.3
1	D	1032	GLU	2.3
1	A	129	VAL	2.3
1	B	531	THR	2.3
1	C	580	LYS	2.3
1	C	849	MET	2.3
1	C	762	GLU	2.3
1	D	1071	ASP	2.3
1	B	551	TYR	2.3
1	A	264	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	454	VAL	2.3
1	D	985	ARG	2.3
1	C	643	GLU	2.3
1	C	718	GLU	2.3
1	B	528	ARG	2.3
1	D	950	GLU	2.3
1	C	620	ALA	2.3
1	A	220	LYS	2.3
1	D	990	GLU	2.3
1	A	101	ARG	2.3
1	A	159	ASP	2.3
1	B	303	LEU	2.3
1	B	474	CYS	2.3
1	B	546	ALA	2.2
1	A	125	ARG	2.2
1	A	228	LEU	2.2
1	A	165	VAL	2.2
1	D	856	ILE	2.2
1	A	66	ASP	2.2
1	A	280	ASP	2.2
1	D	927	GLU	2.2
1	A	173	GLU	2.2
1	D	932	ASP	2.2
1	B	513	SER	2.2
1	C	847	ASN	2.2
1	B	520	GLU	2.2
1	D	957	ARG	2.2
1	C	579	LEU	2.2
1	B	504	LYS	2.2
1	A	215	SER	2.2
1	A	117	GLU	2.1
1	B	288	ILE	2.1
1	C	639	LEU	2.1
1	A	163	GLU	2.1
1	D	1002	GLU	2.1
1	A	14	ASP	2.1
1	C	647	THR	2.1
1	A	62	GLU	2.1
1	C	723	ALA	2.1
1	D	945	GLN	2.1
1	A	90	ARG	2.1
1	A	265	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	861	GLN	2.1
1	D	1038	SER	2.1
1	C	612	VAL	2.1
1	C	636	GLN	2.1
1	D	924	GLU	2.1
1	C	583	LYS	2.1
1	C	842	LEU	2.1
1	B	500	GLN	2.1
1	B	559	ASP	2.1
1	A	44	VAL	2.1
1	B	457	GLU	2.1
1	D	1027	ASP	2.1
1	A	281	MET	2.0
1	D	921	GLU	2.0
1	A	274	LEU	2.0
1	C	687	ALA	2.0
1	B	475	ALA	2.0
1	B	524	GLU	2.0
1	D	943	ARG	2.0
1	C	852	ILE	2.0
1	A	225	ILE	2.0
1	A	194	GLU	2.0
1	C	707	GLU	2.0
1	C	721	HIS	2.0
1	A	197	ILE	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 carbohydrates 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.