



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2018 – 06:27 PM EST

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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030736

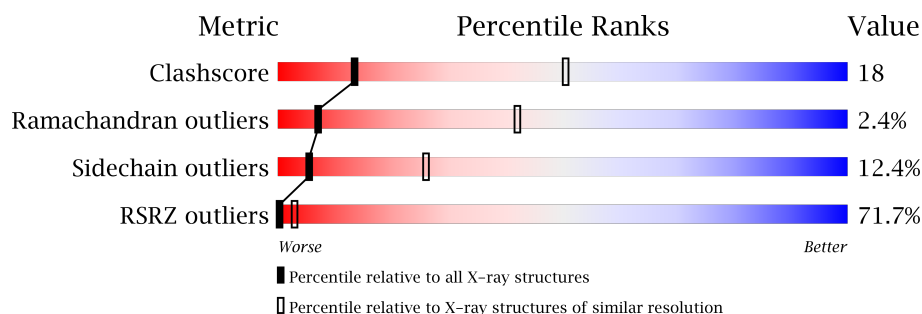
# 1 Overall quality at a glance

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	112137	1035 (10.00-3.80)
Ramachandran outliers	110173	1003 (10.00-3.76)
Sidechain outliers	110143	1098 (10.00-3.70)
RSRZ outliers	101464	1003 (10.00-3.72)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	<div> <div>70%</div> <div> <div>64%</div> <div>24%</div> <div>8%</div> <div>.</div> </div> </div>
1	B	284	<div> <div>83%</div> <div> <div>68%</div> <div>22%</div> <div>8%</div> <div>.</div> </div> </div>
1	C	284	<div> <div>68%</div> <div> <div>62%</div> <div>26%</div> <div>8%</div> <div>.</div> </div> </div>
1	D	284	<div> <div>65%</div> <div> <div>60%</div> <div>28%</div> <div>8%</div> <div>.</div> </div> </div>

## 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.

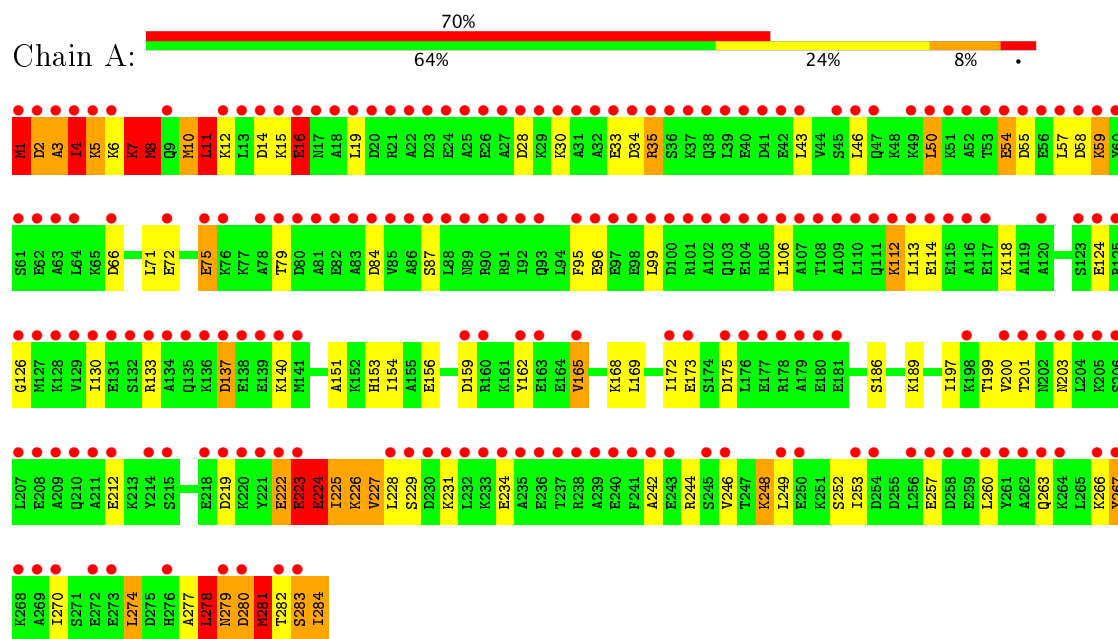
- Molecule 1 is a protein called TROPOMYOSIN.

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			

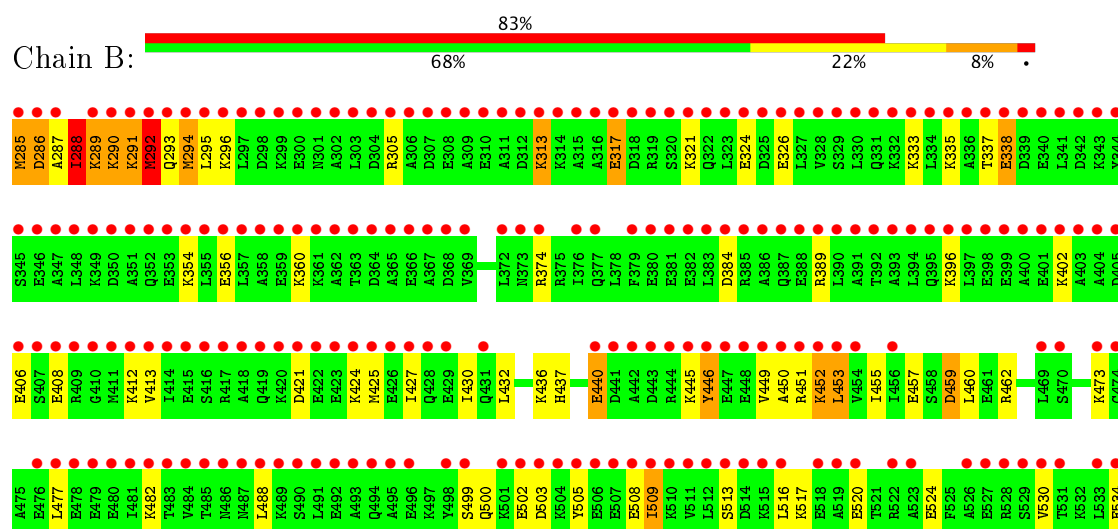
### 3 Residue-property plots

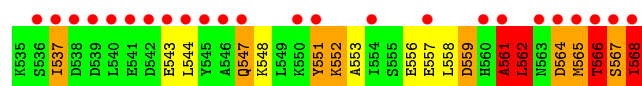
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

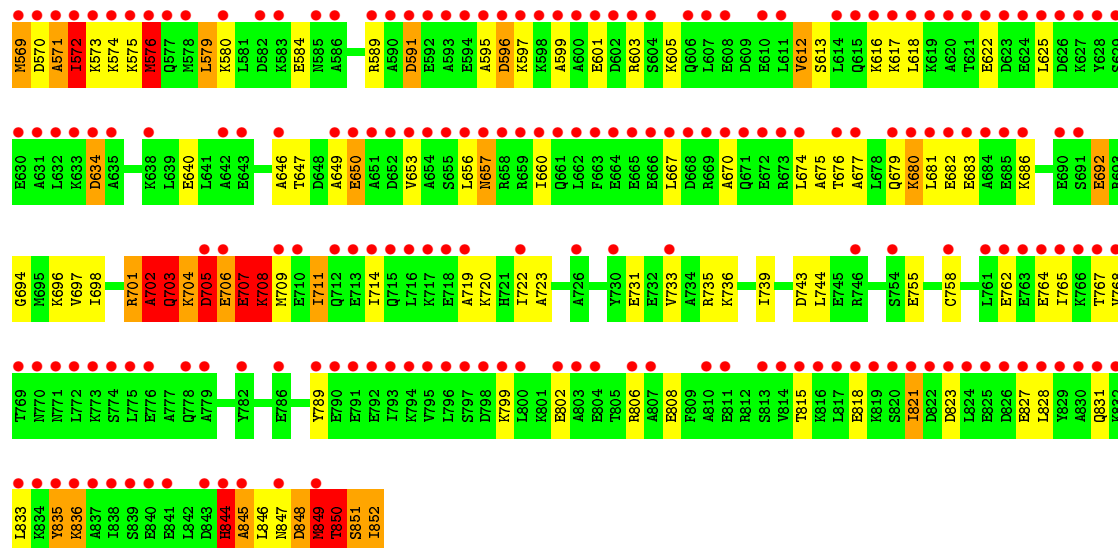


#### • Molecule 1: TROPOMYOSIN

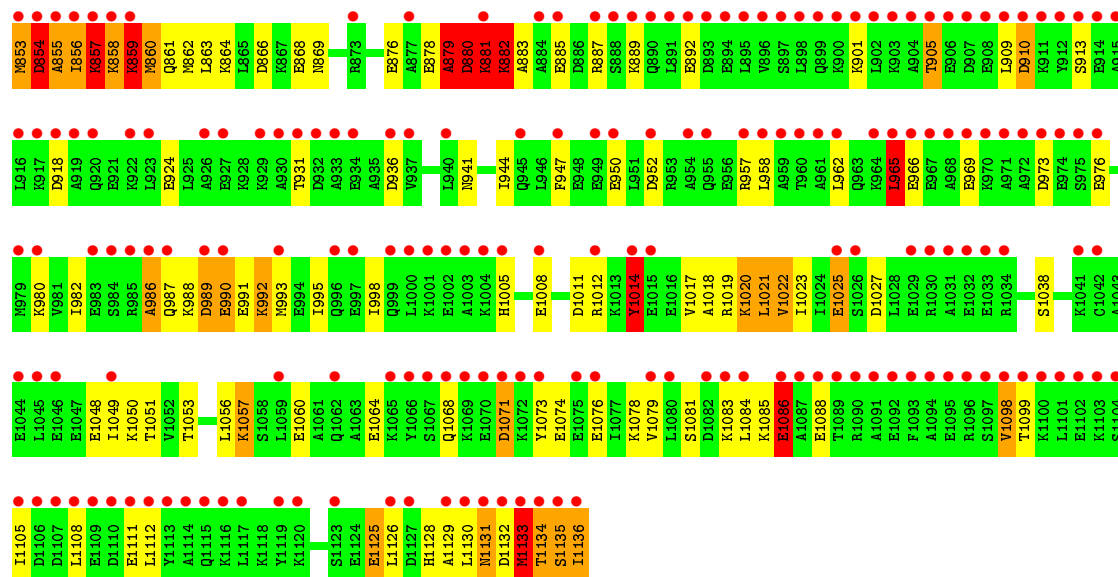




• Molecule 1: TROPOMYOSIN



• Molecule 1: TROPOMYOSIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 6.73Å)	Xtriage
Refinement program	XTALVIEW, 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 <sup>2</sup> )	210.9	Xtriage
Anisotropy	1.027	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.54 , 457.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.34$ , $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.67	EDS
Total number of atoms	9160	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	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(°)	Ideal(°)
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(°)	Ideal(°)
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(°)	Ideal(°)
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(°)	Ideal(°)
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(°)	Ideal(°)
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(°)	Ideal(°)
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 ⓘ

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: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

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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: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: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: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: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:C:702:ALA:C	1:C:708:LYS:HD3	2.22	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: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:253:ILE:O	1:A:257:GLU:HB2	2.02	0.59
1:A:7:LYS:CD	1:A:8:MET:HG2	2.33	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: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: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: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: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:B:445:LYS:O	1:B:449:VAL:HG12	2.07	0.55
1:C:572:ILE:HG13	1:C:572:ILE:CA	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: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:A:137:ASP:CG	1:A:140:LYS:HZ1	2.11	0.53
1:C:701:ARG:O	1:C:708:LYS:CD	2.56	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: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: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: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:876:GLU:O	1:D:879:ALA:HB3	2.11	0.50
1:A:242:ALA:O	1:A:246:VAL:HG23	2.12	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:114:GLU:HG2	1:A:118:LYS:NZ	2.27	0.49
1:A:1:MET:O	1:A:4:ILE:N	2.45	0.49
1:B:402:LYS:O	1:B:406:GLU:HG3	2.11	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: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:317:GLU:O	1:B:321:LYS:HG3	2.13	0.48
1:B:558:LEU:O	1:B:562:LEU:HB2	2.12	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:597:LYS:NZ	1:C:601:GLU:OE2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:A:203:ASN:HB3	1:B:488:LEU:HD11	1.98	0.46
1:B:564:ASP:C	1:B:566:THR:N	2.69	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:C:601:GLU:O	1:C:605:LYS:HG3	2.15	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: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: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: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: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:A:16:GLU:O	1:A:19:LEU:HB2	2.16	0.45
1:A:4:ILE:CG1	1:B:288:ILE:HG21	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:MET:HG2	1:B:293:GLN:HG3	1.99	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:A:75:GLU:CD	1:B:354:LYS:HZ3	2.20	0.45
1:C:653:VAL:O	1:C:657:ASN:HB2	2.16	0.45
1:B:356:GLU:OE2	1:B:360:LYS:NZ	2.49	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:D:859:LYS:H	1:D:859:LYS:CA	2.07	0.45
1:A:248:LYS:NZ	1:A:252:SER:OG	2.50	0.45
1:A:4:ILE:HG22	1:A:7:LYS:HG2	1.99	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:HG21	1:D:856:ILE:HD13	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:D:864:LYS:NZ	1:D:868:GLU:OE2	2.51	0.44
1:C:844:HIS:O	1:C:845:ALA:C	2.56	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:A:169:LEU:O	1:A:172:ILE:HG22	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:D:1108:LEU:O	1:D:1112:LEU:HD13	2.18	0.43
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:B:513:SER:O	1:B:517:LYS:NZ	2.52	0.43
1:C:649:ALA:O	1:C:653:VAL:HG23	2.19	0.43
1:C:704:LYS:O	1:C:708:LYS:CB	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ARG:NH1	1:B:324:GLU:OE2	2.51	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:C:698:ILE:HG21	1:D:982:ILE:HG23	2.01	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:D:988:LYS:O	1:D:992:LYS:HD2	2.18	0.43
1:A:151:ALA:O	1:A:154:ILE:HG22	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:54:GLU:OE1	1:B:333:LYS:NZ	2.51	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:C:848:ASP:C	1:C:851:SER:N	2.72	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:12:LYS:NZ	1:A:16:GLU:OE1	2.52	0.42
1:A:11:LEU:HD23	1:B:295:LEU:O	2.19	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: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: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: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

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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:A:7:LYS:O	1:A:10:MET:N	2.54	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: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: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:A:1:MET:H2	1:A:4:ILE:HG12	1.83	0.41
1:C:704:LYS:C	1:C:708:LYS:CG	2.89	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: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: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:612:VAL:HG22	1:C:616:LYS:HZ2	1.86	0.40
1:C:680:LYS:HZ3	1:D:965:LEU:HA	1.87	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

### 5.3.1 Protein backbone

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	35
1	B	282/284 (99%)	250 (89%)	28 (10%)	4 (1%)	13	54
1	C	282/284 (99%)	246 (87%)	30 (11%)	6 (2%)	8	45
1	D	282/284 (99%)	246 (87%)	28 (10%)	8 (3%)	6	39
All	All	1128/1136 (99%)	983 (87%)	118 (10%)	27 (2%)	7	42

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 ⓘ

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%)	3	20
1	B	245/245 (100%)	220 (90%)	25 (10%)	8	33
1	C	245/245 (100%)	217 (89%)	28 (11%)	7	28
1	D	245/245 (100%)	212 (86%)	33 (14%)	4	24
All	All	980/980 (100%)	858 (88%)	122 (12%)	5	26

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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	284/284 (100%)	3.25	200 (70%) <b>0</b> <b>3</b>	174, 174, 174, 174	0
1	B	284/284 (100%)	3.70	237 (83%) <b>0</b> <b>2</b>	174, 174, 174, 174	0
1	C	284/284 (100%)	3.41	192 (67%) <b>0</b> <b>3</b>	174, 174, 174, 174	0
1	D	284/284 (100%)	2.96	185 (65%) <b>0</b> <b>3</b>	174, 174, 174, 174	0
All	All	1136/1136 (100%)	3.33	814 (71%) <b>0</b> <b>3</b>	174, 174, 174, 174	0

All (814) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	657	ASN	14.7
1	A	2	ASP	14.6
1	C	596	ASP	12.6
1	A	36	SER	11.5
1	C	658	ARG	11.4
1	D	905	THR	11.1
1	C	660	ILE	11.0
1	C	653	VAL	10.6
1	A	30	LYS	10.6
1	A	33	GLU	10.4
1	A	40	GLU	10.1
1	B	483	THR	10.0
1	A	34	ASP	9.9
1	D	901	LYS	9.7
1	D	898	LEU	9.6
1	C	604	SER	9.4
1	A	137	ASP	9.1
1	B	380	GLU	8.9
1	C	599	ALA	8.9
1	A	25	ALA	8.9
1	A	32	ALA	8.9

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Mol	Chain	Res	Type	RSRZ
1	C	831	GLN	8.9
1	B	479	GLU	8.8
1	C	654	ALA	8.8
1	C	655	SER	8.8
1	B	346	GLU	8.8
1	C	661	GLN	8.7
1	D	858	LYS	8.7
1	C	825	GLU	8.6
1	B	480	GLU	8.6
1	C	826	ASP	8.6
1	A	29	LYS	8.6
1	D	1134	THR	8.6
1	B	342	ASP	8.5
1	B	484	VAL	8.5
1	B	286	ASP	8.5
1	C	600	ALA	8.5
1	A	39	LEU	8.3
1	C	659	ARG	8.2
1	D	894	GLU	8.2
1	A	28	ASP	8.1
1	A	35	ARG	8.1
1	D	892	GLU	7.8
1	A	20	ASP	7.8
1	C	656	LEU	7.8
1	C	840	GLU	7.7
1	B	350	ASP	7.7
1	A	38	GLN	7.7
1	D	899	GLN	7.6
1	A	22	ALA	7.6
1	C	603	ARG	7.6
1	B	343	LYS	7.6
1	C	839	SER	7.6
1	B	541	GLU	7.5
1	D	888	SER	7.5
1	C	827	GLU	7.3
1	C	629	SER	7.3
1	D	912	TYR	7.3
1	B	487	ASN	7.3
1	A	24	GLU	7.3
1	C	594	GLU	7.2
1	C	822	ASP	7.2
1	C	824	LEU	7.1

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Mol	Chain	Res	Type	RSRZ
1	C	821	ILE	7.1
1	A	21	ARG	7.1
1	D	907	ASP	7.1
1	C	828	LEU	7.0
1	D	908	GLU	7.0
1	B	407	SER	7.0
1	C	832	LYS	6.9
1	A	26	GLU	6.9
1	B	486	ASN	6.8
1	A	95	PHE	6.8
1	D	1104	SER	6.8
1	B	353	GLU	6.8
1	B	485	THR	6.8
1	C	593	ALA	6.8
1	D	911	LYS	6.8
1	A	84	ASP	6.8
1	A	3	ALA	6.7
1	B	488	LEU	6.7
1	A	205	LYS	6.7
1	B	396	LYS	6.7
1	D	902	LEU	6.6
1	C	820	SER	6.6
1	C	836	LYS	6.6
1	B	491	LEU	6.6
1	B	564	ASP	6.6
1	A	1	MET	6.6
1	A	5	LYS	6.6
1	C	829	TYR	6.6
1	C	771	ASN	6.6
1	D	1069	LYS	6.6
1	D	895	LEU	6.5
1	A	92	ILE	6.5
1	B	494	GLN	6.5
1	B	482	LYS	6.5
1	C	823	ASP	6.5
1	B	363	THR	6.5
1	B	379	PHE	6.5
1	C	664	GLU	6.4
1	A	263	GLN	6.4
1	D	906	GLU	6.4
1	D	910	ASP	6.4
1	C	597	LYS	6.4

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Mol	Chain	Res	Type	RSRZ
1	C	837	ALA	6.3
1	D	854	ASP	6.3
1	D	855	ALA	6.3
1	A	31	ALA	6.3
1	B	383	LEU	6.2
1	D	1116	LYS	6.2
1	C	607	LEU	6.2
1	D	904	ALA	6.2
1	B	492	GLU	6.1
1	A	80	ASP	6.1
1	A	111	GLN	6.1
1	B	409	ARG	6.1
1	C	595	ALA	6.1
1	A	99	LEU	6.1
1	B	543	GLU	6.1
1	A	56	GLU	6.1
1	B	384	ASP	6.1
1	B	408	GLU	6.1
1	D	897	SER	6.0
1	B	323	LEU	6.0
1	C	571	ALA	6.0
1	D	885	GLU	6.0
1	A	37	LYS	6.0
1	B	400	ALA	6.0
1	C	833	LEU	5.9
1	D	909	LEU	5.9
1	D	914	GLU	5.9
1	C	818	GLU	5.9
1	C	590	ALA	5.9
1	C	838	ILE	5.9
1	B	481	ILE	5.8
1	B	421	ASP	5.8
1	B	540	LEU	5.8
1	B	338	GLU	5.8
1	D	1133	MET	5.8
1	C	628	TYR	5.8
1	D	1101	LEU	5.8
1	D	933	ALA	5.7
1	C	841	GLU	5.7
1	D	965	LEU	5.7
1	B	393	ALA	5.7
1	B	537	ILE	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	53	THR	5.7
1	D	913	SER	5.6
1	D	891	LEU	5.6
1	A	81	ALA	5.6
1	D	1135	SER	5.6
1	B	387	GLN	5.6
1	A	96	GLU	5.6
1	D	903	LYS	5.6
1	B	337	THR	5.6
1	B	356	GLU	5.6
1	C	577	GLN	5.6
1	B	538	ASP	5.6
1	A	204	LEU	5.6
1	B	354	LYS	5.5
1	B	362	ALA	5.5
1	C	663	PHE	5.5
1	A	239	ALA	5.5
1	C	817	LEU	5.5
1	A	112	LYS	5.4
1	D	968	ALA	5.4
1	C	622	GLU	5.4
1	B	392	THR	5.4
1	A	235	ALA	5.4
1	B	418	ALA	5.4
1	C	666	GLU	5.4
1	A	60	TYR	5.4
1	B	542	ASP	5.4
1	A	82	GLU	5.4
1	D	900	LYS	5.4
1	A	103	GLN	5.4
1	A	23	ASP	5.4
1	B	339	ASP	5.4
1	B	386	ALA	5.4
1	C	650	GLU	5.3
1	B	347	ALA	5.3
1	A	127	MET	5.3
1	C	652	ASP	5.3
1	A	42	GLU	5.3
1	D	1097	SER	5.3
1	D	1112	LEU	5.3
1	C	662	LEU	5.3
1	B	415	GLU	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	202	ASN	5.2
1	A	130	ILE	5.2
1	D	974	GLU	5.2
1	D	1066	TYR	5.2
1	B	319	ARG	5.2
1	C	778	GLN	5.2
1	C	574	LYS	5.2
1	A	208	GLU	5.2
1	D	1131	ASN	5.2
1	C	670	ALA	5.2
1	A	16	GLU	5.2
1	B	345	SER	5.2
1	C	625	LEU	5.1
1	D	964	LYS	5.1
1	C	790	GLU	5.1
1	D	1108	LEU	5.1
1	A	236	GLU	5.1
1	B	406	GLU	5.1
1	A	267	TYR	5.1
1	B	376	ILE	5.1
1	A	43	LEU	5.1
1	A	201	THR	5.0
1	A	237	THR	5.0
1	B	567	SER	5.0
1	C	602	ASP	5.0
1	B	359	GLU	5.0
1	B	349	LYS	5.0
1	B	360	LYS	5.0
1	B	411	MET	5.0
1	A	88	LEU	5.0
1	D	1030	ARG	5.0
1	B	344	TYR	4.9
1	A	55	ASP	4.9
1	B	361	LYS	4.9
1	C	621	THR	4.9
1	B	358	ALA	4.9
1	C	768	VAL	4.9
1	B	499	SER	4.9
1	B	405	ASP	4.9
1	D	915	ALA	4.9
1	B	478	GLU	4.9
1	B	326	GLU	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	377	GLN	4.9
1	C	592	GLU	4.9
1	D	1096	ARG	4.8
1	B	414	ILE	4.8
1	A	27	ALA	4.8
1	A	109	ALA	4.8
1	C	774	SER	4.8
1	B	330	LEU	4.8
1	C	570	ASP	4.8
1	C	835	TYR	4.8
1	C	634	ASP	4.8
1	B	320	SER	4.7
1	D	934	GLU	4.7
1	C	667	LEU	4.7
1	D	1073	TYR	4.7
1	B	490	SER	4.7
1	C	769	THR	4.7
1	B	331	GLN	4.7
1	B	498	TYR	4.7
1	D	936	ASP	4.7
1	C	635	ALA	4.7
1	D	1115	GLN	4.7
1	B	515	LYS	4.7
1	B	298	ASP	4.7
1	D	1029	GLU	4.6
1	B	526	ALA	4.6
1	A	85	VAL	4.6
1	B	388	GLU	4.6
1	A	206	SER	4.6
1	B	324	GLU	4.6
1	A	138	GLU	4.6
1	C	610	GLU	4.6
1	B	287	ALA	4.6
1	D	969	GLU	4.6
1	B	329	SER	4.6
1	B	340	GLU	4.6
1	B	382	GLU	4.6
1	C	713	GLU	4.6
1	A	116	ALA	4.6
1	B	404	ALA	4.5
1	C	611	LEU	4.5
1	C	770	ASN	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	767	THR	4.5
1	B	495	ALA	4.5
1	B	373	ASN	4.5
1	C	575	LYS	4.5
1	A	6	LYS	4.5
1	D	889	LYS	4.5
1	C	766	LYS	4.5
1	B	533	LEU	4.5
1	A	57	LEU	4.4
1	C	810	ALA	4.4
1	C	598	LYS	4.4
1	D	893	ASP	4.4
1	A	234	GLU	4.4
1	B	506	GLU	4.4
1	B	302	ALA	4.4
1	A	9	GLN	4.4
1	B	530	VAL	4.4
1	A	79	THR	4.4
1	A	115	GLU	4.4
1	B	285	MET	4.4
1	C	813	SER	4.4
1	D	996	GLN	4.4
1	B	510	LYS	4.4
1	B	325	ASP	4.3
1	C	631	ALA	4.3
1	B	381	GLU	4.3
1	B	511	VAL	4.3
1	C	726	ALA	4.3
1	B	293	GLN	4.3
1	C	582	ASP	4.3
1	C	792	GLU	4.3
1	D	1094	ALA	4.3
1	D	975	SER	4.3
1	D	1132	ASP	4.3
1	B	514	ASP	4.3
1	B	390	LEU	4.3
1	A	113	LEU	4.3
1	B	341	LEU	4.3
1	A	108	THR	4.3
1	B	389	ARG	4.3
1	C	814	VAL	4.3
1	B	534	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	601	GLU	4.3
1	A	253	ILE	4.3
1	B	397	LEU	4.3
1	B	403	ALA	4.3
1	B	327	LEU	4.2
1	B	401	GLU	4.2
1	D	1136	ILE	4.2
1	C	705	ASP	4.2
1	A	54	GLU	4.2
1	D	1062	GLN	4.2
1	D	1130	LEU	4.2
1	B	352	GLN	4.2
1	A	15	LYS	4.2
1	A	45	SER	4.2
1	D	1100	LYS	4.2
1	D	1076	GLU	4.2
1	C	834	LYS	4.2
1	D	972	ALA	4.2
1	B	316	ALA	4.2
1	A	87	SER	4.2
1	A	133	ARG	4.2
1	C	830	ALA	4.2
1	B	410	GLY	4.2
1	D	1000	LEU	4.2
1	D	1111	GLU	4.1
1	B	333	LYS	4.1
1	A	257	GLU	4.1
1	C	626	ASP	4.1
1	A	102	ALA	4.1
1	C	638	LYS	4.1
1	A	134	ALA	4.1
1	B	301	ASN	4.1
1	B	519	ALA	4.1
1	C	807	ALA	4.1
1	C	793	ILE	4.1
1	A	242	ALA	4.1
1	A	17	ASN	4.1
1	A	52	ALA	4.1
1	B	300	GLU	4.1
1	A	46	LEU	4.0
1	B	372	LEU	4.0
1	A	83	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	334	LEU	4.0
1	C	591	ASP	4.0
1	B	307	ASP	4.0
1	B	512	LEU	4.0
1	C	706	GLU	4.0
1	B	355	LEU	4.0
1	D	1072	LYS	4.0
1	D	1087	ALA	4.0
1	B	290	LYS	4.0
1	B	364	ASP	4.0
1	B	322	GLN	4.0
1	B	412	LYS	4.0
1	D	1123	SER	4.0
1	A	61	SER	4.0
1	A	238	ARG	4.0
1	A	233	LYS	3.9
1	B	539	ASP	3.9
1	B	398	GLU	3.9
1	C	578	MET	3.9
1	C	619	LYS	3.9
1	D	1065	LYS	3.9
1	B	477	LEU	3.9
1	C	673	ARG	3.9
1	C	680	LYS	3.9
1	D	881	LYS	3.9
1	C	754	SER	3.9
1	A	106	LEU	3.9
1	B	423	GLU	3.9
1	A	232	LEU	3.9
1	A	18	ALA	3.9
1	A	136	LYS	3.9
1	D	922	LYS	3.9
1	B	557	GLU	3.8
1	B	291	LYS	3.8
1	C	796	LEU	3.8
1	D	896	VAL	3.8
1	D	1113	TYR	3.8
1	C	819	LYS	3.8
1	C	775	LEU	3.8
1	B	536	SER	3.8
1	C	716	LEU	3.8
1	C	677	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	318	ASP	3.8
1	A	89	ASN	3.8
1	A	203	ASN	3.8
1	D	1070	GLU	3.8
1	C	682	GLU	3.8
1	A	98	GLU	3.8
1	C	615	GLN	3.8
1	A	124	GLU	3.8
1	A	207	LEU	3.8
1	D	1120	LYS	3.8
1	A	49	LYS	3.8
1	A	59	LYS	3.8
1	C	589	ARG	3.8
1	D	966	GLU	3.8
1	B	365	ALA	3.7
1	D	1109	GLU	3.7
1	D	1099	THR	3.7
1	A	266	LYS	3.7
1	A	107	ALA	3.7
1	A	91	ARG	3.7
1	C	786	GLU	3.7
1	B	424	LYS	3.7
1	C	719	ALA	3.7
1	B	399	GLU	3.7
1	C	651	ALA	3.7
1	B	568	ILE	3.7
1	B	416	SER	3.7
1	C	811	GLU	3.7
1	C	715	GLN	3.7
1	C	816	LYS	3.7
1	B	473	LYS	3.7
1	A	175	ASP	3.7
1	D	971	ALA	3.7
1	B	425	MET	3.7
1	A	243	GLU	3.7
1	D	967	GLU	3.7
1	D	1105	ILE	3.7
1	B	547	GLN	3.7
1	B	391	ALA	3.6
1	D	989	ASP	3.6
1	A	240	GLU	3.6
1	B	357	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	289	LYS	3.6
1	D	1127	ASP	3.6
1	C	797	SER	3.6
1	B	503	ASP	3.6
1	D	1095	GLU	3.6
1	B	449	VAL	3.6
1	B	351	ALA	3.6
1	A	180	GLU	3.6
1	B	518	GLU	3.6
1	D	1080	LEU	3.6
1	D	1092	GLU	3.6
1	B	313	LYS	3.6
1	C	712	GLN	3.6
1	D	1083	LYS	3.6
1	A	176	LEU	3.5
1	A	19	LEU	3.5
1	B	335	LYS	3.5
1	C	632	LEU	3.5
1	C	800	LEU	3.5
1	A	223	GLU	3.5
1	C	671	GLN	3.5
1	D	1098	VAL	3.5
1	D	1110	ASP	3.5
1	B	446	TYR	3.5
1	B	476	GLU	3.5
1	A	269	ALA	3.5
1	D	930	ALA	3.5
1	D	1093	PHE	3.5
1	B	312	ASP	3.5
1	B	507	GLU	3.5
1	C	606	GLN	3.5
1	C	618	LEU	3.5
1	B	310	GLU	3.5
1	B	505	TYR	3.5
1	A	100	ASP	3.5
1	A	250	GLU	3.5
1	A	209	ALA	3.5
1	B	444	ARG	3.5
1	D	973	ASP	3.5
1	D	1102	GLU	3.5
1	C	803	ALA	3.4
1	B	522	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	502	GLU	3.4
1	D	884	ALA	3.4
1	B	306	ALA	3.4
1	D	1090	ARG	3.4
1	C	665	GLU	3.4
1	B	566	THR	3.4
1	C	844	HIS	3.4
1	D	916	LEU	3.4
1	D	1086	GLU	3.4
1	A	282	THR	3.4
1	C	789	TYR	3.4
1	C	630	GLU	3.4
1	C	691	SER	3.4
1	D	1129	ALA	3.4
1	A	110	LEU	3.4
1	C	649	ALA	3.4
1	A	123	SER	3.4
1	D	958	LEU	3.4
1	C	614	LEU	3.3
1	A	140	LYS	3.3
1	C	576	MET	3.3
1	C	624	GLU	3.3
1	C	764	GLU	3.3
1	C	608	GLU	3.3
1	D	926	ALA	3.3
1	C	799	LYS	3.3
1	C	573	LYS	3.3
1	C	773	LYS	3.3
1	A	131	GLU	3.3
1	B	452	LYS	3.3
1	D	1103	LYS	3.3
1	D	970	LYS	3.3
1	B	328	VAL	3.3
1	D	955	GLN	3.3
1	A	172	ILE	3.3
1	A	58	ASP	3.3
1	B	420	LYS	3.3
1	C	686	LYS	3.3
1	D	984	SER	3.2
1	A	12	LYS	3.2
1	D	997	GLU	3.2
1	B	470	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	561	ALA	3.2
1	A	75	GLU	3.2
1	A	93	GLN	3.2
1	B	544	LEU	3.2
1	D	937	VAL	3.2
1	C	765	ILE	3.2
1	D	1107	ASP	3.2
1	B	493	ALA	3.2
1	A	273	GLU	3.2
1	D	919	ALA	3.2
1	D	1119	TYR	3.2
1	A	128	LYS	3.2
1	B	443	ASP	3.2
1	D	923	LEU	3.2
1	D	993	MET	3.2
1	B	332	LYS	3.1
1	D	961	ALA	3.1
1	B	426	GLU	3.1
1	A	241	PHE	3.1
1	B	305	ARG	3.1
1	A	222	GLU	3.1
1	B	489	LYS	3.1
1	D	1091	ALA	3.1
1	B	317	GLU	3.1
1	C	782	TYR	3.1
1	D	890	GLN	3.1
1	B	417	ARG	3.1
1	D	1014	TYR	3.1
1	D	1026	SER	3.1
1	A	78	ALA	3.1
1	D	1008	GLU	3.1
1	B	563	ASN	3.1
1	D	983	GLU	3.0
1	A	231	LYS	3.0
1	B	501	LYS	3.0
1	D	979	MET	3.0
1	A	41	ASP	3.0
1	A	249	LEU	3.0
1	B	441	ASP	3.0
1	B	422	GLU	3.0
1	D	918	ASP	3.0
1	B	336	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	450	ALA	3.0
1	A	105	ARG	3.0
1	B	429	GLU	3.0
1	C	795	VAL	3.0
1	D	859	LYS	3.0
1	D	949	GLU	3.0
1	C	758	CYS	3.0
1	A	50	LEU	3.0
1	C	623	ASP	3.0
1	C	585	ASN	3.0
1	B	453	LEU	3.0
1	D	980	LYS	3.0
1	A	13	LEU	3.0
1	D	1068	GLN	3.0
1	A	259	GLU	3.0
1	C	772	LEU	3.0
1	C	683	GLU	3.0
1	A	160	ARG	2.9
1	D	952	ASP	2.9
1	B	296	LYS	2.9
1	B	560	HIS	2.9
1	A	177	GLU	2.9
1	A	268	LYS	2.9
1	C	794	LYS	2.9
1	A	139	GLU	2.9
1	C	668	ASP	2.9
1	D	1084	LEU	2.9
1	D	929	LYS	2.9
1	C	733	VAL	2.9
1	A	86	ALA	2.9
1	C	684	ALA	2.9
1	D	986	ALA	2.9
1	B	294	MET	2.9
1	B	554	ILE	2.9
1	C	845	ALA	2.9
1	D	1003	ALA	2.9
1	C	722	ILE	2.9
1	B	529	SER	2.9
1	D	962	LEU	2.9
1	C	627	LYS	2.8
1	C	646	ALA	2.8
1	A	72	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	523	ALA	2.8
1	D	1004	LYS	2.8
1	C	616	LYS	2.8
1	D	857	LYS	2.8
1	C	676	THR	2.8
1	A	126	GLY	2.8
1	A	212	GLU	2.8
1	B	428	GLN	2.8
1	B	368	ASP	2.8
1	A	64	LEU	2.8
1	B	469	LEU	2.8
1	D	1042	CYS	2.8
1	D	987	GLN	2.8
1	A	246	VAL	2.8
1	B	440	GLU	2.8
1	C	761	LEU	2.8
1	D	1106	ASP	2.8
1	C	642	ALA	2.8
1	B	297	LEU	2.8
1	C	669	ARG	2.8
1	A	254	ASP	2.8
1	B	550	LYS	2.8
1	C	843	ASP	2.7
1	C	804	GLU	2.7
1	C	709	MET	2.7
1	C	798	ASP	2.7
1	A	272	GLU	2.7
1	B	527	GLU	2.7
1	D	1005	HIS	2.7
1	D	1126	LEU	2.7
1	D	887	ARG	2.7
1	B	395	GLN	2.7
1	C	779	ALA	2.7
1	A	114	GLU	2.7
1	C	776	GLU	2.7
1	A	51	LYS	2.7
1	A	179	ALA	2.7
1	D	1015	GLU	2.7
1	B	385	ARG	2.7
1	A	104	GLU	2.7
1	B	448	GLU	2.7
1	D	940	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	4	ILE	2.7
1	A	47	GLN	2.7
1	A	135	GLN	2.7
1	A	256	LEU	2.7
1	B	309	ALA	2.7
1	A	218	GLU	2.7
1	B	292	MET	2.7
1	C	572	ILE	2.7
1	D	853	MET	2.7
1	A	229	SER	2.7
1	D	947	PHE	2.6
1	B	402	LYS	2.6
1	A	258	ASP	2.6
1	A	120	ALA	2.6
1	C	806	ARG	2.6
1	B	321	LYS	2.6
1	D	1079	VAL	2.6
1	C	674	LEU	2.6
1	A	261	TYR	2.6
1	C	710	GLU	2.6
1	D	1089	THR	2.6
1	B	394	LEU	2.6
1	B	419	GLN	2.6
1	B	565	MET	2.6
1	B	496	GLU	2.6
1	D	1117	LEU	2.6
1	B	427	ILE	2.6
1	D	1033	GLU	2.6
1	D	873	ARG	2.6
1	B	508	GLU	2.6
1	B	295	LEU	2.6
1	C	679	GLN	2.6
1	C	681	LEU	2.6
1	D	1012	ARG	2.6
1	A	211	ALA	2.6
1	B	445	LYS	2.5
1	D	1044	GLU	2.5
1	B	369	VAL	2.5
1	C	746	ARG	2.5
1	A	97	GLU	2.5
1	A	279	ASN	2.5
1	A	245	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	1034	ARG	2.5
1	A	181	GLU	2.5
1	A	283	SER	2.5
1	B	442	ALA	2.5
1	B	509	ILE	2.5
1	D	920	GLN	2.5
1	A	141	MET	2.5
1	D	999	GLN	2.5
1	B	304	ASP	2.5
1	C	633	LYS	2.5
1	B	413	VAL	2.5
1	B	314	LYS	2.5
1	B	348	LEU	2.5
1	A	76	LYS	2.5
1	D	1088	GLU	2.5
1	B	299	LYS	2.4
1	A	260	LEU	2.4
1	C	714	ILE	2.4
1	B	308	GLU	2.4
1	C	802	GLU	2.4
1	B	447	GLU	2.4
1	D	1025	GLU	2.4
1	B	431	GLN	2.4
1	B	367	ALA	2.4
1	C	763	GLU	2.4
1	D	1075	GLU	2.4
1	D	1031	ALA	2.4
1	C	672	GLU	2.4
1	C	617	LYS	2.4
1	A	210	GLN	2.4
1	B	315	ALA	2.4
1	C	685	GLU	2.4
1	A	270	ILE	2.4
1	B	545	TYR	2.4
1	D	1041	LYS	2.4
1	D	1001	LYS	2.4
1	C	690	GLU	2.4
1	D	1045	LEU	2.4
1	B	311	ALA	2.3
1	D	959	ALA	2.3
1	A	63	ALA	2.3
1	C	791	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	917	LYS	2.3
1	A	198	LYS	2.3
1	C	815	THR	2.3
1	A	132	SER	2.3
1	C	717	LYS	2.3
1	D	931	THR	2.3
1	C	569	MET	2.3
1	B	516	LEU	2.3
1	B	374	ARG	2.3
1	C	730	TYR	2.3
1	C	586	ALA	2.3
1	A	214	TYR	2.3
1	B	366	GLU	2.3
1	D	1067	SER	2.3
1	A	276	HIS	2.3
1	B	451	ARG	2.3
1	A	230	ASP	2.3
1	D	976	GLU	2.3
1	C	580	LYS	2.3
1	D	1059	LEU	2.3
1	A	178	ARG	2.2
1	A	264	LYS	2.2
1	D	1046	GLU	2.2
1	A	219	ASP	2.2
1	A	262	ALA	2.2
1	D	1082	ASP	2.2
1	A	220	LYS	2.2
1	D	1032	GLU	2.2
1	B	474	CYS	2.2
1	D	877	ALA	2.2
1	D	960	THR	2.2
1	D	985	ARG	2.2
1	C	762	GLU	2.2
1	B	528	ARG	2.2
1	D	954	ALA	2.2
1	A	200	VAL	2.2
1	D	1071	ASP	2.2
1	C	643	GLU	2.2
1	B	456	ILE	2.2
1	C	718	GLU	2.2
1	A	129	VAL	2.2
1	D	950	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	849	MET	2.2
1	A	101	ARG	2.2
1	B	454	VAL	2.1
1	B	531	THR	2.1
1	D	1049	ILE	2.1
1	A	125	ARG	2.1
1	D	990	GLU	2.1
1	D	1114	ALA	2.1
1	A	159	ASP	2.1
1	B	504	LYS	2.1
1	C	847	ASN	2.1
1	A	66	ASP	2.1
1	D	927	GLU	2.1
1	A	162	TYR	2.1
1	A	221	TYR	2.1
1	A	280	ASP	2.1
1	A	165	VAL	2.1
1	D	957	ARG	2.1
1	A	173	GLU	2.1
1	B	513	SER	2.1
1	B	303	LEU	2.1
1	D	932	ASP	2.1
1	B	520	GLU	2.1
1	B	551	TYR	2.1
1	A	215	SER	2.0
1	A	228	LEU	2.0
1	D	856	ILE	2.0
1	C	620	ALA	2.0
1	A	117	GLU	2.0
1	C	583	LYS	2.0
1	A	163	GLU	2.0
1	D	1002	GLU	2.0
1	B	546	ALA	2.0
1	A	62	GLU	2.0
1	A	90	ARG	2.0
1	A	14	ASP	2.0
1	D	945	GLN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.