



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2024 – 04:16 AM EST

PDB ID : 3H4P
Title : Proteasome 20S core particle from Methanocaldococcus jannaschii
Authors : Jeffrey, P.D.; Zhang, F.; Hu, M.; Tian, G.; Zhang, P.; Finley, D.; Shi, Y.
Deposited on : 2009-04-20
Resolution : 4.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

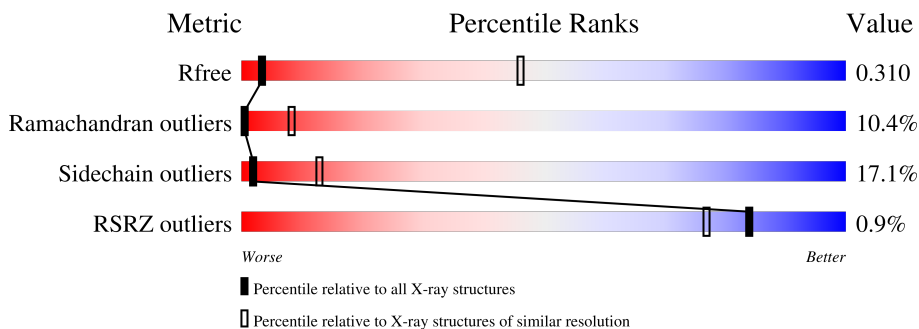
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 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))
R_{free}	130704	1193 (4.50-3.70)
Ramachandran outliers	138981	1005 (4.48-3.72)
Sidechain outliers	138945	1199 (4.50-3.70)
RSRZ outliers	127900	1034 (4.50-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	264	 2% 71% 16% • 12%
1	B	264	 % 69% 17% • 12%
1	C	264	 % 70% 16% • 12%
1	D	264	 % 69% 17% • 12%
1	E	264	 3% 68% 18% • 12%
1	F	264	 2% 68% 18% • 12%
1	G	264	 % 69% 17% • 12%

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Mol	Chain	Length	Quality of chain
1	H	264	66% 20% • 12%
1	I	264	68% 18% • 12%
1	J	264	70% 16% • 12%
1	K	264	69% 18% • 12%
1	L	264	67% 19% • 12%
1	M	264	69% 18% • 12%
1	N	264	70% 17% • 12%
2	a	219	73% 17% • 8%
2	b	219	69% 20% • 8%
2	c	219	74% 14% • 8%
2	d	219	68% 22% • 8%
2	e	219	68% 22% • 8%
2	f	219	70% 18% • 8%
2	g	219	69% 19% • 8%
2	h	219	68% 22% • 8%
2	i	219	68% 21% • 8%
2	j	219	70% 20% • 8%
2	k	219	70% 19% • 8%
2	l	219	69% 19% • 8%
2	m	219	68% 21% • 8%
2	n	219	73% 16% • 8%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 46648 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 Proteasome subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	232	1813	1150	312	346	5	0	0	0
1	B	232	1813	1150	312	346	5	0	0	0
1	C	232	1813	1150	312	346	5	0	0	0
1	D	232	1813	1150	312	346	5	0	0	0
1	E	232	1813	1150	312	346	5	0	0	0
1	F	232	1813	1150	312	346	5	0	0	0
1	G	232	1813	1150	312	346	5	0	0	0
1	H	232	1813	1150	312	346	5	0	0	0
1	I	232	1813	1150	312	346	5	0	0	0
1	J	232	1813	1150	312	346	5	0	0	0
1	K	232	1813	1150	312	346	5	0	0	0
1	L	232	1813	1150	312	346	5	0	0	0
1	M	232	1813	1150	312	346	5	0	0	0
1	N	232	1813	1150	312	346	5	0	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q60177

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP Q60177
A	0	HIS	-	expression tag	UNP Q60177
B	-2	GLY	-	expression tag	UNP Q60177
B	-1	SER	-	expression tag	UNP Q60177
B	0	HIS	-	expression tag	UNP Q60177
C	-2	GLY	-	expression tag	UNP Q60177
C	-1	SER	-	expression tag	UNP Q60177
C	0	HIS	-	expression tag	UNP Q60177
D	-2	GLY	-	expression tag	UNP Q60177
D	-1	SER	-	expression tag	UNP Q60177
D	0	HIS	-	expression tag	UNP Q60177
E	-2	GLY	-	expression tag	UNP Q60177
E	-1	SER	-	expression tag	UNP Q60177
E	0	HIS	-	expression tag	UNP Q60177
F	-2	GLY	-	expression tag	UNP Q60177
F	-1	SER	-	expression tag	UNP Q60177
F	0	HIS	-	expression tag	UNP Q60177
G	-2	GLY	-	expression tag	UNP Q60177
G	-1	SER	-	expression tag	UNP Q60177
G	0	HIS	-	expression tag	UNP Q60177
H	-2	GLY	-	expression tag	UNP Q60177
H	-1	SER	-	expression tag	UNP Q60177
H	0	HIS	-	expression tag	UNP Q60177
I	-2	GLY	-	expression tag	UNP Q60177
I	-1	SER	-	expression tag	UNP Q60177
I	0	HIS	-	expression tag	UNP Q60177
J	-2	GLY	-	expression tag	UNP Q60177
J	-1	SER	-	expression tag	UNP Q60177
J	0	HIS	-	expression tag	UNP Q60177
K	-2	GLY	-	expression tag	UNP Q60177
K	-1	SER	-	expression tag	UNP Q60177
K	0	HIS	-	expression tag	UNP Q60177
L	-2	GLY	-	expression tag	UNP Q60177
L	-1	SER	-	expression tag	UNP Q60177
L	0	HIS	-	expression tag	UNP Q60177
M	-2	GLY	-	expression tag	UNP Q60177
M	-1	SER	-	expression tag	UNP Q60177
M	0	HIS	-	expression tag	UNP Q60177
N	-2	GLY	-	expression tag	UNP Q60177
N	-1	SER	-	expression tag	UNP Q60177
N	0	HIS	-	expression tag	UNP Q60177

- Molecule 2 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	a	202	1519	964	248	298	9	0	0	0
2	b	202	1519	964	248	298	9	0	0	0
2	c	202	1519	964	248	298	9	0	0	0
2	d	202	1519	964	248	298	9	0	0	0
2	e	202	1519	964	248	298	9	0	0	0
2	f	202	1519	964	248	298	9	0	0	0
2	g	202	1519	964	248	298	9	0	0	0
2	h	202	1519	964	248	298	9	0	0	0
2	i	202	1519	964	248	298	9	0	0	0
2	j	202	1519	964	248	298	9	0	0	0
2	k	202	1519	964	248	298	9	0	0	0
2	l	202	1519	964	248	298	9	0	0	0
2	m	202	1519	964	248	298	9	0	0	0
2	n	202	1519	964	248	298	9	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	6	MET	-	expression tag	UNP Q58634
b	6	MET	-	expression tag	UNP Q58634
c	6	MET	-	expression tag	UNP Q58634
d	6	MET	-	expression tag	UNP Q58634
e	6	MET	-	expression tag	UNP Q58634
f	6	MET	-	expression tag	UNP Q58634
g	6	MET	-	expression tag	UNP Q58634
h	6	MET	-	expression tag	UNP Q58634
i	6	MET	-	expression tag	UNP Q58634
j	6	MET	-	expression tag	UNP Q58634
k	6	MET	-	expression tag	UNP Q58634
l	6	MET	-	expression tag	UNP Q58634

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Chain	Residue	Modelled	Actual	Comment	Reference
m	6	MET	-	expression tag	UNP Q58634
n	6	MET	-	expression tag	UNP Q58634



- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta

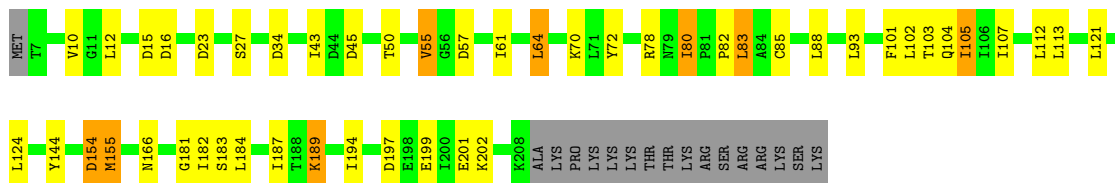


- Molecule 2: Proteasome subunit beta

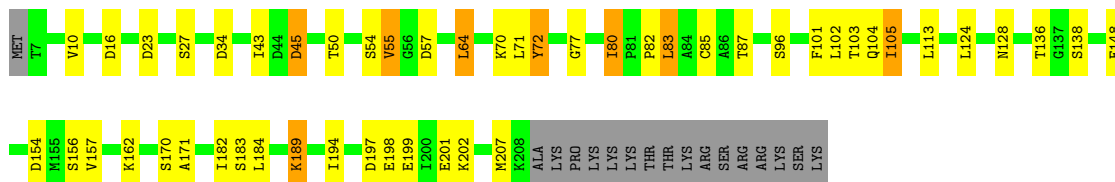


- Molecule 2: Proteasome subunit beta

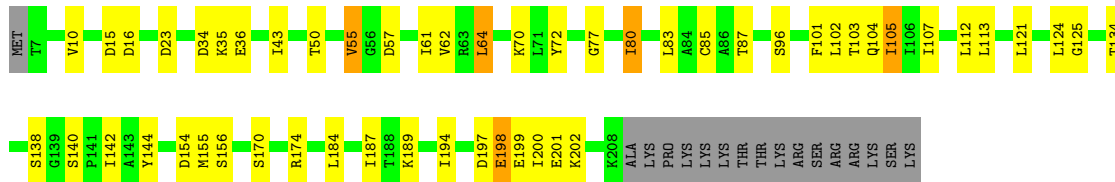




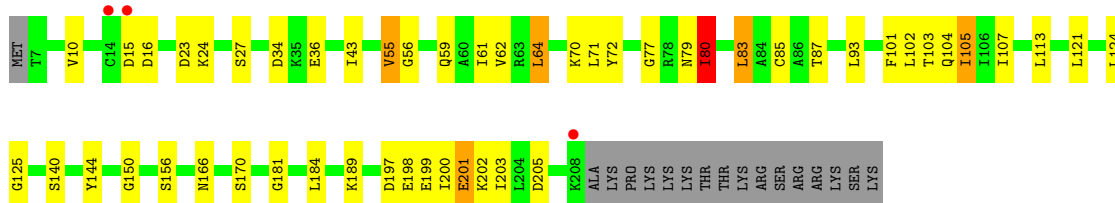
• Molecule 2: Proteasome subunit beta



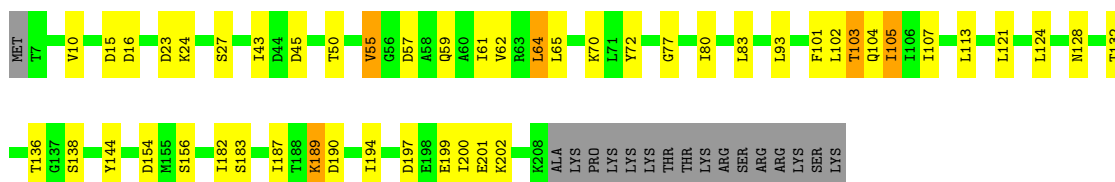
• Molecule 2: Proteasome subunit beta



• Molecule 2: Proteasome subunit beta

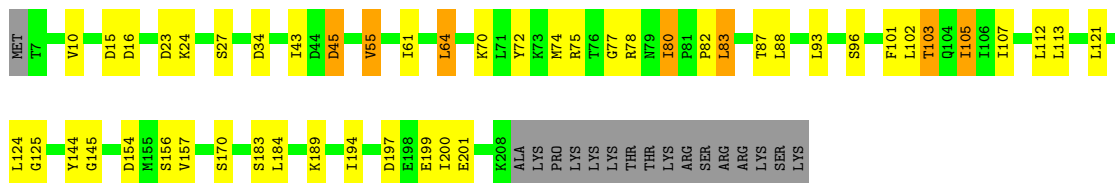


• Molecule 2: Proteasome subunit beta

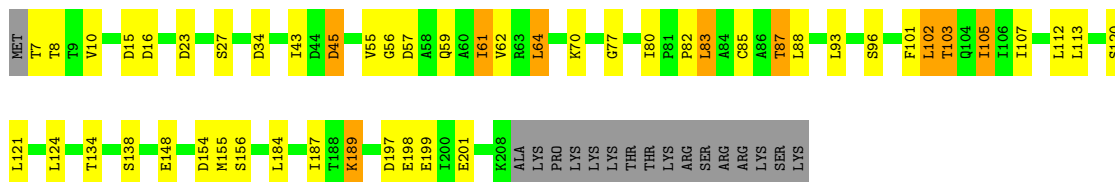


• Molecule 2: Proteasome subunit beta

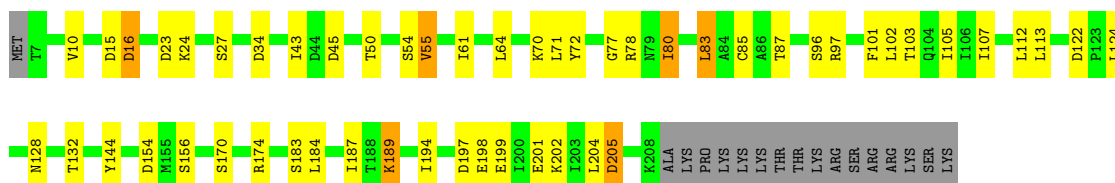




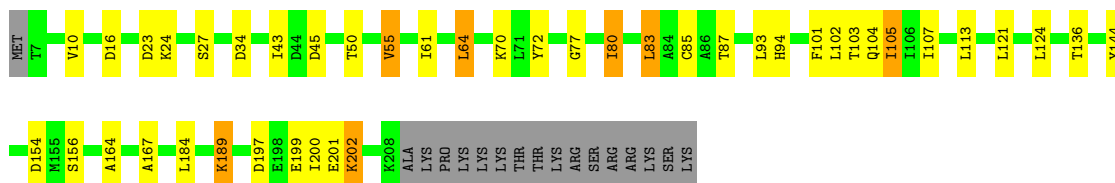
• Molecule 2: Proteasome subunit beta



• Molecule 2: Proteasome subunit beta



• Molecule 2: Proteasome subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	206.72Å 219.54Å 149.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.98 – 4.10 49.98 – 4.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.98-4.10) 99.8 (49.98-4.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 4.14Å)	Xtrriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.254 , 0.325 0.243 , 0.310	Depositor DCC
R_{free} test set	2740 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	118.1	Xtrriage
Anisotropy	0.499	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 121.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	46648	wwPDB-VP
Average B, all atoms (Å ²)	141.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.62 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6646e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.49	0/1832	0.66	0/2468
1	B	0.47	0/1832	0.67	0/2468
1	C	0.50	0/1832	0.69	0/2468
1	D	0.57	1/1832 (0.1%)	0.76	2/2468 (0.1%)
1	E	0.48	0/1832	0.69	1/2468 (0.0%)
1	F	0.57	0/1832	0.72	1/2468 (0.0%)
1	G	0.55	0/1832	0.73	0/2468
1	H	0.50	0/1832	0.69	1/2468 (0.0%)
1	I	0.49	0/1832	0.70	1/2468 (0.0%)
1	J	0.53	0/1832	0.69	0/2468
1	K	0.51	0/1832	0.69	0/2468
1	L	0.53	0/1832	0.70	0/2468
1	M	0.48	0/1832	0.67	0/2468
1	N	0.47	0/1832	0.65	0/2468
2	a	0.52	0/1536	0.72	0/2070
2	b	0.52	0/1536	0.74	1/2070 (0.0%)
2	c	0.51	0/1536	0.74	2/2070 (0.1%)
2	d	0.53	0/1536	0.77	1/2070 (0.0%)
2	e	0.55	0/1536	0.77	4/2070 (0.2%)
2	f	0.60	0/1536	0.80	1/2070 (0.0%)
2	g	0.58	0/1536	0.79	1/2070 (0.0%)
2	h	0.53	0/1536	0.75	1/2070 (0.0%)
2	i	0.57	0/1536	0.79	2/2070 (0.1%)
2	j	0.61	0/1536	0.84	1/2070 (0.0%)
2	k	0.59	0/1536	0.79	1/2070 (0.0%)
2	l	0.54	0/1536	0.79	3/2070 (0.1%)
2	m	0.51	0/1536	0.75	1/2070 (0.0%)
2	n	0.50	0/1536	0.74	1/2070 (0.0%)
All	All	0.53	1/47152 (0.0%)	0.73	26/63532 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	91	ASP	CB-CG	5.38	1.63	1.51

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	i	64	LEU	CA-CB-CG	7.58	132.73	115.30
2	e	64	LEU	CA-CB-CG	7.57	132.70	115.30
2	d	64	LEU	CA-CB-CG	7.28	132.04	115.30
2	l	64	LEU	CA-CB-CG	6.86	131.09	115.30
2	n	64	LEU	CA-CB-CG	6.73	130.77	115.30
2	j	64	LEU	CA-CB-CG	6.71	130.74	115.30
2	c	64	LEU	CA-CB-CG	6.56	130.38	115.30
1	F	191	LEU	CA-CB-CG	6.53	130.31	115.30
2	g	64	LEU	CA-CB-CG	6.52	130.29	115.30
2	k	64	LEU	CA-CB-CG	6.45	130.13	115.30
2	h	64	LEU	CA-CB-CG	6.42	130.07	115.30
2	m	64	LEU	CA-CB-CG	6.35	129.91	115.30
2	f	64	LEU	CA-CB-CG	6.16	129.48	115.30
1	D	191	LEU	CA-CB-CG	5.98	129.06	115.30
1	D	138	LEU	CA-CB-CG	-5.79	101.99	115.30
2	l	102	LEU	CA-CB-CG	5.69	128.39	115.30
2	b	64	LEU	CA-CB-CG	5.69	128.39	115.30
1	E	158	LEU	CA-CB-CG	5.57	128.10	115.30
2	i	80	ILE	CB-CA-C	-5.49	100.62	111.60
1	H	191	LEU	CA-CB-CG	5.48	127.91	115.30
2	e	28	LEU	CA-CB-CG	-5.46	102.74	115.30
2	l	88	LEU	CA-CB-CG	-5.34	103.03	115.30
2	e	80	ILE	CB-CA-C	-5.31	100.98	111.60
1	I	191	LEU	CA-CB-CG	5.05	126.93	115.30
2	e	89	LEU	CA-CB-CG	-5.04	103.70	115.30
2	c	98	MET	CB-CG-SD	5.01	127.44	112.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	230/264 (87%)	163 (71%)	43 (19%)	24 (10%)	0	8
1	B	230/264 (87%)	162 (70%)	46 (20%)	22 (10%)	0	10
1	C	230/264 (87%)	155 (67%)	51 (22%)	24 (10%)	0	8
1	D	230/264 (87%)	158 (69%)	47 (20%)	25 (11%)	0	7
1	E	230/264 (87%)	158 (69%)	47 (20%)	25 (11%)	0	7
1	F	230/264 (87%)	152 (66%)	53 (23%)	25 (11%)	0	7
1	G	230/264 (87%)	156 (68%)	51 (22%)	23 (10%)	0	9
1	H	230/264 (87%)	153 (66%)	49 (21%)	28 (12%)	0	5
1	I	230/264 (87%)	159 (69%)	44 (19%)	27 (12%)	0	6
1	J	230/264 (87%)	161 (70%)	45 (20%)	24 (10%)	0	8
1	K	230/264 (87%)	151 (66%)	51 (22%)	28 (12%)	0	5
1	L	230/264 (87%)	162 (70%)	39 (17%)	29 (13%)	0	5
1	M	230/264 (87%)	159 (69%)	45 (20%)	26 (11%)	0	6
1	N	230/264 (87%)	159 (69%)	48 (21%)	23 (10%)	0	9
2	a	200/219 (91%)	135 (68%)	45 (22%)	20 (10%)	0	9
2	b	200/219 (91%)	129 (64%)	53 (26%)	18 (9%)	1	12
2	c	200/219 (91%)	140 (70%)	45 (22%)	15 (8%)	1	15
2	d	200/219 (91%)	132 (66%)	46 (23%)	22 (11%)	0	7
2	e	200/219 (91%)	136 (68%)	46 (23%)	18 (9%)	1	12
2	f	200/219 (91%)	142 (71%)	42 (21%)	16 (8%)	1	14
2	g	200/219 (91%)	132 (66%)	43 (22%)	25 (12%)	0	5
2	h	200/219 (91%)	136 (68%)	44 (22%)	20 (10%)	0	9
2	i	200/219 (91%)	130 (65%)	46 (23%)	24 (12%)	0	5
2	j	200/219 (91%)	145 (72%)	39 (20%)	16 (8%)	1	14
2	k	200/219 (91%)	126 (63%)	50 (25%)	24 (12%)	0	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	l	200/219 (91%)	143 (72%)	37 (18%)	20 (10%)	0	9
2	m	200/219 (91%)	139 (70%)	43 (22%)	18 (9%)	1	12
2	n	200/219 (91%)	136 (68%)	46 (23%)	18 (9%)	1	12
All	All	6020/6762 (89%)	4109 (68%)	1284 (21%)	627 (10%)	0	8

All (627) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	TYR
1	A	43	CYS
1	A	132	PRO
1	A	155	SER
1	A	168	SER
1	A	191	LEU
1	A	208	GLU
1	A	219	ASP
1	B	19	GLU
1	B	23	TYR
1	B	43	CYS
1	B	155	SER
1	B	208	GLU
1	B	219	ASP
1	C	23	TYR
1	C	25	VAL
1	C	43	CYS
1	C	168	SER
1	C	208	GLU
1	C	219	ASP
1	D	19	GLU
1	D	23	TYR
1	D	43	CYS
1	D	115	LYS
1	D	155	SER
1	D	208	GLU
1	D	219	ASP
1	E	23	TYR
1	E	43	CYS
1	E	168	SER
1	E	208	GLU
1	E	219	ASP
1	F	19	GLU

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Mol	Chain	Res	Type
1	F	23	TYR
1	F	43	CYS
1	F	154	PRO
1	F	155	SER
1	F	168	SER
1	F	208	GLU
1	F	219	ASP
1	G	19	GLU
1	G	23	TYR
1	G	43	CYS
1	G	168	SER
1	G	178	GLU
1	G	219	ASP
2	a	70	LYS
2	a	103	THR
2	a	201	GLU
2	b	54	SER
2	b	55	VAL
2	b	70	LYS
2	b	103	THR
2	b	156	SER
2	b	197	ASP
2	c	103	THR
2	c	156	SER
2	c	197	ASP
2	d	55	VAL
2	d	70	LYS
2	d	103	THR
2	d	105	ILE
2	d	156	SER
2	d	174	ARG
2	d	197	ASP
2	e	55	VAL
2	e	103	THR
2	e	197	ASP
2	f	83	LEU
2	f	103	THR
2	f	197	ASP
2	g	45	ASP
2	g	64	LEU
2	g	83	LEU
2	g	103	THR

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Mol	Chain	Res	Type
2	g	105	ILE
2	g	197	ASP
1	H	19	GLU
1	H	23	TYR
1	H	43	CYS
1	H	91	ASP
1	H	155	SER
1	H	191	LEU
1	H	208	GLU
1	I	23	TYR
1	I	43	CYS
1	I	130	VAL
1	I	204	ASP
1	I	208	GLU
1	I	219	ASP
1	I	243	GLU
1	J	23	TYR
1	J	43	CYS
1	J	154	PRO
1	J	168	SER
1	J	191	LEU
1	J	208	GLU
1	J	219	ASP
1	K	19	GLU
1	K	23	TYR
1	K	43	CYS
1	K	155	SER
1	K	208	GLU
1	K	219	ASP
1	L	19	GLU
1	L	23	TYR
1	L	43	CYS
1	L	91	ASP
1	L	208	GLU
1	L	219	ASP
1	M	19	GLU
1	M	23	TYR
1	M	43	CYS
1	M	155	SER
1	M	168	SER
1	M	191	LEU
1	M	208	GLU

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Mol	Chain	Res	Type
1	M	219	ASP
1	N	23	TYR
1	N	43	CYS
1	N	91	ASP
1	N	168	SER
1	N	208	GLU
1	N	219	ASP
2	h	103	THR
2	h	156	SER
2	h	197	ASP
2	h	200	ILE
2	h	201	GLU
2	i	55	VAL
2	i	70	LYS
2	i	103	THR
2	i	105	ILE
2	i	156	SER
2	i	170	SER
2	i	197	ASP
2	i	201	GLU
2	j	103	THR
2	j	105	ILE
2	j	156	SER
2	j	197	ASP
2	j	201	GLU
2	k	45	ASP
2	k	75	ARG
2	k	103	THR
2	k	105	ILE
2	k	156	SER
2	k	170	SER
2	k	197	ASP
2	l	55	VAL
2	l	70	LYS
2	l	83	LEU
2	l	103	THR
2	l	105	ILE
2	l	156	SER
2	l	197	ASP
2	m	54	SER
2	m	103	THR
2	m	156	SER

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Mol	Chain	Res	Type
2	m	197	ASP
2	n	103	THR
2	n	156	SER
2	n	201	GLU
1	A	91	ASP
1	A	170	ARG
1	A	237	VAL
1	B	21	ARG
1	B	25	VAL
1	B	56	THR
1	B	168	SER
1	C	91	ASP
1	C	115	LYS
1	C	130	VAL
1	C	154	PRO
1	C	191	LEU
1	D	55	ILE
1	D	65	ILE
1	D	154	PRO
1	D	178	GLU
1	D	183	ASP
1	D	191	LEU
1	D	237	VAL
1	E	65	ILE
1	E	91	ASP
1	E	130	VAL
1	E	155	SER
1	E	191	LEU
1	F	21	ARG
1	F	35	GLY
1	F	65	ILE
1	F	130	VAL
1	F	185	ILE
1	F	191	LEU
1	G	80	SER
1	G	91	ASP
1	G	120	ILE
1	G	130	VAL
1	G	154	PRO
1	G	155	SER
1	G	163	ALA
1	G	183	ASP

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Mol	Chain	Res	Type
2	a	55	VAL
2	a	83	LEU
2	a	105	ILE
2	a	148	GLU
2	a	156	SER
2	a	197	ASP
2	b	64	LEU
2	b	77	GLY
2	b	83	LEU
2	c	24	LYS
2	c	64	LEU
2	c	70	LYS
2	c	77	GLY
2	c	105	ILE
2	d	45	ASP
2	d	77	GLY
2	e	36	GLU
2	e	54	SER
2	e	70	LYS
2	e	77	GLY
2	e	105	ILE
2	f	55	VAL
2	f	64	LEU
2	f	70	LYS
2	f	105	ILE
2	f	112	LEU
2	g	54	SER
2	g	55	VAL
2	g	70	LYS
2	g	77	GLY
2	g	104	GLN
2	g	156	SER
2	g	171	ALA
1	H	56	THR
1	H	115	LYS
1	H	129	GLY
1	H	154	PRO
1	H	178	GLU
1	H	204	ASP
1	H	219	ASP
1	H	228	GLU
1	H	230	ILE

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Mol	Chain	Res	Type
1	H	237	VAL
1	I	19	GLU
1	I	91	ASP
1	I	115	LYS
1	I	155	SER
1	I	168	SER
1	I	170	ARG
1	I	191	LEU
1	J	19	GLU
1	J	56	THR
1	J	65	ILE
1	J	155	SER
1	K	35	GLY
1	K	44	LYS
1	K	80	SER
1	K	91	ASP
1	K	132	PRO
1	K	168	SER
1	K	178	GLU
1	K	183	ASP
1	K	237	VAL
1	K	243	GLU
1	L	56	THR
1	L	73	ASP
1	L	115	LYS
1	L	154	PRO
1	L	155	SER
1	L	163	ALA
1	L	168	SER
1	L	178	GLU
1	L	237	VAL
1	M	25	VAL
1	M	91	ASP
1	M	163	ALA
1	M	237	VAL
1	N	55	ILE
1	N	163	ALA
1	N	178	GLU
1	N	237	VAL
2	h	36	GLU
2	h	55	VAL
2	h	62	VAL

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Mol	Chain	Res	Type
2	h	64	LEU
2	h	70	LYS
2	h	174	ARG
2	i	36	GLU
2	i	56	GLY
2	i	77	GLY
2	i	79	ASN
2	i	83	LEU
2	i	200	ILE
2	j	64	LEU
2	j	70	LYS
2	j	77	GLY
2	j	189	LYS
2	j	200	ILE
2	k	55	VAL
2	k	61	ILE
2	k	64	LEU
2	k	70	LYS
2	k	83	LEU
2	k	157	VAL
2	k	201	GLU
2	l	45	ASP
2	l	59	GLN
2	l	77	GLY
2	l	112	LEU
2	l	148	GLU
2	m	55	VAL
2	m	77	GLY
2	m	112	LEU
2	m	170	SER
2	m	201	GLU
2	m	204	LEU
2	n	24	LYS
2	n	77	GLY
2	n	197	ASP
2	n	200	ILE
1	A	19	GLU
1	A	130	VAL
1	A	154	PRO
1	A	163	ALA
1	A	174	MET
1	A	178	GLU

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Mol	Chain	Res	Type
1	A	183	ASP
1	B	91	ASP
1	B	104	TYR
1	B	154	PRO
1	B	191	LEU
1	B	232	LYS
1	C	19	GLU
1	C	21	ARG
1	C	236	LYS
1	D	33	ARG
1	D	56	THR
1	D	228	GLU
1	E	19	GLU
1	E	154	PRO
1	E	170	ARG
1	F	104	TYR
1	F	183	ASP
1	F	236	LYS
1	G	104	TYR
1	G	228	GLU
2	a	77	GLY
2	a	112	LEU
2	a	189	LYS
2	a	200	ILE
2	b	112	LEU
2	b	201	GLU
2	b	207	MET
2	c	83	LEU
2	c	202	LYS
2	d	138	SER
2	e	155	MET
2	f	78	ARG
2	f	155	MET
2	f	181	GLY
2	f	189	LYS
2	f	201	GLU
2	g	71	LEU
2	g	157	VAL
2	g	170	SER
2	g	182	ILE
2	g	201	GLU
1	H	163	ALA

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Mol	Chain	Res	Type
1	H	168	SER
1	I	55	ILE
1	I	154	PRO
1	J	55	ILE
1	J	178	GLU
1	J	183	ASP
1	J	185	ILE
1	J	197	ALA
1	J	204	ASP
1	K	65	ILE
1	K	104	TYR
1	K	154	PRO
1	K	163	ALA
1	K	193	LEU
1	L	44	LYS
1	L	174	MET
1	L	204	ASP
1	M	21	ARG
1	M	104	TYR
1	M	154	PRO
1	M	157	ALA
1	M	178	GLU
1	N	21	ARG
1	N	56	THR
1	N	154	PRO
1	N	183	ASP
1	N	191	LEU
1	N	232	LYS
2	h	77	GLY
2	h	170	SER
2	i	71	LEU
2	j	24	LYS
2	j	59	GLN
2	j	138	SER
2	k	74	MET
2	k	77	GLY
2	k	78	ARG
2	l	189	LYS
2	m	24	LYS
2	m	70	LYS
2	m	189	LYS
2	n	55	VAL

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Mol	Chain	Res	Type
2	n	64	LEU
2	n	70	LYS
2	n	105	ILE
2	n	189	LYS
1	A	55	ILE
1	A	56	THR
1	A	228	GLU
1	B	183	ASP
1	C	114	ALA
1	C	155	SER
1	C	163	ALA
1	C	183	ASP
1	C	237	VAL
1	D	15	VAL
1	D	163	ALA
1	D	193	LEU
1	E	104	TYR
1	E	115	LYS
1	E	163	ALA
1	E	236	LYS
1	F	56	THR
1	F	91	ASP
1	G	115	LYS
1	G	191	LEU
2	a	59	GLN
2	a	138	SER
2	c	16	ASP
2	d	24	LYS
2	d	80	ILE
2	d	112	LEU
2	d	125	GLY
2	d	146	VAL
2	d	170	SER
2	d	201	GLU
2	e	112	LEU
2	e	166	ASN
2	e	181	GLY
2	e	201	GLU
2	f	80	ILE
2	g	207	MET
1	H	21	ARG
1	H	65	ILE

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Mol	Chain	Res	Type
1	H	130	VAL
1	I	21	ARG
1	I	104	TYR
1	I	163	ALA
1	J	237	VAL
1	K	24	GLN
1	K	124	TYR
1	K	228	GLU
1	L	16	PHE
1	L	130	VAL
1	L	183	ASP
1	L	191	LEU
1	L	228	GLU
1	M	144	LYS
1	M	174	MET
1	M	183	ASP
1	N	19	GLU
2	h	105	ILE
2	h	112	LEU
2	h	125	GLY
2	i	62	VAL
2	i	64	LEU
2	i	150	GLY
2	j	65	LEU
2	k	112	LEU
2	l	56	GLY
2	l	64	LEU
2	m	16	ASP
2	m	78	ARG
2	m	83	LEU
2	m	174	ARG
2	n	83	LEU
2	n	164	ALA
2	n	167	ALA
1	A	73	ASP
1	A	104	TYR
1	A	236	LYS
1	B	157	ALA
1	B	204	ASP
1	B	228	GLU
1	C	104	TYR
1	C	174	MET

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Mol	Chain	Res	Type
1	D	25	VAL
1	D	104	TYR
1	D	174	MET
1	D	236	LYS
1	E	80	SER
1	E	87	ARG
1	E	185	ILE
1	F	80	SER
1	F	204	ASP
1	G	208	GLU
2	a	64	LEU
2	a	78	ARG
2	a	80	ILE
2	a	170	SER
2	b	24	LYS
2	b	189	LYS
2	c	189	LYS
2	d	98	MET
2	e	65	LEU
2	e	80	ILE
2	f	166	ASN
2	g	72	TYR
2	g	80	ILE
2	g	82	PRO
2	g	148	GLU
2	g	162	LYS
1	H	44	LYS
1	H	183	ASP
1	I	44	LYS
1	I	65	ILE
1	I	183	ASP
1	I	228	GLU
1	I	237	VAL
1	J	87	ARG
1	J	91	ASP
1	J	104	TYR
1	J	145	ASN
1	K	73	ASP
1	K	197	ALA
1	L	15	VAL
1	L	114	ALA
1	L	145	ASN

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Mol	Chain	Res	Type
1	M	195	ILE
1	M	228	GLU
1	N	62	ILE
1	N	104	TYR
1	N	155	SER
1	N	236	LYS
2	h	80	ILE
2	h	138	SER
2	h	198	GLU
2	i	24	LYS
2	i	59	GLN
2	i	80	ILE
2	j	55	VAL
2	k	24	LYS
2	l	8	THR
2	l	61	ILE
1	B	237	VAL
1	C	56	THR
1	F	47	VAL
1	G	35	GLY
1	G	157	ALA
1	G	185	ILE
1	G	204	ASP
2	a	125	GLY
2	b	80	ILE
2	b	82	PRO
2	b	200	ILE
2	c	55	VAL
2	c	80	ILE
2	c	112	LEU
2	d	124	LEU
2	d	159	GLU
2	e	24	LYS
2	g	189	LYS
1	H	87	ARG
1	H	114	ALA
1	K	236	LYS
1	M	132	PRO
1	N	96	GLU
2	h	142	ILE
2	i	125	GLY
2	i	166	ASN

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Mol	Chain	Res	Type
2	k	125	GLY
2	k	145	GLY
2	l	87	THR
2	n	80	ILE
2	n	94	HIS
2	n	202	LYS
1	B	185	ILE
1	E	132	PRO
1	E	237	VAL
1	F	55	ILE
1	F	120	ILE
1	F	237	VAL
2	d	142	ILE
1	H	128	GLY
1	H	185	ILE
1	I	156	GLY
1	J	88	VAL
1	K	130	VAL
1	L	132	PRO
1	L	170	ARG
1	M	55	ILE
1	M	65	ILE
1	M	185	ILE
2	l	62	VAL
2	m	80	ILE
1	C	132	PRO
2	d	62	VAL
1	I	129	GLY
1	I	185	ILE
2	i	181	GLY
1	B	65	ILE
1	E	15	VAL
1	E	35	GLY
1	E	88	VAL
2	e	145	GLY
2	f	82	PRO
1	L	230	ILE
2	j	62	VAL
2	k	80	ILE
2	k	200	ILE
2	l	82	PRO
1	C	15	VAL

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Mol	Chain	Res	Type
1	D	185	ILE
2	e	203	ILE
1	J	15	VAL
1	N	230	ILE
2	k	82	PRO
2	b	146	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	195/224 (87%)	171 (88%)	24 (12%)	4 22
1	B	195/224 (87%)	167 (86%)	28 (14%)	3 18
1	C	195/224 (87%)	170 (87%)	25 (13%)	4 21
1	D	195/224 (87%)	170 (87%)	25 (13%)	4 21
1	E	195/224 (87%)	166 (85%)	29 (15%)	3 17
1	F	195/224 (87%)	165 (85%)	30 (15%)	2 16
1	G	195/224 (87%)	166 (85%)	29 (15%)	3 17
1	H	195/224 (87%)	162 (83%)	33 (17%)	2 14
1	I	195/224 (87%)	166 (85%)	29 (15%)	3 17
1	J	195/224 (87%)	170 (87%)	25 (13%)	4 21
1	K	195/224 (87%)	170 (87%)	25 (13%)	4 21
1	L	195/224 (87%)	166 (85%)	29 (15%)	3 17
1	M	195/224 (87%)	169 (87%)	26 (13%)	4 21
1	N	195/224 (87%)	170 (87%)	25 (13%)	4 21
2	a	163/179 (91%)	135 (83%)	28 (17%)	2 12
2	b	163/179 (91%)	126 (77%)	37 (23%)	1 5
2	c	163/179 (91%)	133 (82%)	30 (18%)	1 10
2	d	163/179 (91%)	128 (78%)	35 (22%)	1 6
2	e	163/179 (91%)	129 (79%)	34 (21%)	1 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	f	163/179 (91%)	125 (77%)	38 (23%)	1	5
2	g	163/179 (91%)	131 (80%)	32 (20%)	1	8
2	h	163/179 (91%)	126 (77%)	37 (23%)	1	5
2	i	163/179 (91%)	132 (81%)	31 (19%)	1	9
2	j	163/179 (91%)	126 (77%)	37 (23%)	1	5
2	k	163/179 (91%)	132 (81%)	31 (19%)	1	9
2	l	163/179 (91%)	127 (78%)	36 (22%)	1	6
2	m	163/179 (91%)	124 (76%)	39 (24%)	0	5
2	n	163/179 (91%)	132 (81%)	31 (19%)	1	9
All	All	5012/5642 (89%)	4154 (83%)	858 (17%)	2	13

All (858) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	VAL
1	A	17	SER
1	A	19	GLU
1	A	37	THR
1	A	45	ASP
1	A	51	VAL
1	A	58	LYS
1	A	60	VAL
1	A	68	ILE
1	A	73	ASP
1	A	82	LEU
1	A	83	VAL
1	A	90	ILE
1	A	117	ILE
1	A	135	VAL
1	A	153	ASP
1	A	159	ILE
1	A	184	ASP
1	A	205	ILE
1	A	208	GLU
1	A	211	ASP
1	A	212	VAL
1	A	225	ILE
1	A	242	ASN
1	B	17	SER

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Mol	Chain	Res	Type
1	B	19	GLU
1	B	36	THR
1	B	45	ASP
1	B	51	VAL
1	B	55	ILE
1	B	58	LYS
1	B	60	VAL
1	B	68	ILE
1	B	82	LEU
1	B	83	VAL
1	B	88	VAL
1	B	90	ILE
1	B	102	LEU
1	B	117	ILE
1	B	121	LYS
1	B	135	VAL
1	B	136	SER
1	B	139	ILE
1	B	153	ASP
1	B	159	ILE
1	B	180	GLU
1	B	205	ILE
1	B	208	GLU
1	B	211	ASP
1	B	222	PHE
1	B	225	ILE
1	B	242	ASN
1	C	15	VAL
1	C	17	SER
1	C	19	GLU
1	C	36	THR
1	C	37	THR
1	C	45	ASP
1	C	49	LEU
1	C	58	LYS
1	C	68	ILE
1	C	82	LEU
1	C	83	VAL
1	C	95	LEU
1	C	99	ILE
1	C	117	ILE
1	C	118	CYS

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Mol	Chain	Res	Type
1	C	121	LYS
1	C	135	VAL
1	C	153	ASP
1	C	159	ILE
1	C	193	LEU
1	C	205	ILE
1	C	208	GLU
1	C	210	VAL
1	C	212	VAL
1	C	242	ASN
1	D	15	VAL
1	D	19	GLU
1	D	37	THR
1	D	45	ASP
1	D	49	LEU
1	D	58	LYS
1	D	60	VAL
1	D	68	ILE
1	D	82	LEU
1	D	88	VAL
1	D	90	ILE
1	D	102	LEU
1	D	117	ILE
1	D	121	LYS
1	D	135	VAL
1	D	153	ASP
1	D	159	ILE
1	D	180	GLU
1	D	205	ILE
1	D	208	GLU
1	D	210	VAL
1	D	211	ASP
1	D	212	VAL
1	D	222	PHE
1	D	242	ASN
1	E	13	ILE
1	E	15	VAL
1	E	19	GLU
1	E	36	THR
1	E	37	THR
1	E	45	ASP
1	E	49	LEU

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Mol	Chain	Res	Type
1	E	55	ILE
1	E	58	LYS
1	E	60	VAL
1	E	67	LYS
1	E	68	ILE
1	E	82	LEU
1	E	103	THR
1	E	117	ILE
1	E	121	LYS
1	E	130	VAL
1	E	135	VAL
1	E	153	ASP
1	E	159	ILE
1	E	180	GLU
1	E	184	ASP
1	E	205	ILE
1	E	208	GLU
1	E	210	VAL
1	E	211	ASP
1	E	212	VAL
1	E	222	PHE
1	E	242	ASN
1	F	13	ILE
1	F	15	VAL
1	F	19	GLU
1	F	25	VAL
1	F	36	THR
1	F	37	THR
1	F	45	ASP
1	F	47	VAL
1	F	58	LYS
1	F	60	VAL
1	F	68	ILE
1	F	79	THR
1	F	82	LEU
1	F	88	VAL
1	F	90	ILE
1	F	109	SER
1	F	117	ILE
1	F	118	CYS
1	F	121	LYS
1	F	135	VAL

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Mol	Chain	Res	Type
1	F	136	SER
1	F	159	ILE
1	F	168	SER
1	F	177	LEU
1	F	180	GLU
1	F	205	ILE
1	F	208	GLU
1	F	211	ASP
1	F	222	PHE
1	F	242	ASN
1	G	13	ILE
1	G	15	VAL
1	G	17	SER
1	G	19	GLU
1	G	36	THR
1	G	45	ASP
1	G	55	ILE
1	G	58	LYS
1	G	60	VAL
1	G	68	ILE
1	G	82	LEU
1	G	83	VAL
1	G	88	VAL
1	G	102	LEU
1	G	103	THR
1	G	117	ILE
1	G	121	LYS
1	G	135	VAL
1	G	153	ASP
1	G	159	ILE
1	G	168	SER
1	G	180	GLU
1	G	205	ILE
1	G	208	GLU
1	G	210	VAL
1	G	211	ASP
1	G	212	VAL
1	G	222	PHE
1	G	242	ASN
2	a	10	VAL
2	a	15	ASP
2	a	16	ASP

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Mol	Chain	Res	Type
2	a	23	ASP
2	a	27	SER
2	a	43	ILE
2	a	45	ASP
2	a	50	THR
2	a	55	VAL
2	a	57	ASP
2	a	80	ILE
2	a	83	LEU
2	a	85	CYS
2	a	87	THR
2	a	93	LEU
2	a	96	SER
2	a	101	PHE
2	a	102	LEU
2	a	105	ILE
2	a	124	LEU
2	a	128	ASN
2	a	136	THR
2	a	144	TYR
2	a	154	ASP
2	a	187	ILE
2	a	189	LYS
2	a	194	ILE
2	a	199	GLU
2	b	10	VAL
2	b	15	ASP
2	b	16	ASP
2	b	23	ASP
2	b	27	SER
2	b	30	ASN
2	b	34	ASP
2	b	43	ILE
2	b	45	ASP
2	b	50	THR
2	b	55	VAL
2	b	61	ILE
2	b	72	TYR
2	b	80	ILE
2	b	83	LEU
2	b	85	CYS
2	b	97	ARG

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Mol	Chain	Res	Type
2	b	101	PHE
2	b	102	LEU
2	b	104	GLN
2	b	105	ILE
2	b	107	ILE
2	b	113	LEU
2	b	121	LEU
2	b	122	ASP
2	b	124	LEU
2	b	128	ASN
2	b	134	THR
2	b	144	TYR
2	b	154	ASP
2	b	188	THR
2	b	189	LYS
2	b	194	ILE
2	b	198	GLU
2	b	199	GLU
2	b	201	GLU
2	b	202	LYS
2	c	10	VAL
2	c	15	ASP
2	c	16	ASP
2	c	23	ASP
2	c	27	SER
2	c	34	ASP
2	c	35	LYS
2	c	43	ILE
2	c	50	THR
2	c	55	VAL
2	c	61	ILE
2	c	72	TYR
2	c	80	ILE
2	c	83	LEU
2	c	85	CYS
2	c	93	LEU
2	c	97	ARG
2	c	101	PHE
2	c	102	LEU
2	c	104	GLN
2	c	105	ILE
2	c	107	ILE

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Mol	Chain	Res	Type
2	c	113	LEU
2	c	124	LEU
2	c	154	ASP
2	c	184	LEU
2	c	189	LYS
2	c	194	ILE
2	c	199	GLU
2	c	202	LYS
2	d	7	THR
2	d	10	VAL
2	d	15	ASP
2	d	16	ASP
2	d	23	ASP
2	d	27	SER
2	d	34	ASP
2	d	43	ILE
2	d	55	VAL
2	d	57	ASP
2	d	59	GLN
2	d	72	TYR
2	d	78	ARG
2	d	80	ILE
2	d	83	LEU
2	d	85	CYS
2	d	87	THR
2	d	93	LEU
2	d	101	PHE
2	d	102	LEU
2	d	103	THR
2	d	105	ILE
2	d	113	LEU
2	d	120	SER
2	d	121	LEU
2	d	124	LEU
2	d	128	ASN
2	d	140	SER
2	d	144	TYR
2	d	154	ASP
2	d	184	LEU
2	d	187	ILE
2	d	189	LYS
2	d	194	ILE

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Mol	Chain	Res	Type
2	d	199	GLU
2	e	10	VAL
2	e	15	ASP
2	e	16	ASP
2	e	23	ASP
2	e	27	SER
2	e	30	ASN
2	e	34	ASP
2	e	35	LYS
2	e	43	ILE
2	e	45	ASP
2	e	55	VAL
2	e	57	ASP
2	e	59	GLN
2	e	61	ILE
2	e	72	TYR
2	e	80	ILE
2	e	83	LEU
2	e	85	CYS
2	e	87	THR
2	e	96	SER
2	e	101	PHE
2	e	102	LEU
2	e	105	ILE
2	e	107	ILE
2	e	121	LEU
2	e	124	LEU
2	e	134	THR
2	e	144	TYR
2	e	154	ASP
2	e	183	SER
2	e	184	LEU
2	e	189	LYS
2	e	198	GLU
2	e	199	GLU
2	f	10	VAL
2	f	12	LEU
2	f	15	ASP
2	f	16	ASP
2	f	23	ASP
2	f	27	SER
2	f	34	ASP

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Mol	Chain	Res	Type
2	f	43	ILE
2	f	45	ASP
2	f	50	THR
2	f	55	VAL
2	f	57	ASP
2	f	61	ILE
2	f	72	TYR
2	f	80	ILE
2	f	83	LEU
2	f	85	CYS
2	f	88	LEU
2	f	93	LEU
2	f	101	PHE
2	f	102	LEU
2	f	104	GLN
2	f	105	ILE
2	f	107	ILE
2	f	113	LEU
2	f	121	LEU
2	f	124	LEU
2	f	144	TYR
2	f	154	ASP
2	f	155	MET
2	f	182	ILE
2	f	183	SER
2	f	184	LEU
2	f	187	ILE
2	f	189	LYS
2	f	194	ILE
2	f	199	GLU
2	f	202	LYS
2	g	10	VAL
2	g	16	ASP
2	g	23	ASP
2	g	27	SER
2	g	34	ASP
2	g	43	ILE
2	g	45	ASP
2	g	50	THR
2	g	55	VAL
2	g	57	ASP
2	g	72	TYR

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Mol	Chain	Res	Type
2	g	80	ILE
2	g	83	LEU
2	g	85	CYS
2	g	87	THR
2	g	96	SER
2	g	101	PHE
2	g	102	LEU
2	g	105	ILE
2	g	113	LEU
2	g	124	LEU
2	g	128	ASN
2	g	136	THR
2	g	138	SER
2	g	154	ASP
2	g	183	SER
2	g	184	LEU
2	g	189	LYS
2	g	194	ILE
2	g	198	GLU
2	g	199	GLU
2	g	202	LYS
1	H	13	ILE
1	H	15	VAL
1	H	17	SER
1	H	19	GLU
1	H	25	VAL
1	H	36	THR
1	H	37	THR
1	H	43	CYS
1	H	45	ASP
1	H	49	LEU
1	H	58	LYS
1	H	60	VAL
1	H	68	ILE
1	H	82	LEU
1	H	83	VAL
1	H	88	VAL
1	H	90	ILE
1	H	102	LEU
1	H	117	ILE
1	H	118	CYS
1	H	121	LYS

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Mol	Chain	Res	Type
1	H	135	VAL
1	H	153	ASP
1	H	159	ILE
1	H	184	ASP
1	H	196	THR
1	H	205	ILE
1	H	208	GLU
1	H	211	ASP
1	H	212	VAL
1	H	221	GLN
1	H	222	PHE
1	H	242	ASN
1	I	15	VAL
1	I	19	GLU
1	I	25	VAL
1	I	36	THR
1	I	37	THR
1	I	45	ASP
1	I	51	VAL
1	I	58	LYS
1	I	60	VAL
1	I	68	ILE
1	I	82	LEU
1	I	83	VAL
1	I	85	ASP
1	I	88	VAL
1	I	117	ILE
1	I	118	CYS
1	I	121	LYS
1	I	135	VAL
1	I	153	ASP
1	I	159	ILE
1	I	196	THR
1	I	205	ILE
1	I	208	GLU
1	I	210	VAL
1	I	211	ASP
1	I	212	VAL
1	I	222	PHE
1	I	242	ASN
1	I	243	GLU
1	J	15	VAL

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Mol	Chain	Res	Type
1	J	19	GLU
1	J	25	VAL
1	J	36	THR
1	J	37	THR
1	J	45	ASP
1	J	49	LEU
1	J	58	LYS
1	J	60	VAL
1	J	68	ILE
1	J	82	LEU
1	J	83	VAL
1	J	90	ILE
1	J	96	GLU
1	J	117	ILE
1	J	118	CYS
1	J	135	VAL
1	J	153	ASP
1	J	180	GLU
1	J	205	ILE
1	J	208	GLU
1	J	211	ASP
1	J	222	PHE
1	J	225	ILE
1	J	242	ASN
1	K	15	VAL
1	K	19	GLU
1	K	36	THR
1	K	37	THR
1	K	45	ASP
1	K	55	ILE
1	K	58	LYS
1	K	60	VAL
1	K	68	ILE
1	K	82	LEU
1	K	83	VAL
1	K	88	VAL
1	K	117	ILE
1	K	121	LYS
1	K	135	VAL
1	K	153	ASP
1	K	159	ILE
1	K	168	SER

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Mol	Chain	Res	Type
1	K	180	GLU
1	K	205	ILE
1	K	207	PRO
1	K	208	GLU
1	K	211	ASP
1	K	222	PHE
1	K	242	ASN
1	L	13	ILE
1	L	15	VAL
1	L	17	SER
1	L	19	GLU
1	L	25	VAL
1	L	37	THR
1	L	43	CYS
1	L	45	ASP
1	L	49	LEU
1	L	58	LYS
1	L	60	VAL
1	L	68	ILE
1	L	82	LEU
1	L	90	ILE
1	L	95	LEU
1	L	102	LEU
1	L	117	ILE
1	L	135	VAL
1	L	153	ASP
1	L	159	ILE
1	L	180	GLU
1	L	196	THR
1	L	205	ILE
1	L	208	GLU
1	L	210	VAL
1	L	211	ASP
1	L	222	PHE
1	L	225	ILE
1	L	242	ASN
1	M	13	ILE
1	M	15	VAL
1	M	17	SER
1	M	19	GLU
1	M	37	THR
1	M	51	VAL

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Mol	Chain	Res	Type
1	M	58	LYS
1	M	60	VAL
1	M	68	ILE
1	M	73	ASP
1	M	82	LEU
1	M	88	VAL
1	M	90	ILE
1	M	99	ILE
1	M	102	LEU
1	M	117	ILE
1	M	135	VAL
1	M	153	ASP
1	M	159	ILE
1	M	162	LYS
1	M	180	GLU
1	M	205	ILE
1	M	208	GLU
1	M	211	ASP
1	M	212	VAL
1	M	242	ASN
1	N	15	VAL
1	N	19	GLU
1	N	25	VAL
1	N	36	THR
1	N	37	THR
1	N	45	ASP
1	N	49	LEU
1	N	58	LYS
1	N	60	VAL
1	N	68	ILE
1	N	82	LEU
1	N	83	VAL
1	N	90	ILE
1	N	99	ILE
1	N	102	LEU
1	N	117	ILE
1	N	135	VAL
1	N	159	ILE
1	N	180	GLU
1	N	184	ASP
1	N	205	ILE
1	N	208	GLU

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Mol	Chain	Res	Type
1	N	211	ASP
1	N	212	VAL
1	N	242	ASN
2	h	10	VAL
2	h	15	ASP
2	h	16	ASP
2	h	23	ASP
2	h	34	ASP
2	h	35	LYS
2	h	43	ILE
2	h	50	THR
2	h	55	VAL
2	h	57	ASP
2	h	61	ILE
2	h	72	TYR
2	h	80	ILE
2	h	83	LEU
2	h	85	CYS
2	h	87	THR
2	h	96	SER
2	h	101	PHE
2	h	102	LEU
2	h	104	GLN
2	h	105	ILE
2	h	107	ILE
2	h	113	LEU
2	h	121	LEU
2	h	124	LEU
2	h	134	THR
2	h	140	SER
2	h	144	TYR
2	h	154	ASP
2	h	155	MET
2	h	184	LEU
2	h	187	ILE
2	h	189	LYS
2	h	194	ILE
2	h	198	GLU
2	h	199	GLU
2	h	202	LYS
2	i	10	VAL
2	i	15	ASP

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Mol	Chain	Res	Type
2	i	16	ASP
2	i	23	ASP
2	i	27	SER
2	i	34	ASP
2	i	43	ILE
2	i	55	VAL
2	i	61	ILE
2	i	72	TYR
2	i	80	ILE
2	i	83	LEU
2	i	85	CYS
2	i	87	THR
2	i	93	LEU
2	i	101	PHE
2	i	102	LEU
2	i	104	GLN
2	i	105	ILE
2	i	107	ILE
2	i	113	LEU
2	i	121	LEU
2	i	124	LEU
2	i	140	SER
2	i	144	TYR
2	i	184	LEU
2	i	189	LYS
2	i	198	GLU
2	i	199	GLU
2	i	202	LYS
2	i	203	ILE
2	j	10	VAL
2	j	15	ASP
2	j	16	ASP
2	j	23	ASP
2	j	27	SER
2	j	43	ILE
2	j	45	ASP
2	j	50	THR
2	j	55	VAL
2	j	57	ASP
2	j	61	ILE
2	j	72	TYR
2	j	80	ILE

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Mol	Chain	Res	Type
2	j	83	LEU
2	j	93	LEU
2	j	101	PHE
2	j	102	LEU
2	j	103	THR
2	j	104	GLN
2	j	105	ILE
2	j	107	ILE
2	j	113	LEU
2	j	121	LEU
2	j	124	LEU
2	j	128	ASN
2	j	132	THR
2	j	136	THR
2	j	144	TYR
2	j	154	ASP
2	j	182	ILE
2	j	183	SER
2	j	187	ILE
2	j	189	LYS
2	j	190	ASP
2	j	194	ILE
2	j	199	GLU
2	j	202	LYS
2	k	10	VAL
2	k	15	ASP
2	k	16	ASP
2	k	23	ASP
2	k	27	SER
2	k	34	ASP
2	k	43	ILE
2	k	45	ASP
2	k	55	VAL
2	k	72	TYR
2	k	80	ILE
2	k	83	LEU
2	k	87	THR
2	k	88	LEU
2	k	93	LEU
2	k	96	SER
2	k	101	PHE
2	k	102	LEU

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Mol	Chain	Res	Type
2	k	103	THR
2	k	105	ILE
2	k	107	ILE
2	k	113	LEU
2	k	121	LEU
2	k	124	LEU
2	k	144	TYR
2	k	154	ASP
2	k	183	SER
2	k	184	LEU
2	k	189	LYS
2	k	194	ILE
2	k	199	GLU
2	l	7	THR
2	l	10	VAL
2	l	15	ASP
2	l	16	ASP
2	l	23	ASP
2	l	27	SER
2	l	34	ASP
2	l	43	ILE
2	l	45	ASP
2	l	57	ASP
2	l	61	ILE
2	l	80	ILE
2	l	83	LEU
2	l	85	CYS
2	l	87	THR
2	l	93	LEU
2	l	96	SER
2	l	101	PHE
2	l	102	LEU
2	l	103	THR
2	l	105	ILE
2	l	107	ILE
2	l	113	LEU
2	l	120	SER
2	l	121	LEU
2	l	124	LEU
2	l	134	THR
2	l	138	SER
2	l	154	ASP

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Mol	Chain	Res	Type
2	l	155	MET
2	l	184	LEU
2	l	187	ILE
2	l	189	LYS
2	l	198	GLU
2	l	199	GLU
2	l	201	GLU
2	m	10	VAL
2	m	15	ASP
2	m	16	ASP
2	m	23	ASP
2	m	27	SER
2	m	34	ASP
2	m	43	ILE
2	m	45	ASP
2	m	50	THR
2	m	55	VAL
2	m	61	ILE
2	m	71	LEU
2	m	72	TYR
2	m	80	ILE
2	m	83	LEU
2	m	85	CYS
2	m	87	THR
2	m	96	SER
2	m	97	ARG
2	m	101	PHE
2	m	102	LEU
2	m	105	ILE
2	m	107	ILE
2	m	113	LEU
2	m	122	ASP
2	m	124	LEU
2	m	128	ASN
2	m	132	THR
2	m	144	TYR
2	m	154	ASP
2	m	183	SER
2	m	184	LEU
2	m	187	ILE
2	m	189	LYS
2	m	194	ILE

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Mol	Chain	Res	Type
2	m	198	GLU
2	m	199	GLU
2	m	202	LYS
2	m	205	ASP
2	n	10	VAL
2	n	16	ASP
2	n	23	ASP
2	n	27	SER
2	n	34	ASP
2	n	43	ILE
2	n	45	ASP
2	n	50	THR
2	n	55	VAL
2	n	61	ILE
2	n	72	TYR
2	n	80	ILE
2	n	83	LEU
2	n	85	CYS
2	n	87	THR
2	n	93	LEU
2	n	101	PHE
2	n	102	LEU
2	n	104	GLN
2	n	105	ILE
2	n	107	ILE
2	n	113	LEU
2	n	121	LEU
2	n	124	LEU
2	n	136	THR
2	n	144	TYR
2	n	154	ASP
2	n	184	LEU
2	n	189	LYS
2	n	199	GLU
2	n	202	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	g	128	ASN
1	N	98	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	232/264 (87%)	-0.08	4 (1%) 70 60	127, 157, 221, 336	0
1	B	232/264 (87%)	0.02	3 (1%) 77 68	118, 151, 270, 519	0
1	C	232/264 (87%)	-0.25	2 (0%) 84 77	114, 132, 205, 333	0
1	D	232/264 (87%)	-0.39	1 (0%) 92 87	59, 134, 205, 245	0
1	E	232/264 (87%)	-0.14	7 (3%) 50 39	82, 139, 252, 355	0
1	F	232/264 (87%)	-0.18	4 (1%) 70 60	92, 116, 204, 346	0
1	G	232/264 (87%)	-0.32	2 (0%) 84 77	106, 128, 215, 284	0
1	H	232/264 (87%)	-0.30	1 (0%) 92 87	131, 148, 187, 271	0
1	I	232/264 (87%)	-0.23	4 (1%) 70 60	90, 136, 212, 299	0
1	J	232/264 (87%)	-0.02	9 (3%) 39 31	81, 141, 259, 366	0
1	K	232/264 (87%)	-0.28	0 100 100	112, 139, 220, 291	0
1	L	232/264 (87%)	-0.25	0 100 100	113, 135, 208, 253	0
1	M	232/264 (87%)	-0.02	8 (3%) 45 36	126, 143, 253, 507	0
1	N	232/264 (87%)	-0.15	2 (0%) 84 77	130, 147, 186, 303	0
2	a	202/219 (92%)	-0.41	1 (0%) 91 85	118, 138, 170, 185	0
2	b	202/219 (92%)	-0.14	4 (1%) 65 56	113, 131, 161, 180	0
2	c	202/219 (92%)	-0.36	0 100 100	101, 119, 195, 251	0
2	d	202/219 (92%)	-0.40	1 (0%) 91 85	107, 124, 162, 194	0
2	e	202/219 (92%)	-0.42	1 (0%) 91 85	93, 111, 159, 203	0
2	f	202/219 (92%)	-0.37	0 100 100	100, 115, 150, 175	0
2	g	202/219 (92%)	-0.33	0 100 100	110, 125, 149, 171	0
2	h	202/219 (92%)	-0.40	0 100 100	123, 139, 174, 186	0
2	i	202/219 (92%)	-0.36	3 (1%) 73 63	110, 123, 155, 170	0
2	j	202/219 (92%)	-0.48	0 100 100	72, 87, 159, 212	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	k	202/219 (92%)	-0.43	0 100 100	80, 102, 177, 209	0
2	l	202/219 (92%)	-0.41	0 100 100	104, 120, 160, 193	0
2	m	202/219 (92%)	-0.35	0 100 100	102, 122, 213, 254	0
2	n	202/219 (92%)	-0.26	0 100 100	122, 148, 181, 195	0
All	All	6076/6762 (89%)	-0.27	57 (0%) 84 77	59, 134, 207, 519	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	244	GLU	6.5
1	J	13	ILE	5.3
1	E	236	LYS	5.2
1	J	244	GLU	4.6
1	A	244	GLU	4.3
1	J	241	LEU	3.9
1	J	238	LYS	3.8
1	F	243	GLU	3.7
1	B	243	GLU	3.6
1	I	13	ILE	3.3
1	C	243	GLU	3.1
2	i	15	ASP	3.1
1	M	244	GLU	3.1
1	M	238	LYS	3.0
2	e	15	ASP	3.0
1	N	238	LYS	3.0
1	F	13	ILE	2.9
2	i	14	CYS	2.9
2	i	208	LYS	2.8
1	E	13	ILE	2.8
1	E	15	VAL	2.8
2	b	108	GLY	2.8
1	H	13	ILE	2.7
1	M	243	GLU	2.7
1	J	192	GLU	2.7
1	I	244	GLU	2.6
1	I	239	LYS	2.6
1	B	244	GLU	2.6
2	d	98	MET	2.6
1	E	16	PHE	2.5
1	J	242	ASN	2.5
1	G	13	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	244	GLU	2.4
1	A	241	LEU	2.4
1	M	241	LEU	2.4
1	J	243	GLU	2.4
1	A	13	ILE	2.4
1	B	21	ARG	2.3
1	F	45	ASP	2.3
1	J	237	VAL	2.3
1	E	233	LEU	2.3
1	C	241	LEU	2.2
1	N	13	ILE	2.2
2	a	14	CYS	2.2
1	A	179	LYS	2.2
1	J	45	ASP	2.1
1	M	242	ASN	2.1
2	b	13	ILE	2.1
1	D	241	LEU	2.1
1	M	207	PRO	2.1
1	G	236	LYS	2.1
1	M	52	ASP	2.1
2	b	157	VAL	2.0
1	E	239	LYS	2.0
2	b	14	CYS	2.0
1	M	200	LYS	2.0
1	I	15	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.