



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:08 AM GMT

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 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/ValidationPDFNotes.html>

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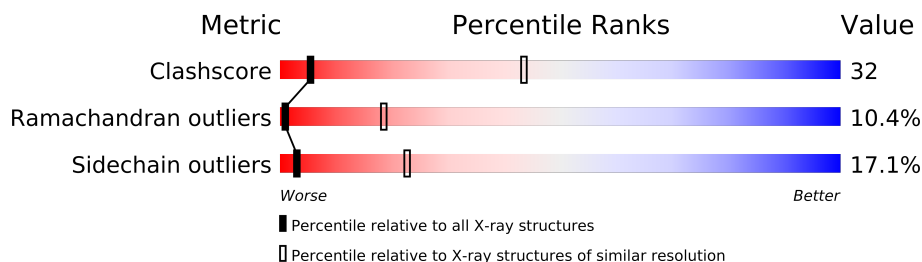
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : **FAILED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
Clashscore	79885	1248 (4.70-3.50)
Ramachandran outliers	78287	1183 (4.70-3.50)
Sidechain outliers	78261	1168 (4.70-3.50)











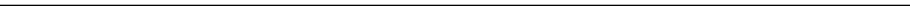
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	264	
1	B	264	
1	C	264	
1	D	264	
1	E	264	
1	F	264	
1	G	264	
1	H	264	
1	I	264	
1	J	264	
1	K	264	
1	L	264	
1	M	264	
1	N	264	
2	a	219	
2	b	219	
2	c	219	

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Mol	Chain	Length	Quality of chain
2	d	219	
2	e	219	
2	f	219	
2	g	219	
2	h	219	
2	i	219	
2	j	219	
2	k	219	
2	l	219	
2	m	219	
2	n	219	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 46648 atoms, of which 0 are hydrogen and 0 are deuterium.

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
1	A	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			
1	B	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			
1	C	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			
1	D	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			
1	E	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			
1	F	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			
1	G	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			
1	H	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			
1	I	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			
1	J	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			
1	K	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			
1	L	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			
1	M	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			
1	N	232	Total	C	N	O	S	0	0	0
			1813	1150	312	346	5			

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
2	a	202	Total 1519	C 964	N 248	O 298	S 9	0	0	0
2	b	202	Total 1519	C 964	N 248	O 298	S 9	0	0	0
2	c	202	Total 1519	C 964	N 248	O 298	S 9	0	0	0
2	d	202	Total 1519	C 964	N 248	O 298	S 9	0	0	0
2	e	202	Total 1519	C 964	N 248	O 298	S 9	0	0	0
2	f	202	Total 1519	C 964	N 248	O 298	S 9	0	0	0
2	g	202	Total 1519	C 964	N 248	O 298	S 9	0	0	0
2	h	202	Total 1519	C 964	N 248	O 298	S 9	0	0	0
2	i	202	Total 1519	C 964	N 248	O 298	S 9	0	0	0
2	j	202	Total 1519	C 964	N 248	O 298	S 9	0	0	0
2	k	202	Total 1519	C 964	N 248	O 298	S 9	0	0	0
2	l	202	Total 1519	C 964	N 248	O 298	S 9	0	0	0
2	m	202	Total 1519	C 964	N 248	O 298	S 9	0	0	0
2	n	202	Total 1519	C 964	N 248	O 298	S 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

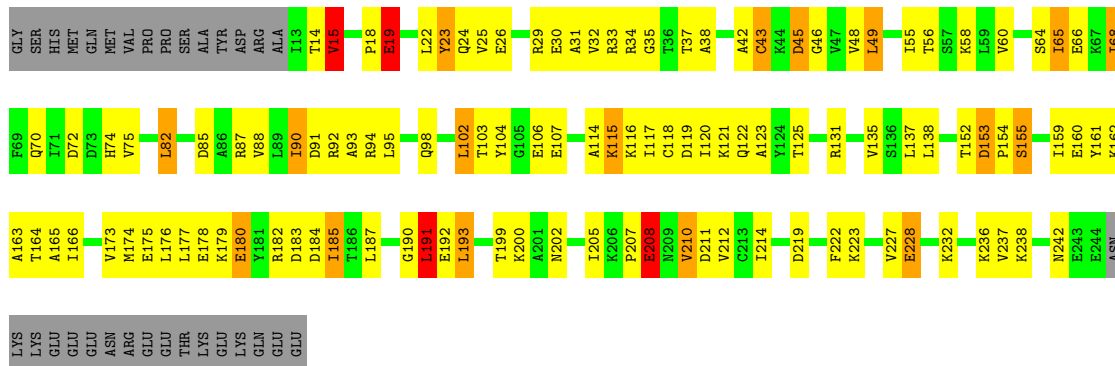






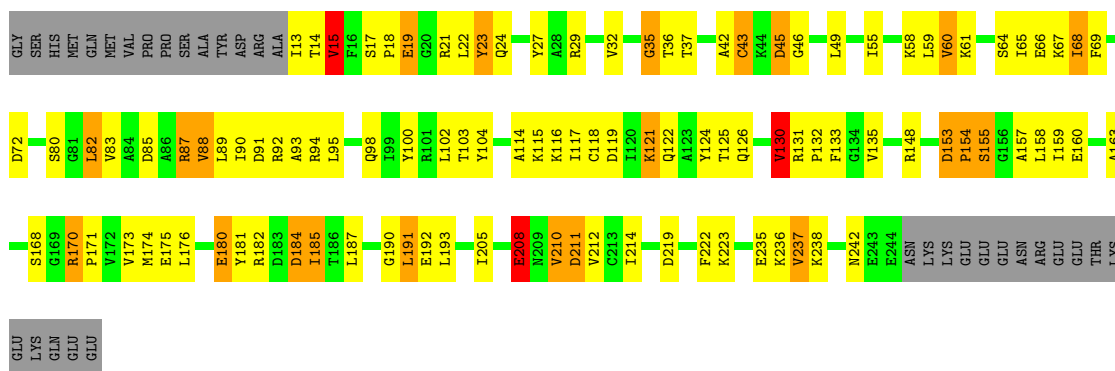
- Molecule 1: Proteasome subunit alpha

Chain D:



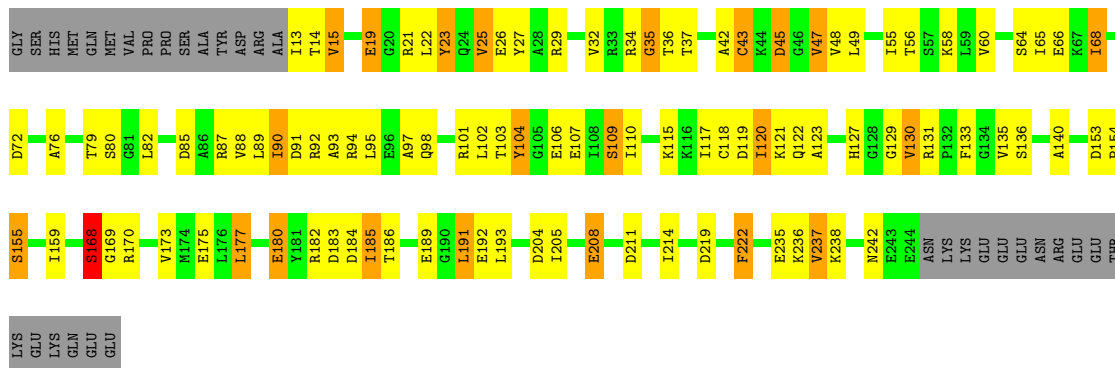
- Molecule 1: Proteasome subunit alpha

Chain E:



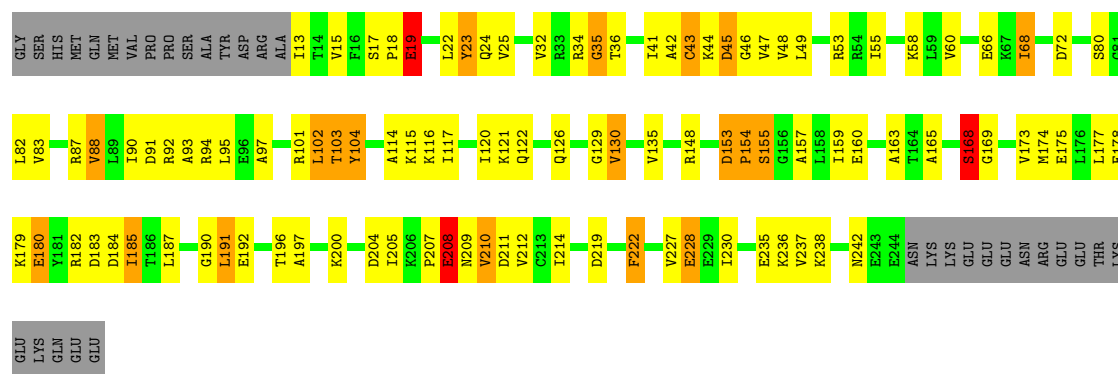
- Molecule 1: Proteasome subunit alpha

Chain F:



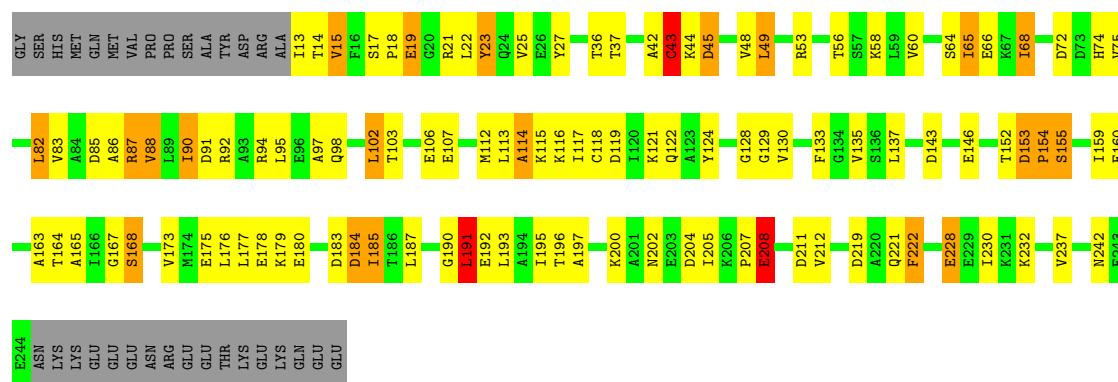
- Molecule 1: Proteasome subunit alpha

Chain G:



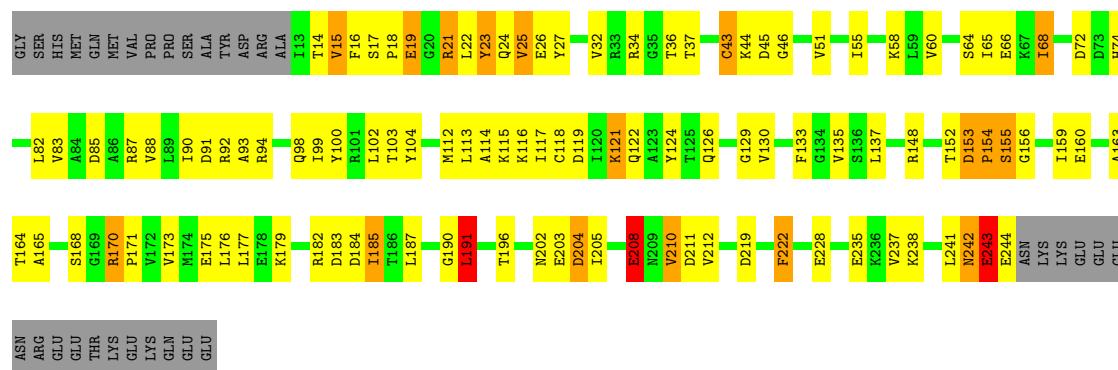
- Molecule 1: Proteasome subunit alpha

Chain H:



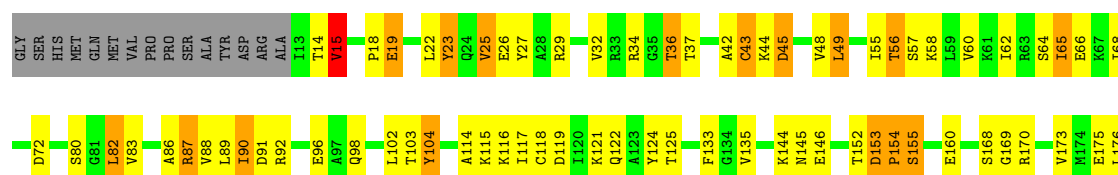
- Molecule 1: Proteasome subunit alpha

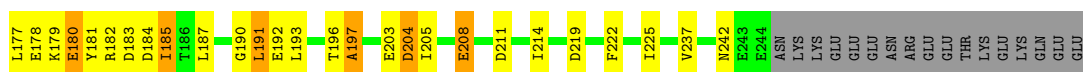
Chain I:



- Molecule 1: Proteasome subunit alpha

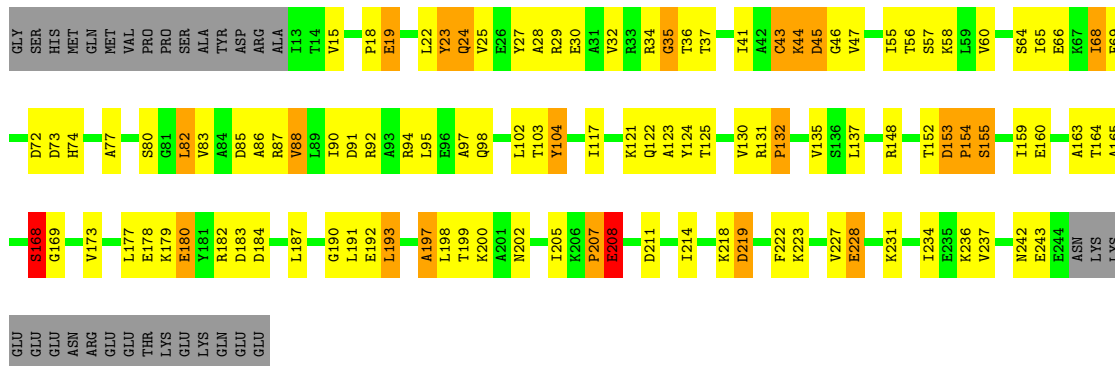
Chain J:





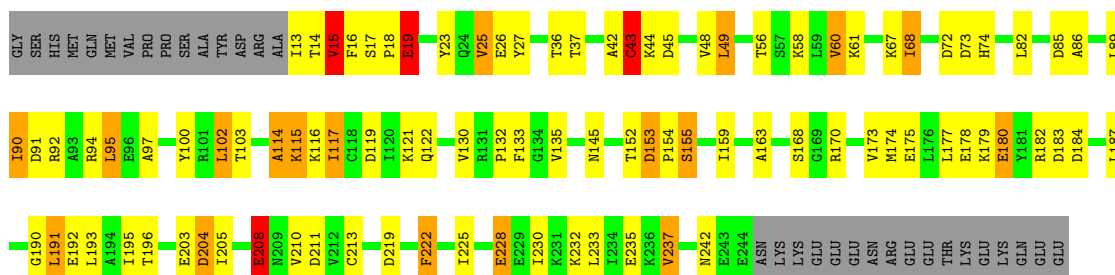
- Molecule 1: Proteasome subunit alpha

Chain K:



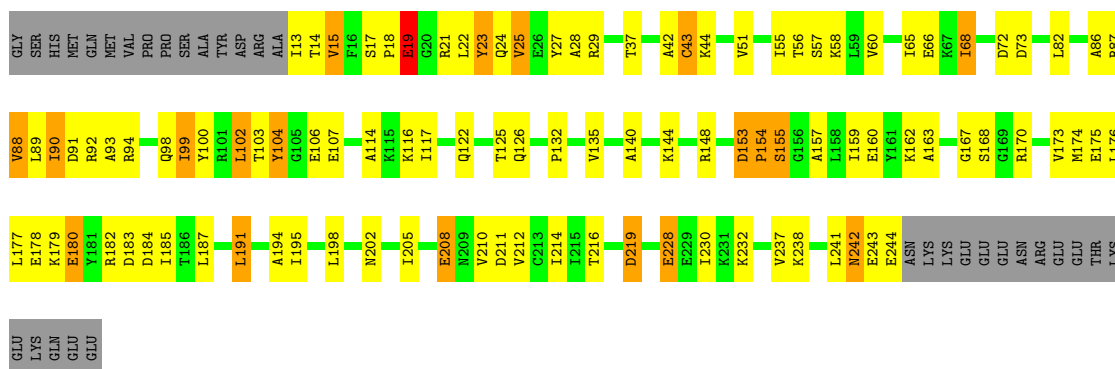
- Molecule 1: Proteasome subunit alpha

Chain L: 



- Molecule 1: Proteasome subunit alpha

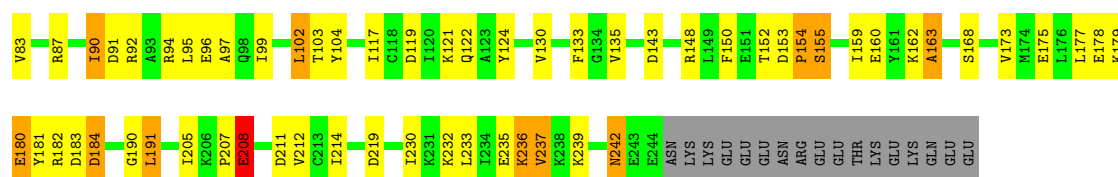
Chain M:



- Molecule 1: Proteasome subunit alpha

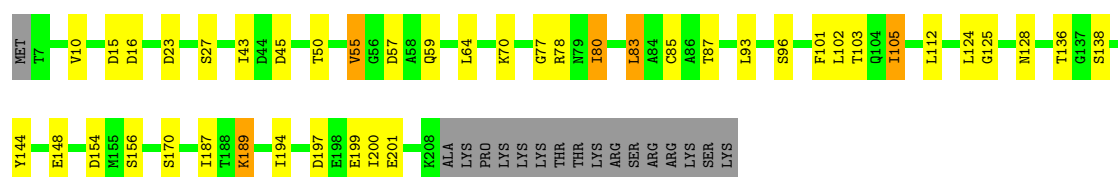
Chain N:





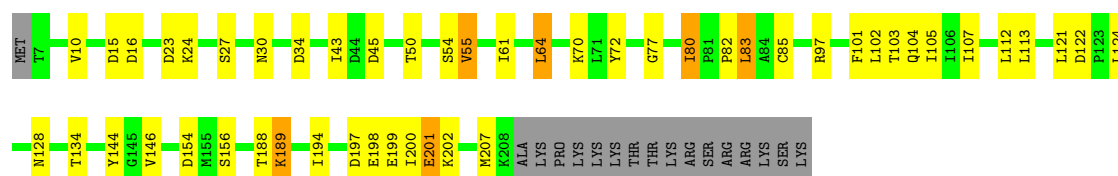
• Molecule 2: Proteasome subunit beta

Chain a:



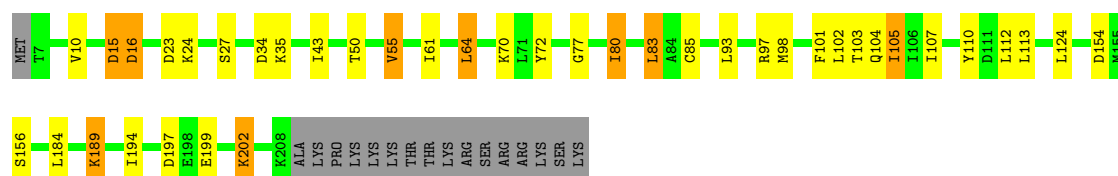
• Molecule 2: Proteasome subunit beta

Chain b:



• Molecule 2: Proteasome subunit beta

Chain c:



• Molecule 2: Proteasome subunit beta

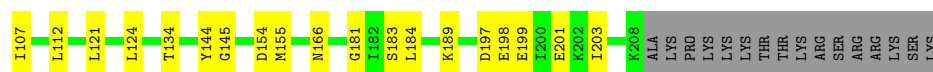
Chain d:



• Molecule 2: Proteasome subunit beta

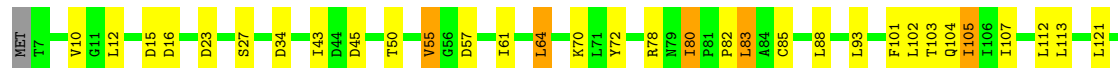
Chain e:





- Molecule 2: Proteasome subunit beta

Chain f:



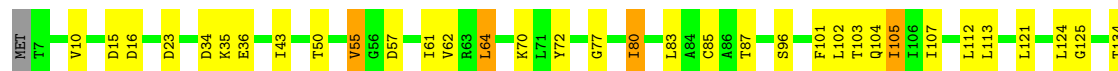
- Molecule 2: Proteasome subunit beta

Chain g:



- Molecule 2: Proteasome subunit beta

Chain h:



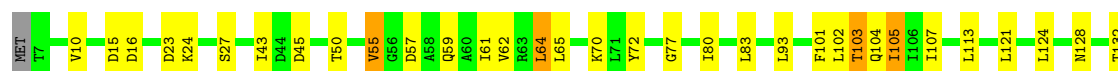
- Molecule 2: Proteasome subunit beta

Chain i:



- Molecule 2: Proteasome subunit beta

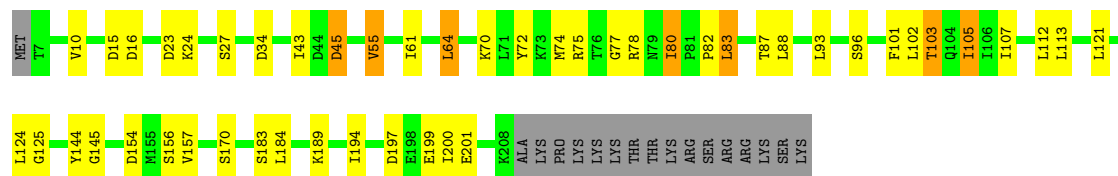
Chain j:



- Molecule 2: Proteasome subunit beta

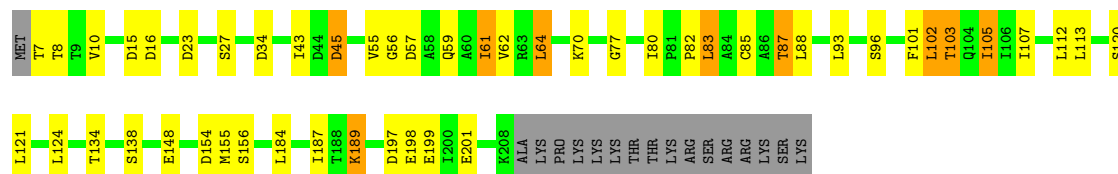


Chain k: 



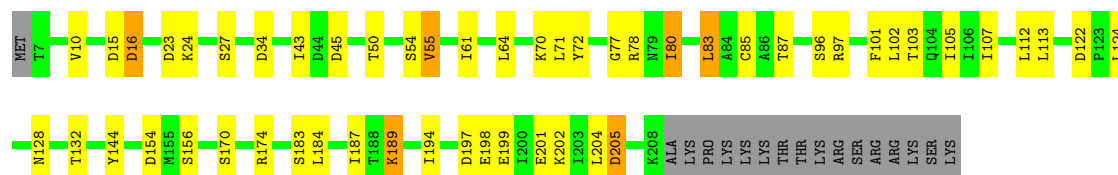
• Molecule 2: Proteasome subunit beta

Chain l: 



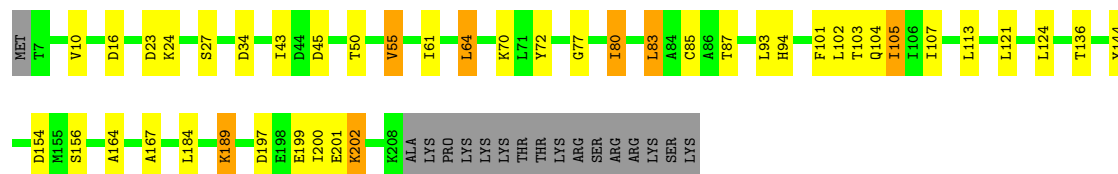
• Molecule 2: Proteasome subunit beta

Chain m: 



• Molecule 2: Proteasome subunit beta

Chain n: 



## 4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	206.72Å 219.54Å 149.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.98 – 4.10	Depositor
% Data completeness (in resolution range)	99.8 (49.98-4.10)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.49 (at 4.14Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.254 , 0.325	Depositor
Wilson B-factor (Å <sup>2</sup> )	118.1	Xtriage
Anisotropy	0.499	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	9 of 53849 reflections (0.017%)	Xtriage
Total number of atoms	46648	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	141.0	wwPDB-VP

Xtriage'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.*

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

## 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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1813	0	0	60	0
1	B	1813	0	0	55	2
1	C	1813	0	0	47	0
1	D	1813	0	0	73	0
1	E	1813	0	0	77	1
1	F	1813	0	0	55	1
1	G	1813	0	0	65	0
1	H	1813	0	0	61	0
1	I	1813	0	0	65	1
1	J	1813	0	0	59	0
1	K	1813	0	0	68	0
1	L	1813	0	0	55	0
1	M	1813	0	0	60	2
1	N	1813	0	0	49	0
2	a	1519	0	0	0	0
2	b	1519	0	0	0	0
2	c	1519	0	0	0	2
2	d	1519	0	0	0	0
2	e	1519	0	0	0	0
2	f	1519	0	0	0	1
2	g	1519	0	0	0	0
2	h	1519	0	0	0	0
2	i	1519	0	0	0	2
2	j	1519	0	0	0	0
2	k	1519	0	0	0	0
2	l	1519	0	0	0	0
2	m	1519	0	0	0	1
2	n	1519	0	0	0	0
All	All	46648	0	0	793	7

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 32.

All (793) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:153:ASP:O	1:H:155:SER:N	2.06	0.89
1:G:207:PRO:O	1:G:208:GLU:CG	2.21	0.88
1:I:90:ILE:O	1:I:92:ARG:N	2.13	0.82
1:D:153:ASP:O	1:D:155:SER:N	2.12	0.82
1:I:153:ASP:O	1:I:155:SER:N	2.13	0.81
1:L:114:ALA:O	1:L:116:LYS:N	2.14	0.80
1:L:153:ASP:O	1:L:155:SER:N	2.16	0.79
1:G:153:ASP:O	1:G:155:SER:N	2.17	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:153:ASP:O	1:J:155:SER:N	2.17	0.76
1:L:90:ILE:O	1:L:92:ARG:N	2.19	0.76
1:F:153:ASP:O	1:F:155:SER:N	2.19	0.75
1:E:153:ASP:O	1:E:155:SER:N	2.22	0.73
1:A:68:ILE:N	1:A:68:ILE:CD1	2.52	0.73
1:D:207:PRO:O	1:D:208:GLU:CG	2.36	0.72
1:K:153:ASP:O	1:K:155:SER:N	2.22	0.72
1:D:160:GLU:CB	1:E:64:SER:CB	2.68	0.72
1:L:68:ILE:CD1	1:L:68:ILE:N	2.53	0.71
1:J:87:ARG:O	1:J:90:ILE:N	2.23	0.71
1:H:114:ALA:O	1:H:116:LYS:N	2.25	0.69
1:H:72:ASP:OD2	1:H:98:GLN:NE2	2.25	0.69
1:B:153:ASP:O	1:B:155:SER:N	2.26	0.68
1:A:90:ILE:O	1:A:92:ARG:N	2.27	0.68
1:J:121:LYS:NZ	1:J:152:THR:OG1	2.27	0.68
1:D:72:ASP:OD2	1:D:98:GLN:NE2	2.27	0.68
1:G:43:CYS:SG	1:G:44:LYS:N	2.68	0.67
1:N:90:ILE:O	1:N:92:ARG:N	2.27	0.67
1:I:90:ILE:C	1:I:92:ARG:N	2.48	0.67
1:K:68:ILE:CD1	1:K:68:ILE:N	2.58	0.66
1:M:153:ASP:O	1:M:155:SER:N	2.28	0.66
1:K:103:THR:O	1:K:104:TYR:CG	2.48	0.66
1:C:153:ASP:O	1:C:155:SER:N	2.29	0.66
1:G:182:ARG:O	1:G:184:ASP:N	2.29	0.66
1:D:114:ALA:O	1:D:116:LYS:N	2.29	0.66
1:A:153:ASP:O	1:A:155:SER:N	2.30	0.64
1:E:32:VAL:O	1:E:35:GLY:N	2.31	0.64
1:E:208:GLU:C	1:E:210:VAL:N	2.51	0.64
1:C:122:GLN:NE2	1:D:85:ASP:OD2	2.31	0.64
1:H:90:ILE:O	1:H:92:ARG:N	2.30	0.63
1:C:102:LEU:O	1:C:103:THR:CB	4.00	0.62
1:M:122:GLN:O	1:M:125:THR:N	2.31	0.62
1:F:90:ILE:O	1:F:94:ARG:N	2.31	0.62
1:H:228:GLU:O	1:H:232:LYS:N	2.32	0.62
1:G:182:ARG:C	1:G:184:ASP:N	2.53	0.62
1:D:187:LEU:O	1:D:191:LEU:N	2.33	0.62
1:B:155:SER:OG	1:B:155:SER:O	2.17	0.62
1:K:43:CYS:SG	1:K:46:GLY:O	2.57	0.61
1:I:242:ASN:O	1:I:244:GLU:N	2.33	0.61
1:H:90:ILE:C	1:H:92:ARG:N	2.53	0.61
1:G:72:ASP:OD2	1:G:101:ARG:NH1	2.32	0.61
1:K:43:CYS:SG	1:K:44:LYS:N	2.74	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:182:ARG:O	1:E:185:ILE:CG2	2.49	0.61
1:D:68:ILE:N	1:D:68:ILE:CD1	2.64	0.60
1:L:90:ILE:C	1:L:92:ARG:N	2.54	0.60
1:H:119:ASP:OD1	1:I:87:ARG:NH2	2.34	0.60
1:C:114:ALA:O	1:C:116:LYS:N	2.35	0.60
1:G:177:LEU:O	1:G:179:LYS:N	2.34	0.60
1:G:68:ILE:CD1	1:G:68:ILE:N	2.65	0.60
1:A:90:ILE:C	1:A:92:ARG:N	2.55	0.59
1:L:72:ASP:O	1:L:74:HIS:N	2.35	0.59
1:K:180:GLU:N	1:K:180:GLU:CD	2.56	0.59
1:J:64:SER:O	1:J:66:GLU:N	2.36	0.59
1:H:192:GLU:O	1:H:193:LEU:C	2.40	0.59
1:M:68:ILE:CD1	1:M:68:ILE:N	2.66	0.58
1:J:29:ARG:O	1:J:32:VAL:N	2.36	0.58
1:N:102:LEU:O	1:N:103:THR:CB	4.07	0.58
1:I:124:TYR:CD1	1:I:133:PHE:CE2	2.92	0.58
1:N:150:PHE:CE1	1:N:160:GLU:CB	2.86	0.58
1:D:182:ARG:O	1:D:184:ASP:N	2.36	0.58
1:G:148:ARG:CD	1:G:160:GLU:OE1	2.51	0.58
1:N:124:TYR:CD1	1:N:133:PHE:CZ	2.92	0.58
1:H:207:PRO:O	1:H:208:GLU:CG	2.51	0.58
1:F:168:SER:OG	1:F:169:GLY:N	2.35	0.58
1:C:208:GLU:C	1:C:210:VAL:N	2.56	0.58
1:K:85:ASP:OD1	1:K:131:ARG:NH1	2.37	0.58
1:F:186:THR:OG1	1:F:189:GLU:CB	2.52	0.57
1:I:68:ILE:N	1:I:68:ILE:CD1	2.67	0.57
1:N:153:ASP:O	1:N:155:SER:N	2.37	0.57
1:G:90:ILE:O	1:G:94:ARG:N	2.37	0.57
1:I:72:ASP:OD2	1:I:98:GLN:NE2	2.37	0.57
1:H:187:LEU:O	1:H:191:LEU:N	2.38	0.57
1:K:64:SER:O	1:K:66:GLU:N	2.38	0.57
1:J:25:VAL:CG2	1:J:26:GLU:N	2.67	0.57
1:D:182:ARG:C	1:D:184:ASP:N	2.58	0.57
1:F:25:VAL:CG2	1:F:26:GLU:N	2.68	0.56
1:E:29:ARG:O	1:E:32:VAL:N	2.38	0.56
1:D:32:VAL:O	1:D:34:ARG:N	2.39	0.56
1:M:153:ASP:OD1	1:M:154:PRO:N	2.38	0.56
1:H:42:ALA:O	1:H:43:CYS:SG	2.62	0.56
1:H:68:ILE:CD1	1:H:68:ILE:N	2.68	0.56
1:D:173:VAL:C	1:D:175:GLU:N	2.59	0.56
1:E:118:CYS:SG	1:E:157:ALA:N	2.78	0.56
1:C:119:ASP:OD1	1:D:87:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:90:ILE:O	1:E:92:ARG:N	2.38	0.56
1:M:102:LEU:CD2	1:M:103:THR:N	3.17	0.56
1:D:90:ILE:C	1:D:92:ARG:N	2.58	0.56
1:M:241:LEU:C	1:M:242:ASN:CG	2.63	0.56
1:F:182:ARG:C	1:F:184:ASP:N	2.59	0.56
1:L:48:VAL:CG1	1:L:49:LEU:N	2.68	0.56
1:A:48:VAL:CG1	1:A:49:LEU:N	2.68	0.56
1:J:180:GLU:N	1:J:180:GLU:CD	2.59	0.56
1:G:180:GLU:CD	1:G:180:GLU:N	2.59	0.56
1:K:22:LEU:O	1:K:23:TYR:O	2.24	0.56
1:D:14:THR:O	1:D:15:VAL:CG1	2.54	0.55
1:D:115:LYS:NZ	1:E:66:GLU:OE1	2.39	0.55
1:G:197:ALA:O	1:G:200:LYS:N	2.39	0.55
1:M:90:ILE:C	1:M:92:ARG:N	2.59	0.55
1:F:180:GLU:CD	1:F:180:GLU:N	2.60	0.55
1:D:162:LYS:N	1:E:59:LEU:O	2.39	0.55
1:E:184:ASP:O	1:E:185:ILE:C	2.44	0.55
1:E:45:ASP:OD2	1:E:45:ASP:N	2.39	0.55
1:C:45:ASP:OD2	1:C:45:ASP:N	2.38	0.55
1:D:18:PRO:O	1:E:27:TYR:CE1	2.60	0.55
1:E:119:ASP:OD1	1:F:87:ARG:NE	2.40	0.55
1:E:187:LEU:O	1:E:191:LEU:N	2.40	0.55
1:I:153:ASP:OD1	1:I:154:PRO:N	2.41	0.54
1:C:90:ILE:O	1:C:92:ARG:N	2.40	0.54
1:A:25:VAL:CG2	1:A:26:GLU:N	2.69	0.54
1:H:124:TYR:CD1	1:H:133:PHE:CZ	2.96	0.54
1:A:22:LEU:O	1:A:23:TYR:O	2.26	0.54
1:N:90:ILE:C	1:N:92:ARG:N	2.61	0.54
1:C:90:ILE:C	1:C:92:ARG:N	2.60	0.54
1:K:18:PRO:C	1:L:27:TYR:CD1	2.81	0.54
1:L:19:GLU:N	1:L:19:GLU:OE1	2.40	0.54
1:K:23:TYR:O	1:K:24:GLN:C	2.43	0.54
1:D:64:SER:O	1:D:66:GLU:N	2.40	0.54
1:L:114:ALA:C	1:L:116:LYS:N	2.59	0.54
1:K:82:LEU:CD1	1:K:82:LEU:N	2.70	0.54
1:D:102:LEU:O	1:D:103:THR:CB	3.98	0.54
1:E:87:ARG:O	1:E:90:ILE:N	2.41	0.54
1:G:90:ILE:C	1:G:92:ARG:N	2.61	0.54
1:G:32:VAL:C	1:G:34:ARG:N	2.61	0.54
1:G:214:ILE:N	1:G:214:ILE:CD1	2.71	0.54
1:A:153:ASP:OD1	1:A:154:PRO:N	2.41	0.53
1:C:102:LEU:C	1:C:102:LEU:CD2	2.99	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:90:ILE:O	1:M:94:ARG:N	2.42	0.53
1:A:133:PHE:CE2	1:G:126:GLN:NE2	2.77	0.53
1:A:137:LEU:N	1:A:152:THR:OG1	2.41	0.53
1:B:87:ARG:O	1:B:90:ILE:N	2.41	0.53
1:E:114:ALA:O	1:E:116:LYS:N	2.41	0.53
1:A:53:ARG:O	1:A:209:ASN:OD1	2.26	0.53
1:L:180:GLU:CD	1:L:180:GLU:N	2.62	0.53
1:J:42:ALA:O	1:J:43:CYS:CB	2.56	0.53
1:G:90:ILE:O	1:G:92:ARG:N	2.41	0.53
1:E:126:GLN:NE2	1:F:133:PHE:CE2	2.76	0.53
1:K:137:LEU:N	1:K:152:THR:OG1	2.42	0.53
1:J:190:GLY:O	1:J:191:LEU:C	2.46	0.53
1:H:143:ASP:N	1:H:146:GLU:O	2.42	0.53
1:I:18:PRO:O	1:J:27:TYR:CD1	2.62	0.53
1:K:182:ARG:O	1:K:184:ASP:N	2.42	0.53
1:K:23:TYR:O	1:K:25:VAL:N	2.42	0.53
1:B:68:ILE:CD1	1:B:68:ILE:N	2.72	0.53
1:L:119:ASP:OD1	1:M:87:ARG:NH2	2.42	0.52
1:F:173:VAL:O	1:F:177:LEU:CD1	2.58	0.52
1:A:173:VAL:O	1:A:176:LEU:N	2.42	0.52
1:F:235:GLU:O	1:F:237:VAL:N	2.42	0.52
1:M:23:TYR:O	1:M:24:GLN:C	2.48	0.52
1:I:87:ARG:O	1:I:90:ILE:N	2.42	0.52
1:K:198:LEU:O	1:K:199:THR:C	2.47	0.52
1:N:32:VAL:C	1:N:34:ARG:N	2.61	0.52
1:G:227:VAL:O	1:G:228:GLU:CB	2.57	0.52
1:G:43:CYS:SG	1:G:46:GLY:O	2.68	0.52
1:E:90:ILE:C	1:E:92:ARG:N	2.62	0.52
1:K:86:ALA:O	1:K:87:ARG:C	2.46	0.52
1:K:87:ARG:O	1:K:88:VAL:C	2.45	0.52
1:F:173:VAL:C	1:F:175:GLU:N	2.62	0.52
1:F:123:ALA:O	1:F:127:HIS:ND1	2.43	0.52
1:K:182:ARG:C	1:K:184:ASP:N	2.63	0.52
1:B:112:MET:O	1:B:113:LEU:C	2.46	0.52
1:B:114:ALA:O	1:B:116:LYS:N	2.43	0.52
1:J:173:VAL:O	1:J:176:LEU:N	2.42	0.52
1:F:22:LEU:O	1:F:23:TYR:O	2.28	0.52
1:D:192:GLU:O	1:D:193:LEU:C	2.47	0.52
1:F:106:GLU:O	1:F:107:GLU:C	2.47	0.52
1:I:173:VAL:C	1:I:175:GLU:N	2.63	0.52
1:D:102:LEU:CD2	1:D:102:LEU:C	2.78	0.52
1:D:118:CYS:O	1:E:87:ARG:NH2	2.43	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:95:LEU:C	1:G:97:ALA:N	2.62	0.52
1:L:192:GLU:O	1:L:193:LEU:C	2.48	0.52
1:J:214:ILE:N	1:J:214:ILE:CD1	2.72	0.52
1:F:90:ILE:C	1:F:92:ARG:N	2.63	0.52
1:D:119:ASP:OD1	1:E:87:ARG:NE	2.43	0.52
1:M:148:ARG:CD	1:M:160:GLU:OE1	2.58	0.52
1:I:190:GLY:O	1:I:191:LEU:C	2.47	0.52
1:A:27:TYR:CD1	1:G:18:PRO:O	2.63	0.52
1:N:68:ILE:CD1	1:N:68:ILE:N	2.73	0.52
1:K:197:ALA:O	1:K:200:LYS:N	2.43	0.51
1:K:190:GLY:O	1:K:191:LEU:C	2.48	0.51
1:F:48:VAL:CG1	1:F:49:LEU:N	2.72	0.51
1:H:153:ASP:C	1:H:153:ASP:OD1	2.49	0.51
1:D:18:PRO:C	1:E:27:TYR:CD1	2.83	0.51
1:D:32:VAL:C	1:D:34:ARG:N	2.63	0.51
1:H:42:ALA:C	1:H:43:CYS:SG	2.89	0.51
1:E:180:GLU:CD	1:E:180:GLU:N	2.63	0.51
1:E:192:GLU:O	1:E:193:LEU:C	2.47	0.51
1:K:69:PHE:N	1:K:77:ALA:O	2.43	0.51
1:D:228:GLU:O	1:D:232:LYS:N	2.43	0.51
1:B:18:PRO:O	1:C:27:TYR:CD1	2.64	0.51
1:H:82:LEU:CD1	1:H:82:LEU:N	2.73	0.51
1:G:45:ASP:OD2	1:G:45:ASP:N	2.44	0.51
1:E:17:SER:OG	1:E:21:ARG:O	2.29	0.51
1:M:173:VAL:C	1:M:175:GLU:N	2.64	0.51
1:H:177:LEU:O	1:H:179:LYS:N	2.44	0.51
1:D:137:LEU:N	1:D:152:THR:OG1	2.43	0.51
1:G:168:SER:OG	1:G:169:GLY:N	2.42	0.51
1:K:187:LEU:O	1:K:191:LEU:N	2.44	0.51
1:E:122:GLN:OE1	1:E:122:GLN:C	2.49	0.51
1:E:87:ARG:O	1:E:88:VAL:C	2.49	0.51
1:J:160:GLU:N	1:K:64:SER:OG	2.44	0.51
1:N:32:VAL:O	1:N:34:ARG:N	2.44	0.51
1:A:27:TYR:CD1	1:G:18:PRO:C	2.84	0.51
1:H:87:ARG:O	1:H:88:VAL:C	2.49	0.51
1:E:22:LEU:O	1:E:23:TYR:O	2.29	0.51
1:M:22:LEU:O	1:M:23:TYR:O	2.27	0.51
1:M:19:GLU:N	1:M:19:GLU:OE1	2.44	0.51
1:G:45:ASP:OD1	1:G:45:ASP:N	3.99	0.51
1:E:82:LEU:CD1	1:E:82:LEU:N	2.74	0.51
1:G:41:ILE:O	1:G:47:VAL:CG2	2.59	0.50
1:G:42:ALA:O	1:G:43:CYS:CB	2.60	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:29:ARG:O	1:F:32:VAL:N	2.45	0.50
1:E:64:SER:O	1:E:66:GLU:N	2.44	0.50
1:D:65:ILE:CG1	1:D:65:ILE:O	2.57	0.50
1:H:102:LEU:C	1:H:102:LEU:CD2	2.91	0.50
1:I:241:LEU:C	1:I:242:ASN:CG	2.70	0.50
1:M:167:GLY:N	1:M:170:ARG:CG	2.74	0.50
1:L:228:GLU:O	1:L:232:LYS:N	2.45	0.50
1:K:72:ASP:O	1:K:74:HIS:N	2.44	0.50
1:I:122:GLN:OE1	1:I:122:GLN:C	2.50	0.50
1:G:103:THR:O	1:G:104:TYR:CG	2.65	0.50
1:K:90:ILE:C	1:K:92:ARG:N	2.64	0.50
1:L:14:THR:CG2	1:L:15:VAL:CG2	2.89	0.50
1:H:27:TYR:CD1	1:N:18:PRO:O	2.64	0.50
1:K:18:PRO:O	1:L:27:TYR:CD1	2.65	0.50
1:J:87:ARG:O	1:J:89:LEU:N	2.45	0.50
1:C:173:VAL:C	1:C:175:GLU:N	2.64	0.50
1:N:32:VAL:O	1:N:35:GLY:N	2.45	0.50
1:L:25:VAL:CG2	1:L:26:GLU:N	2.75	0.50
1:N:235:GLU:O	1:N:237:VAL:N	2.45	0.50
1:A:29:ARG:O	1:A:30:GLU:C	2.50	0.50
1:C:150:PHE:CE1	1:C:160:GLU:CB	2.95	0.50
1:C:182:ARG:NH1	1:C:184:ASP:OD2	2.44	0.50
1:J:103:THR:O	1:J:104:TYR:CG	2.65	0.50
1:F:119:ASP:O	1:F:120:ILE:C	2.49	0.50
1:J:192:GLU:O	1:J:193:LEU:C	2.50	0.50
1:J:48:VAL:CG1	1:J:49:LEU:N	2.74	0.49
1:E:68:ILE:CD1	1:E:68:ILE:N	2.75	0.49
1:E:93:ALA:C	1:E:95:LEU:N	2.65	0.49
1:F:32:VAL:C	1:F:34:ARG:N	2.66	0.49
1:A:87:ARG:O	1:A:88:VAL:C	2.49	0.49
1:C:153:ASP:OD1	1:C:154:PRO:N	2.46	0.49
1:N:102:LEU:CD2	1:N:102:LEU:C	2.95	0.49
1:G:222:PHE:CD1	1:G:222:PHE:C	2.86	0.49
1:K:102:LEU:O	1:K:103:THR:CB	4.06	0.49
1:C:173:VAL:O	1:C:176:LEU:N	2.44	0.49
1:A:102:LEU:O	1:A:103:THR:CB	4.05	0.49
1:A:235:GLU:O	1:A:237:VAL:N	2.45	0.49
1:I:208:GLU:C	1:I:210:VAL:N	2.66	0.49
1:B:180:GLU:CD	1:B:180:GLU:N	2.65	0.49
1:B:22:LEU:O	1:B:23:TYR:O	2.30	0.49
1:F:102:LEU:O	1:F:103:THR:CB	4.02	0.49
1:G:182:ARG:NH1	1:G:184:ASP:OD2	2.45	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:102:LEU:CD2	1:J:103:THR:N	3.50	0.49
1:B:103:THR:O	1:B:104:TYR:CG	2.65	0.49
1:B:143:ASP:OD2	1:B:148:ARG:NH2	2.46	0.49
1:B:148:ARG:CD	1:B:160:GLU:OE1	2.60	0.49
1:A:85:ASP:OD2	1:G:122:GLN:NE2	2.46	0.49
1:F:182:ARG:O	1:F:184:ASP:N	2.46	0.49
1:H:173:VAL:C	1:H:175:GLU:N	2.66	0.49
1:B:124:TYR:CD1	1:B:133:PHE:CZ	3.01	0.49
1:H:176:LEU:O	1:H:180:GLU:OE1	2.30	0.49
1:E:235:GLU:O	1:E:237:VAL:N	2.46	0.49
1:F:182:ARG:NH1	1:F:184:ASP:OD2	2.46	0.49
1:D:43:CYS:SG	1:D:46:GLY:O	2.71	0.49
1:M:86:ALA:O	1:M:87:ARG:C	2.49	0.49
1:C:24:GLN:O	1:C:25:VAL:C	2.50	0.49
1:E:190:GLY:O	1:E:191:LEU:C	2.51	0.49
1:N:177:LEU:O	1:N:179:LYS:N	2.45	0.49
1:A:114:ALA:O	1:A:116:LYS:N	2.44	0.49
1:G:95:LEU:O	1:G:97:ALA:N	2.45	0.49
1:E:173:VAL:C	1:E:175:GLU:N	2.66	0.49
1:G:153:ASP:OD1	1:G:153:ASP:C	2.50	0.48
1:J:153:ASP:OD1	1:J:153:ASP:C	2.52	0.48
1:F:89:LEU:O	1:F:93:ALA:N	2.46	0.48
1:G:22:LEU:O	1:G:23:TYR:O	2.31	0.48
1:B:90:ILE:C	1:B:92:ARG:N	2.66	0.48
1:I:170:ARG:CB	1:I:171:PRO:CD	2.90	0.48
1:F:42:ALA:O	1:F:43:CYS:SG	2.71	0.48
1:N:182:ARG:C	1:N:184:ASP:N	2.66	0.48
1:I:243:GLU:O	1:I:243:GLU:CG	2.61	0.48
1:J:153:ASP:C	1:J:155:SER:N	2.66	0.48
1:A:119:ASP:OD1	1:B:87:ARG:NH2	2.46	0.48
1:E:121:LYS:CG	1:E:133:PHE:CD1	2.96	0.48
1:H:18:PRO:O	1:I:27:TYR:CD1	2.66	0.48
1:D:82:LEU:CD1	1:D:82:LEU:N	2.76	0.48
1:B:153:ASP:OD1	1:B:154:PRO:N	2.46	0.48
1:J:115:LYS:O	1:J:119:ASP:OD2	2.30	0.48
1:M:126:GLN:O	1:N:130:VAL:CG2	2.61	0.48
1:N:239:LYS:O	1:N:242:ASN:OD1	2.32	0.48
1:G:190:GLY:O	1:G:191:LEU:C	2.52	0.48
1:K:192:GLU:O	1:K:193:LEU:C	2.52	0.48
1:J:114:ALA:O	1:J:116:LYS:N	2.46	0.48
1:H:14:THR:CG2	1:H:15:VAL:N	2.76	0.48
1:J:72:ASP:OD2	1:J:98:GLN:NE2	2.46	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:24:GLN:O	1:B:25:VAL:C	2.51	0.48
1:H:222:PHE:CD1	1:H:222:PHE:C	2.86	0.48
1:J:182:ARG:C	1:J:184:ASP:N	2.67	0.48
1:E:14:THR:CG2	1:E:15:VAL:N	2.75	0.48
1:E:181:TYR:CG	1:E:182:ARG:N	2.81	0.48
1:E:43:CYS:SG	1:E:46:GLY:O	2.72	0.48
1:H:106:GLU:O	1:H:107:GLU:C	2.51	0.48
1:G:208:GLU:OE1	1:G:208:GLU:C	2.51	0.48
1:F:14:THR:CG2	1:F:15:VAL:CG2	2.92	0.48
1:J:187:LEU:O	1:J:191:LEU:N	2.46	0.48
1:A:173:VAL:C	1:A:175:GLU:N	2.67	0.48
1:H:18:PRO:C	1:I:27:TYR:CD1	2.87	0.48
1:L:60:VAL:O	1:L:61:LYS:C	2.52	0.48
1:J:45:ASP:OD2	1:J:45:ASP:N	2.46	0.48
1:J:103:THR:O	1:J:104:TYR:CD2	2.67	0.48
1:L:14:THR:CG2	1:L:15:VAL:N	2.75	0.48
1:H:153:ASP:OD1	1:H:154:PRO:N	2.47	0.47
1:L:86:ALA:O	1:L:89:LEU:N	3.23	0.47
1:E:72:ASP:OD2	1:E:98:GLN:NE2	2.47	0.47
1:I:242:ASN:O	1:I:244:GLU:CG	2.62	0.47
1:M:87:ARG:O	1:M:88:VAL:C	2.53	0.47
1:M:90:ILE:O	1:M:92:ARG:N	2.47	0.47
1:D:182:ARG:NH1	1:D:184:ASP:OD2	2.47	0.47
1:N:233:LEU:C	1:N:235:GLU:N	2.67	0.47
1:J:14:THR:O	1:J:15:VAL:CG1	2.61	0.47
1:I:137:LEU:N	1:I:152:THR:OG1	2.47	0.47
1:A:177:LEU:O	1:A:179:LYS:N	2.47	0.47
1:G:24:GLN:O	1:G:25:VAL:C	2.52	0.47
1:A:184:ASP:O	1:A:185:ILE:C	2.52	0.47
1:J:177:LEU:O	1:J:179:LYS:N	2.47	0.47
1:I:184:ASP:O	1:I:185:ILE:C	2.53	0.47
1:L:173:VAL:C	1:L:175:GLU:N	2.68	0.47
1:N:61:LYS:O	1:N:63:ARG:N	2.47	0.47
1:J:90:ILE:C	1:J:92:ARG:N	2.67	0.47
1:M:242:ASN:C	1:M:244:GLU:N	2.67	0.47
1:H:45:ASP:N	1:H:45:ASP:OD2	2.47	0.47
1:J:62:ILE:CG2	1:J:62:ILE:O	2.62	0.47
1:D:19:GLU:OE1	1:D:19:GLU:N	2.47	0.47
1:N:25:VAL:CG2	1:N:26:GLU:N	2.78	0.47
1:N:153:ASP:OD1	1:N:154:PRO:N	2.48	0.47
1:E:148:ARG:CD	1:E:160:GLU:OE1	2.62	0.47
1:H:102:LEU:O	1:H:103:THR:CB	4.02	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:153:ASP:C	1:I:155:SER:N	2.65	0.47
1:F:72:ASP:OD2	1:F:98:GLN:NE2	2.47	0.47
1:C:103:THR:O	1:C:104:TYR:CD2	2.67	0.47
1:C:102:LEU:CD2	1:C:103:THR:N	3.39	0.47
1:I:102:LEU:CD2	1:I:102:LEU:C	2.89	0.47
1:B:218:LYS:O	1:B:219:ASP:CB	2.63	0.47
1:K:164:THR:OG1	1:K:165:ALA:N	2.47	0.47
1:M:180:GLU:N	1:M:180:GLU:CD	2.68	0.47
1:D:30:GLU:O	1:D:31:ALA:C	2.52	0.47
1:B:22:LEU:CD2	1:B:22:LEU:C	2.83	0.47
1:K:41:ILE:O	1:K:47:VAL:CG2	2.63	0.47
1:C:168:SER:OG	1:C:169:GLY:N	2.46	0.47
1:F:32:VAL:O	1:F:35:GLY:N	2.48	0.47
1:J:36:THR:O	1:J:80:SER:OG	2.32	0.47
1:F:76:ALA:O	1:F:140:ALA:N	2.48	0.47
1:G:114:ALA:O	1:G:116:LYS:N	2.48	0.47
1:I:126:GLN:NE2	1:J:133:PHE:CE2	2.83	0.47
1:I:124:TYR:CE1	1:I:133:PHE:CE2	3.03	0.47
1:M:173:VAL:O	1:M:175:GLU:N	2.48	0.47
1:K:148:ARG:CD	1:K:160:GLU:OE1	2.63	0.47
1:A:131:ARG:O	1:A:132:PRO:O	2.33	0.47
1:E:181:TYR:CD2	1:E:182:ARG:N	2.83	0.46
1:J:32:VAL:C	1:J:34:ARG:N	2.68	0.46
1:C:93:ALA:C	1:C:95:LEU:N	2.68	0.46
1:E:214:ILE:O	1:E:223:LYS:N	2.48	0.46
1:L:90:ILE:O	1:L:94:ARG:N	2.48	0.46
1:N:90:ILE:O	1:N:94:ARG:N	2.48	0.46
1:F:119:ASP:O	1:F:122:GLN:N	2.48	0.46
1:D:208:GLU:C	1:D:210:VAL:N	2.69	0.46
1:I:25:VAL:CG2	1:I:26:GLU:N	2.78	0.46
1:K:154:PRO:O	1:K:155:SER:CB	2.63	0.46
1:H:95:LEU:C	1:H:97:ALA:N	2.67	0.46
1:N:23:TYR:O	1:N:24:GLN:C	2.53	0.46
1:H:42:ALA:O	1:H:43:CYS:CB	2.63	0.46
1:J:203:GLU:O	1:J:204:ASP:CB	2.64	0.46
1:K:214:ILE:O	1:K:223:LYS:N	2.49	0.46
1:K:214:ILE:N	1:K:223:LYS:O	2.49	0.46
1:I:222:PHE:CD1	1:I:222:PHE:C	2.88	0.46
1:B:19:GLU:N	1:B:19:GLU:OE1	2.49	0.46
1:E:85:ASP:N	1:E:85:ASP:OD2	2.48	0.46
1:I:203:GLU:O	1:I:204:ASP:CB	2.63	0.46
1:G:102:LEU:O	1:G:103:THR:CB	4.02	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:102:LEU:O	1:M:103:THR:CG2	4.22	0.46
1:M:173:VAL:O	1:M:176:LEU:N	2.48	0.46
1:M:194:ALA:O	1:M:198:LEU:N	2.49	0.46
1:F:14:THR:CG2	1:F:15:VAL:N	2.77	0.46
1:G:153:ASP:OD1	1:G:154:PRO:N	2.49	0.46
1:L:235:GLU:O	1:L:237:VAL:N	2.48	0.46
1:D:180:GLU:N	1:D:180:GLU:CD	2.69	0.46
1:A:102:LEU:C	1:A:102:LEU:CD2	3.02	0.46
1:H:222:PHE:CD1	1:H:222:PHE:O	2.69	0.46
1:B:216:THR:C	1:B:218:LYS:N	2.69	0.46
1:B:235:GLU:O	1:B:237:VAL:N	2.49	0.46
1:J:173:VAL:C	1:J:175:GLU:N	2.68	0.46
1:M:102:LEU:C	1:M:102:LEU:CD2	2.84	0.46
1:G:32:VAL:O	1:G:35:GLY:N	2.48	0.46
1:M:24:GLN:O	1:M:25:VAL:C	2.54	0.46
1:M:14:THR:CG2	1:M:15:VAL:N	2.78	0.46
1:F:115:LYS:NZ	1:G:66:GLU:OE1	2.48	0.46
1:F:68:ILE:N	1:F:68:ILE:CD1	2.79	0.46
1:E:153:ASP:C	1:E:155:SER:N	2.69	0.46
1:D:173:VAL:O	1:D:176:LEU:N	2.49	0.46
1:L:182:ARG:O	1:L:184:ASP:N	2.49	0.46
1:A:214:ILE:N	1:A:214:ILE:CD1	2.79	0.46
1:M:106:GLU:O	1:M:107:GLU:C	2.54	0.46
1:K:34:ARG:O	1:K:35:GLY:O	2.33	0.46
1:G:238:LYS:N	1:G:238:LYS:CD	2.79	0.46
1:C:238:LYS:N	1:C:238:LYS:CD	2.79	0.46
1:J:196:THR:O	1:J:197:ALA:C	2.54	0.45
1:M:140:ALA:CB	1:M:148:ARG:O	2.64	0.45
1:J:122:GLN:O	1:J:125:THR:CB	2.64	0.45
1:I:114:ALA:O	1:I:116:LYS:N	2.49	0.45
1:A:36:THR:OG1	1:A:67:LYS:CE	2.63	0.45
1:C:29:ARG:O	1:C:32:VAL:N	2.49	0.45
1:B:214:ILE:N	1:B:214:ILE:CD1	2.79	0.45
1:J:82:LEU:N	1:J:82:LEU:CD1	2.79	0.45
1:A:90:ILE:O	1:A:94:ARG:N	2.48	0.45
1:B:18:PRO:C	1:C:27:TYR:CD1	2.89	0.45
1:B:173:VAL:C	1:B:175:GLU:N	2.69	0.45
1:F:129:GLY:O	1:F:130:VAL:CB	2.65	0.45
1:N:180:GLU:CD	1:N:180:GLU:N	2.70	0.45
1:I:90:ILE:O	1:I:94:ARG:N	2.48	0.45
1:E:100:TYR:CD2	1:E:100:TYR:C	2.89	0.45
1:E:122:GLN:O	1:E:122:GLN:CD	2.55	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:180:GLU:N	1:H:180:GLU:OE2	2.50	0.45
1:H:48:VAL:CG1	1:H:49:LEU:N	2.78	0.45
1:B:197:ALA:O	1:B:200:LYS:N	2.50	0.45
1:N:208:GLU:OE1	1:N:208:GLU:C	2.55	0.45
1:E:83:VAL:CG1	1:E:83:VAL:O	2.64	0.45
1:M:228:GLU:O	1:M:232:LYS:N	2.49	0.45
1:M:202:ASN:C	1:M:202:ASN:OD1	2.54	0.45
1:A:45:ASP:OD2	1:A:45:ASP:N	2.50	0.45
1:F:214:ILE:CD1	1:F:214:ILE:N	2.79	0.45
1:A:187:LEU:O	1:A:191:LEU:N	2.49	0.45
1:F:72:ASP:OD2	1:F:101:ARG:NH1	2.50	0.45
1:L:115:LYS:NZ	1:M:66:GLU:OE1	2.50	0.45
1:G:32:VAL:O	1:G:34:ARG:N	2.50	0.45
1:B:227:VAL:O	1:B:228:GLU:CB	2.64	0.45
1:L:180:GLU:N	1:L:180:GLU:OE2	2.49	0.45
1:J:184:ASP:O	1:J:185:ILE:C	2.54	0.45
1:K:227:VAL:O	1:K:228:GLU:CB	2.64	0.45
1:L:121:LYS:NZ	1:L:152:THR:OG1	2.50	0.45
1:F:103:THR:O	1:F:104:TYR:CG	2.69	0.45
1:F:22:LEU:C	1:F:22:LEU:CD2	2.85	0.45
1:D:32:VAL:O	1:D:35:GLY:N	2.50	0.45
1:K:95:LEU:C	1:K:97:ALA:N	2.70	0.45
1:L:182:ARG:NH1	1:L:184:ASP:OD2	2.50	0.45
1:B:63:ARG:N	1:B:63:ARG:CD	2.78	0.45
1:N:45:ASP:N	1:N:45:ASP:OD2	2.50	0.45
1:A:19:GLU:O	1:B:34:ARG:NH2	2.49	0.45
1:I:238:LYS:N	1:I:238:LYS:CD	2.79	0.45
1:K:28:ALA:O	1:K:29:ARG:C	2.54	0.45
1:D:161:TYR:CE2	1:E:60:VAL:CG2	3.00	0.45
1:A:87:ARG:O	1:A:90:ILE:N	2.50	0.45
1:A:153:ASP:C	1:A:153:ASP:OD1	2.54	0.45
1:K:90:ILE:O	1:K:94:ARG:N	2.50	0.45
1:I:64:SER:O	1:I:66:GLU:N	2.50	0.45
1:C:190:GLY:O	1:C:191:LEU:C	2.55	0.45
1:F:153:ASP:C	1:F:155:SER:N	2.69	0.45
1:H:14:THR:O	1:H:15:VAL:CG1	2.65	0.45
1:E:102:LEU:CD2	1:E:102:LEU:C	2.85	0.45
1:J:90:ILE:O	1:J:92:ARG:N	2.50	0.45
1:K:95:LEU:O	1:K:98:GLN:N	2.50	0.45
1:L:42:ALA:O	1:L:43:CYS:CB	2.65	0.45
1:C:214:ILE:CD1	1:C:214:ILE:N	2.80	0.45
1:K:90:ILE:O	1:K:92:ARG:N	2.50	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:103:THR:O	1:M:104:TYR:CG	2.70	0.44
1:L:102:LEU:O	1:L:103:THR:CB	4.02	0.44
1:B:102:LEU:CD2	1:B:103:THR:N	3.18	0.44
1:F:42:ALA:O	1:F:43:CYS:CB	2.64	0.44
1:J:14:THR:CG2	1:J:15:VAL:N	2.79	0.44
1:G:87:ARG:O	1:G:88:VAL:C	2.55	0.44
1:L:95:LEU:C	1:L:97:ALA:N	2.70	0.44
1:A:170:ARG:O	1:A:171:PRO:C	2.56	0.44
1:N:214:ILE:CD1	1:N:214:ILE:N	2.80	0.44
1:H:87:ARG:NH2	1:N:119:ASP:OD1	2.50	0.44
1:H:90:ILE:O	1:H:94:ARG:N	2.50	0.44
1:C:103:THR:O	1:C:104:TYR:CG	2.70	0.44
1:B:165:ALA:O	1:B:174:MET:SD	2.75	0.44
1:A:42:ALA:O	1:A:43:CYS:CB	2.65	0.44
1:F:222:PHE:CD1	1:F:222:PHE:C	2.91	0.44
1:E:153:ASP:OD1	1:E:154:PRO:N	2.50	0.44
1:G:114:ALA:C	1:G:116:LYS:N	2.70	0.44
1:I:22:LEU:O	1:I:23:TYR:O	2.35	0.44
1:L:122:GLN:CD	1:L:122:GLN:C	2.76	0.44
1:D:93:ALA:C	1:D:95:LEU:N	2.71	0.44
1:D:102:LEU:CD2	1:D:103:THR:N	3.31	0.44
1:K:87:ARG:O	1:K:90:ILE:N	2.50	0.44
1:A:213:CYS:SG	1:A:222:PHE:CZ	3.11	0.44
1:A:192:GLU:O	1:A:193:LEU:C	2.56	0.44
1:A:60:VAL:O	1:A:61:LYS:C	2.56	0.44
1:I:153:ASP:OD1	1:I:153:ASP:C	2.56	0.44
1:L:153:ASP:C	1:L:153:ASP:OD1	2.56	0.44
1:D:22:LEU:O	1:D:23:TYR:O	2.35	0.44
1:J:22:LEU:O	1:J:23:TYR:O	2.35	0.44
1:K:18:PRO:O	1:L:27:TYR:CE1	2.70	0.44
1:I:18:PRO:C	1:J:27:TYR:CD1	2.91	0.44
1:H:122:GLN:C	1:H:122:GLN:OE1	2.55	0.44
1:I:23:TYR:O	1:I:24:GLN:C	2.56	0.44
1:D:120:ILE:O	1:D:123:ALA:N	2.51	0.44
1:G:19:GLU:OE1	1:G:19:GLU:N	2.51	0.44
1:F:45:ASP:OD2	1:F:45:ASP:N	2.50	0.44
1:H:190:GLY:O	1:H:191:LEU:O	2.36	0.44
1:D:29:ARG:O	1:D:32:VAL:N	2.51	0.44
1:A:29:ARG:O	1:A:32:VAL:N	2.51	0.44
1:A:114:ALA:C	1:A:116:LYS:N	2.71	0.44
1:N:207:PRO:O	1:N:208:GLU:CG	2.65	0.44
1:C:68:ILE:N	1:C:68:ILE:CD1	2.81	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:65:ILE:CG1	1:J:65:ILE:O	2.66	0.44
1:L:173:VAL:O	1:L:175:GLU:N	2.51	0.44
1:K:82:LEU:CD2	1:K:82:LEU:N	2.79	0.44
1:M:22:LEU:CD2	1:M:23:TYR:N	2.81	0.44
1:I:102:LEU:CD2	1:I:103:THR:N	3.31	0.44
1:M:18:PRO:C	1:N:27:TYR:CD1	2.92	0.44
1:H:18:PRO:O	1:I:27:TYR:CE1	2.70	0.44
1:I:177:LEU:O	1:I:179:LYS:N	2.51	0.44
1:K:102:LEU:CD2	1:K:102:LEU:C	2.87	0.43
1:L:72:ASP:C	1:L:74:HIS:N	2.72	0.43
1:E:173:VAL:O	1:E:176:LEU:N	2.51	0.43
1:B:180:GLU:N	1:B:180:GLU:OE2	2.51	0.43
1:M:14:THR:O	1:M:15:VAL:CG1	2.66	0.43
1:D:125:THR:CG2	1:E:131:ARG:NH2	2.81	0.43
1:C:16:PHE:CB	1:D:24:GLN:OE1	2.66	0.43
1:G:165:ALA:O	1:G:174:MET:SD	2.76	0.43
1:K:95:LEU:O	1:K:97:ALA:N	2.51	0.43
1:N:182:ARG:O	1:N:184:ASP:N	2.51	0.43
1:A:14:THR:CG2	1:A:15:VAL:CG2	2.95	0.43
1:M:214:ILE:CD1	1:M:214:ILE:N	2.81	0.43
1:B:202:ASN:C	1:B:202:ASN:OD1	2.56	0.43
1:A:180:GLU:N	1:A:180:GLU:CD	2.72	0.43
1:A:180:GLU:OE2	1:A:180:GLU:N	2.51	0.43
1:J:102:LEU:O	1:J:103:THR:CB	4.00	0.43
1:I:72:ASP:CB	1:I:74:HIS:CE1	3.01	0.43
1:I:90:ILE:O	1:I:93:ALA:N	2.51	0.43
1:C:153:ASP:C	1:C:155:SER:N	2.72	0.43
1:C:173:VAL:O	1:C:175:GLU:N	2.51	0.43
1:M:72:ASP:OD2	1:M:98:GLN:NE2	2.52	0.43
1:M:160:GLU:CB	1:N:64:SER:CB	2.97	0.43
1:B:26:GLU:O	1:B:29:ARG:N	2.51	0.43
1:B:239:LYS:CD	1:B:240:LYS:NZ	2.81	0.43
1:N:14:THR:O	1:N:15:VAL:CG1	2.67	0.43
1:D:45:ASP:OD2	1:D:45:ASP:N	2.50	0.43
1:D:164:THR:OG1	1:D:165:ALA:N	2.52	0.43
1:I:202:ASN:OD1	1:I:202:ASN:C	2.57	0.43
1:D:42:ALA:O	1:D:43:CYS:CB	2.67	0.43
1:M:22:LEU:C	1:M:22:LEU:CD2	2.87	0.43
1:N:173:VAL:C	1:N:175:GLU:N	2.72	0.43
1:K:29:ARG:O	1:K:30:GLU:C	2.57	0.43
1:H:160:GLU:CB	1:I:64:SER:CB	2.97	0.43
1:D:74:HIS:O	1:D:75:VAL:CG2	2.67	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:190:GLY:O	1:J:191:LEU:O	2.36	0.43
1:A:48:VAL:CG1	1:A:213:CYS:O	2.66	0.43
1:N:95:LEU:O	1:N:97:ALA:N	2.51	0.43
1:G:129:GLY:O	1:G:130:VAL:CB	2.67	0.43
1:I:187:LEU:O	1:I:191:LEU:N	2.51	0.43
1:B:182:ARG:O	1:B:184:ASP:N	2.52	0.43
1:N:43:CYS:SG	1:N:44:LYS:N	2.91	0.43
1:H:114:ALA:C	1:H:116:LYS:N	2.70	0.43
1:A:86:ALA:O	1:A:87:ARG:C	2.56	0.43
1:G:92:ARG:O	1:G:92:ARG:CD	2.67	0.43
1:D:18:PRO:O	1:D:19:GLU:CB	2.67	0.43
1:L:177:LEU:O	1:L:179:LYS:N	2.52	0.43
1:B:102:LEU:CD2	1:B:102:LEU:C	2.87	0.43
1:B:102:LEU:O	1:B:103:THR:CB	4.05	0.43
1:J:182:ARG:O	1:J:184:ASP:N	2.52	0.43
1:H:64:SER:O	1:H:66:GLU:N	2.51	0.43
1:K:56:THR:OG1	1:K:57:SER:N	2.51	0.43
1:B:14:THR:CG2	1:B:15:VAL:N	2.81	0.43
1:H:102:LEU:CD2	1:H:103:THR:N	3.20	0.43
1:I:242:ASN:C	1:I:244:GLU:N	2.71	0.43
1:G:93:ALA:C	1:G:95:LEU:N	2.71	0.43
1:M:114:ALA:O	1:M:116:LYS:N	2.52	0.43
1:K:197:ALA:O	1:K:198:LEU:C	2.55	0.43
1:D:199:THR:O	1:D:200:LYS:C	2.56	0.43
1:N:190:GLY:O	1:N:191:LEU:C	2.56	0.43
1:F:155:SER:OG	1:F:155:SER:O	2.35	0.43
1:F:29:ARG:NH1	1:F:153:ASP:OD2	2.51	0.43
1:I:100:TYR:CD2	1:I:100:TYR:C	2.92	0.43
1:D:70:GLN:NE2	1:D:72:ASP:O	2.51	0.43
1:D:190:GLY:O	1:D:191:LEU:C	2.55	0.43
1:A:173:VAL:O	1:A:175:GLU:N	2.52	0.43
1:L:187:LEU:O	1:L:191:LEU:N	2.52	0.43
1:C:235:GLU:O	1:C:237:VAL:N	2.52	0.43
1:M:43:CYS:SG	1:M:44:LYS:N	2.91	0.43
1:F:184:ASP:O	1:F:185:ILE:C	2.57	0.43
1:E:23:TYR:O	1:E:24:GLN:C	2.57	0.43
1:B:29:ARG:O	1:B:32:VAL:N	2.51	0.43
1:I:126:GLN:NE2	1:J:124:TYR:CE1	2.87	0.43
1:K:214:ILE:N	1:K:214:ILE:CD1	2.81	0.43
1:I:16:PHE:CD1	1:I:17:SER:N	2.86	0.43
1:B:184:ASP:O	1:B:185:ILE:C	2.57	0.43
1:M:42:ALA:O	1:M:43:CYS:CB	2.67	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:221:GLN:NE2	1:C:222:PHE:O	2.52	0.43
1:J:86:ALA:O	1:J:87:ARG:C	2.57	0.42
1:C:114:ALA:C	1:C:116:LYS:N	2.72	0.42
1:G:173:VAL:C	1:G:175:GLU:N	2.71	0.42
1:C:72:ASP:OD2	1:C:98:GLN:NE2	2.52	0.42
1:E:180:GLU:OE2	1:E:180:GLU:N	2.52	0.42
1:C:184:ASP:O	1:C:185:ILE:C	2.57	0.42
1:J:181:TYR:CG	1:J:182:ARG:N	2.87	0.42
1:M:182:ARG:C	1:M:184:ASP:N	2.72	0.42
1:M:56:THR:OG1	1:M:57:SER:N	2.52	0.42
1:I:32:VAL:C	1:I:34:ARG:N	2.72	0.42
1:F:32:VAL:O	1:F:34:ARG:N	2.52	0.42
1:E:14:THR:O	1:E:15:VAL:CG1	2.67	0.42
1:F:95:LEU:C	1:F:97:ALA:N	2.72	0.42
1:F:109:SER:O	1:F:110:ILE:C	2.56	0.42
1:E:122:GLN:C	1:E:122:GLN:CD	2.77	0.42
1:G:210:VAL:CG2	1:G:230:ILE:CG2	2.97	0.42
1:L:36:THR:OG1	1:L:67:LYS:CE	2.67	0.42
1:L:203:GLU:O	1:L:204:ASP:CB	2.67	0.42
1:K:66:GLU:CB	1:K:69:PHE:CE1	3.02	0.42
1:K:131:ARG:O	1:K:132:PRO:O	2.37	0.42
1:B:90:ILE:O	1:B:92:ARG:N	2.52	0.42
1:J:144:LYS:O	1:J:146:GLU:N	2.52	0.42
1:L:213:CYS:SG	1:L:222:PHE:CZ	3.12	0.42
1:E:153:ASP:C	1:E:153:ASP:OD1	2.57	0.42
1:A:90:ILE:CD1	1:A:94:ARG:CD	2.97	0.42
1:M:153:ASP:OD1	1:M:153:ASP:C	2.57	0.42
1:H:86:ALA:O	1:H:87:ARG:C	2.56	0.42
1:D:202:ASN:C	1:D:202:ASN:OD1	2.57	0.42
1:H:53:ARG:CB	1:H:65:ILE:CD1	2.98	0.42
1:M:177:LEU:O	1:M:179:LYS:N	2.52	0.42
1:E:66:GLU:CD	1:E:69:PHE:CE1	2.93	0.42
1:N:124:TYR:CE1	1:N:133:PHE:CZ	3.07	0.42
1:N:181:TYR:CG	1:N:182:ARG:N	2.87	0.42
1:J:114:ALA:C	1:J:116:LYS:N	2.71	0.42
1:J:56:THR:OG1	1:J:57:SER:N	2.53	0.42
1:I:14:THR:CG2	1:I:15:VAL:N	2.81	0.42
1:E:130:VAL:CG1	1:E:130:VAL:O	2.67	0.42
1:I:98:GLN:O	1:I:99:ILE:C	2.57	0.42
1:I:190:GLY:O	1:I:191:LEU:O	2.37	0.42
1:A:126:GLN:CB	1:B:131:ARG:NE	2.83	0.42
1:H:85:ASP:OD2	1:N:122:GLN:NE2	2.53	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:148:ARG:CD	1:I:160:GLU:OE1	2.68	0.42
1:D:227:VAL:O	1:D:228:GLU:CB	2.67	0.42
1:E:125:THR:CG2	1:F:131:ARG:NH2	2.83	0.42
1:E:170:ARG:CB	1:E:171:PRO:CD	2.97	0.42
1:B:153:ASP:C	1:B:153:ASP:OD1	2.58	0.42
1:M:99:ILE:CG2	1:M:100:TYR:N	2.82	0.42
1:I:173:VAL:O	1:I:175:GLU:N	2.53	0.42
1:L:222:PHE:C	1:L:222:PHE:CD1	2.92	0.42
1:I:43:CYS:SG	1:I:46:GLY:O	2.78	0.42
1:F:238:LYS:N	1:F:238:LYS:CD	2.82	0.42
1:C:93:ALA:O	1:C:95:LEU:N	2.52	0.42
1:N:95:LEU:C	1:N:97:ALA:N	2.73	0.42
1:H:180:GLU:N	1:H:180:GLU:CD	2.73	0.42
1:K:32:VAL:C	1:K:34:ARG:N	2.72	0.42
1:A:17:SER:CB	1:A:21:ARG:O	2.68	0.42
1:H:164:THR:OG1	1:H:165:ALA:N	2.53	0.42
1:L:190:GLY:O	1:L:191:LEU:C	2.58	0.42
1:C:182:ARG:C	1:C:184:ASP:N	2.73	0.42
1:G:53:ARG:O	1:G:209:ASN:ND2	2.53	0.42
1:K:45:ASP:N	1:K:45:ASP:OD2	2.52	0.42
1:I:121:LYS:NZ	1:I:152:THR:OG1	2.52	0.41
1:E:181:TYR:O	1:E:182:ARG:CG	2.68	0.41
1:G:180:GLU:OE2	1:G:180:GLU:N	2.53	0.41
1:L:192:GLU:O	1:L:195:ILE:N	2.53	0.41
1:D:48:VAL:CG1	1:D:49:LEU:N	2.83	0.41
1:L:18:PRO:C	1:M:27:TYR:CD1	2.94	0.41
1:N:48:VAL:CG1	1:N:49:LEU:N	2.82	0.41
1:D:122:GLN:OE1	1:D:122:GLN:C	2.58	0.41
1:N:19:GLU:N	1:N:19:GLU:OE1	2.53	0.41
1:D:90:ILE:O	1:D:94:ARG:N	2.53	0.41
1:E:122:GLN:NE2	1:F:85:ASP:OD2	2.53	0.41
1:N:236:LYS:O	1:N:237:VAL:CG2	2.68	0.41
1:E:235:GLU:CA	1:E:235:GLU:OE2	2.68	0.41
1:A:14:THR:CG2	1:A:15:VAL:N	2.82	0.41
1:D:214:ILE:O	1:D:223:LYS:N	2.54	0.41
1:K:218:LYS:O	1:K:219:ASP:CB	2.66	0.41
1:A:222:PHE:C	1:A:222:PHE:CD1	2.94	0.41
1:E:114:ALA:C	1:E:116:LYS:N	2.72	0.41
1:A:53:ARG:CB	1:A:209:ASN:O	2.68	0.41
1:I:164:THR:OG1	1:I:165:ALA:N	2.53	0.41
1:H:22:LEU:O	1:H:23:TYR:O	2.38	0.41
1:K:173:VAL:O	1:K:177:LEU:CD1	2.68	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:19:GLU:O	1:B:34:ARG:CZ	2.68	0.41
1:C:126:GLN:CB	1:D:131:ARG:CZ	2.99	0.41
1:M:28:ALA:O	1:M:29:ARG:C	2.56	0.41
1:C:192:GLU:O	1:C:193:LEU:C	2.58	0.41
1:M:89:LEU:O	1:M:93:ALA:N	2.53	0.41
1:D:38:ALA:N	1:D:166:ILE:O	2.53	0.41
1:M:216:THR:OG1	1:M:219:ASP:OD2	2.37	0.41
1:L:153:ASP:C	1:L:155:SER:N	2.74	0.41
1:K:122:GLN:NE2	1:L:85:ASP:OD2	2.53	0.41
1:D:161:TYR:CD1	1:D:164:THR:CG2	3.04	0.41
1:E:87:ARG:O	1:E:89:LEU:N	2.53	0.41
1:G:34:ARG:O	1:G:35:GLY:O	2.37	0.41
1:M:187:LEU:O	1:M:191:LEU:N	2.53	0.41
1:G:235:GLU:O	1:G:237:VAL:N	2.53	0.41
1:F:64:SER:O	1:F:66:GLU:N	2.53	0.41
1:K:72:ASP:C	1:K:74:HIS:N	2.74	0.41
1:A:137:LEU:CB	1:A:152:THR:OG1	2.68	0.41
1:D:114:ALA:C	1:D:116:LYS:N	2.73	0.41
1:H:197:ALA:O	1:H:200:LYS:N	2.54	0.41
1:C:207:PRO:O	1:C:208:GLU:CG	2.68	0.41
1:H:184:ASP:O	1:H:185:ILE:C	2.59	0.41
1:N:121:LYS:NZ	1:N:152:THR:OG1	2.53	0.41
1:B:238:LYS:CD	1:B:238:LYS:N	2.84	0.41
1:J:153:ASP:OD1	1:J:154:PRO:N	2.54	0.41
1:I:119:ASP:OD1	1:J:87:ARG:NE	2.54	0.41
1:A:100:TYR:CD2	1:A:100:TYR:C	2.94	0.41
1:G:184:ASP:O	1:G:185:ILE:C	2.59	0.41
1:H:202:ASN:C	1:H:202:ASN:OD1	2.59	0.41
1:D:26:GLU:CG	1:D:29:ARG:NE	2.83	0.41
1:E:18:PRO:O	1:F:27:TYR:CD1	2.74	0.41
1:B:22:LEU:CD2	1:B:23:TYR:N	2.83	0.41
1:I:235:GLU:OE2	1:I:235:GLU:CA	2.67	0.41
1:L:117:ILE:CD1	1:L:117:ILE:N	2.84	0.41
1:H:74:HIS:O	1:H:75:VAL:CG2	2.69	0.41
1:K:123:ALA:O	1:K:125:THR:N	2.54	0.41
1:B:87:ARG:O	1:B:88:VAL:C	2.59	0.41
1:C:42:ALA:N	1:C:162:LYS:O	2.54	0.41
1:B:190:GLY:O	1:B:191:LEU:C	2.59	0.41
1:A:72:ASP:OD2	1:A:98:GLN:NE2	2.54	0.41
1:A:95:LEU:C	1:A:97:ALA:N	2.73	0.41
1:N:143:ASP:OD2	1:N:148:ARG:NH2	2.54	0.41
1:B:24:GLN:O	1:B:28:ALA:N	2.53	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:106:GLU:O	1:D:107:GLU:C	2.58	0.41
1:N:162:LYS:O	1:N:163:ALA:CB	2.68	0.41
1:M:238:LYS:CD	1:M:238:LYS:N	2.84	0.41
1:H:92:ARG:O	1:H:92:ARG:CG	2.69	0.41
1:C:100:TYR:O	1:C:102:LEU:N	2.54	0.41
1:D:23:TYR:O	1:D:24:GLN:C	2.58	0.41
1:D:14:THR:CG2	1:D:15:VAL:N	2.82	0.41
1:L:100:TYR:CD2	1:L:100:TYR:C	2.94	0.41
1:B:16:PHE:CD1	1:B:17:SER:N	2.89	0.41
1:C:121:LYS:CG	1:C:133:PHE:CD1	3.04	0.41
1:J:43:CYS:SG	1:J:44:LYS:N	2.93	0.41
1:B:124:TYR:CE1	1:B:133:PHE:CZ	3.09	0.41
1:D:177:LEU:O	1:D:179:LYS:N	2.54	0.41
1:H:167:GLY:O	1:H:168:SER:C	2.59	0.41
1:K:208:GLU:OE1	1:K:208:GLU:C	2.58	0.41
1:N:52:ASP:O	1:N:52:ASP:CG	2.56	0.41
1:H:137:LEU:N	1:H:152:THR:OG1	2.54	0.41
1:G:153:ASP:C	1:G:155:SER:N	2.74	0.41
1:M:154:PRO:O	1:M:155:SER:CB	2.69	0.41
1:E:90:ILE:O	1:E:94:ARG:N	2.54	0.41
1:H:192:GLU:O	1:H:195:ILE:N	2.54	0.41
1:D:184:ASP:O	1:D:185:ILE:C	2.60	0.41
1:G:187:LEU:O	1:G:191:LEU:N	2.54	0.41
1:I:112:MET:O	1:I:113:LEU:C	2.59	0.41
1:F:192:GLU:O	1:F:193:LEU:C	2.59	0.41
1:E:238:LYS:CD	1:E:238:LYS:N	2.84	0.41
1:L:133:PHE:N	1:L:133:PHE:CD1	3.65	0.41
1:A:92:ARG:O	1:A:92:ARG:CD	2.69	0.40
1:G:196:THR:O	1:G:197:ALA:C	2.59	0.40
1:E:173:VAL:O	1:E:175:GLU:N	2.54	0.40
1:B:114:ALA:C	1:B:116:LYS:N	2.73	0.40
1:H:112:MET:O	1:H:113:LEU:C	2.59	0.40
1:E:124:TYR:CD1	1:E:133:PHE:CE2	3.10	0.40
1:K:168:SER:OG	1:K:169:GLY:N	2.52	0.40
1:E:170:ARG:O	1:E:174:MET:N	2.54	0.40
1:D:214:ILE:N	1:D:214:ILE:CD1	2.84	0.40
1:K:207:PRO:O	1:K:208:GLU:CG	2.68	0.40
1:G:192:GLU:OE2	1:G:236:LYS:NZ	2.55	0.40
1:C:170:ARG:CB	1:C:171:PRO:CD	2.98	0.40
1:K:231:LYS:O	1:K:234:ILE:N	2.53	0.40
1:G:173:VAL:O	1:G:177:LEU:CD1	2.69	0.40
1:C:95:LEU:C	1:C:97:ALA:N	2.75	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:182:ARG:C	1:L:184:ASP:N	2.75	0.40
1:I:17:SER:OG	1:I:21:ARG:O	2.39	0.40
1:L:18:PRO:O	1:M:27:TYR:CD1	2.75	0.40
1:D:153:ASP:OD1	1:D:153:ASP:C	2.59	0.40
1:E:59:LEU:N	1:E:59:LEU:CD1	2.84	0.40
1:B:113:LEU:O	1:B:114:ALA:C	2.59	0.40
1:M:18:PRO:O	1:M:19:GLU:CB	2.69	0.40
1:E:68:ILE:CD1	1:E:211:ASP:OD2	2.70	0.40
1:G:48:VAL:CG1	1:G:49:LEU:N	2.85	0.40
1:B:26:GLU:O	1:B:27:TYR:C	2.57	0.40
1:E:42:ALA:O	1:E:43:CYS:CB	2.69	0.40
1:K:177:LEU:O	1:K:179:LYS:N	2.55	0.40
1:L:233:LEU:C	1:L:235:GLU:N	2.74	0.40
1:E:60:VAL:O	1:E:61:LYS:C	2.57	0.40
1:N:87:ARG:O	1:N:90:ILE:N	2.55	0.40
1:K:43:CYS:SG	1:K:46:GLY:N	2.95	0.40
1:G:93:ALA:O	1:G:95:LEU:N	2.55	0.40
1:J:169:GLY:O	1:J:170:ARG:C	2.60	0.40
1:M:210:VAL:CG2	1:M:230:ILE:CG2	2.99	0.40
1:L:208:GLU:OE1	1:L:208:GLU:C	2.60	0.40
1:A:72:ASP:O	1:A:74:HIS:N	2.54	0.40
1:L:119:ASP:OD1	1:M:87:ARG:NE	2.55	0.40
1:J:18:PRO:C	1:K:27:TYR:CD1	2.95	0.40
1:F:168:SER:O	1:F:170:ARG:N	2.55	0.40
1:I:182:ARG:C	1:I:184:ASP:N	2.74	0.40
1:K:199:THR:O	1:K:202:ASN:N	2.55	0.40
1:I:173:VAL:O	1:I:176:LEU:N	2.55	0.40
1:C:48:VAL:CG1	1:C:49:LEU:N	2.84	0.40
1:D:238:LYS:CD	1:D:238:LYS:N	2.85	0.40

All (7) 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	Distance(Å)	Clash(Å)
1:B:232:LYS:O	2:c:110:TYR:OH[2_565]	1.88	0.32
1:I:242:ASN:O	2:m:205:ASP:OD1[4_555]	2.00	0.20
1:M:243:GLU:N	2:i:205:ASP:OD1[4_455]	2.03	0.17
1:E:180:GLU:O	1:E:182:ARG:NH2[2_665]	2.09	0.11
1:B:231:LYS:NZ	2:c:15:ASP:OD1[2_565]	2.17	0.03
1:F:184:ASP:O	2:f:154:ASP:OD1[2_665]	2.19	0.01
1:M:242:ASN:O	2:i:201:GLU:OE1[4_455]	2.19	0.01

## 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	230/264 (87%)	163 (71%)	43 (19%)	24 (10%)	1	18
1	B	230/264 (87%)	162 (70%)	46 (20%)	22 (10%)	1	21
1	C	230/264 (87%)	155 (67%)	51 (22%)	24 (10%)	1	18
1	D	230/264 (87%)	158 (69%)	47 (20%)	25 (11%)	1	17
1	E	230/264 (87%)	158 (69%)	47 (20%)	25 (11%)	1	17
1	F	230/264 (87%)	152 (66%)	53 (23%)	25 (11%)	1	17
1	G	230/264 (87%)	156 (68%)	51 (22%)	23 (10%)	1	20
1	H	230/264 (87%)	153 (66%)	49 (21%)	28 (12%)	1	14
1	I	230/264 (87%)	159 (69%)	44 (19%)	27 (12%)	1	15
1	J	230/264 (87%)	161 (70%)	45 (20%)	24 (10%)	1	18
1	K	230/264 (87%)	151 (66%)	51 (22%)	28 (12%)	1	14
1	L	230/264 (87%)	162 (70%)	39 (17%)	29 (13%)	0	13
1	M	230/264 (87%)	159 (69%)	45 (20%)	26 (11%)	1	16
1	N	230/264 (87%)	159 (69%)	48 (21%)	23 (10%)	1	20
2	a	200/219 (91%)	135 (68%)	45 (22%)	20 (10%)	1	20
2	b	200/219 (91%)	129 (64%)	53 (26%)	18 (9%)	1	24
2	c	200/219 (91%)	140 (70%)	45 (22%)	15 (8%)	2	30
2	d	200/219 (91%)	132 (66%)	46 (23%)	22 (11%)	1	17
2	e	200/219 (91%)	136 (68%)	46 (23%)	18 (9%)	1	24
2	f	200/219 (91%)	142 (71%)	42 (21%)	16 (8%)	1	28
2	g	200/219 (91%)	132 (66%)	43 (22%)	25 (12%)	1	14
2	h	200/219 (91%)	136 (68%)	44 (22%)	20 (10%)	1	20
2	i	200/219 (91%)	130 (65%)	46 (23%)	24 (12%)	1	14
2	j	200/219 (91%)	145 (72%)	39 (20%)	16 (8%)	1	28
2	k	200/219 (91%)	126 (63%)	50 (25%)	24 (12%)	1	14
2	l	200/219 (91%)	143 (72%)	37 (18%)	20 (10%)	1	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	m	200/219 (91%)	139 (70%)	43 (22%)	18 (9%)	1	24
2	n	200/219 (91%)	136 (68%)	46 (23%)	18 (9%)	1	24
All	All	6020/6762 (89%)	4109 (68%)	1284 (21%)	627 (10%)	1	18

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
1	F	23	TYR

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Mol	Chain	Res	Type
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
2	g	105	ILE

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Mol	Chain	Res	Type
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
1	M	219	ASP

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Mol	Chain	Res	Type
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
2	m	197	ASP

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Mol	Chain	Res	Type
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
2	a	55	VAL

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Mol	Chain	Res	Type
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
1	H	237	VAL

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Mol	Chain	Res	Type
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
2	h	64	LEU

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Mol	Chain	Res	Type
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
1	A	183	ASP

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Mol	Chain	Res	Type
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
1	H	168	SER

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Mol	Chain	Res	Type
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
2	n	64	LEU

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Mol	Chain	Res	Type
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
1	H	130	VAL

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Mol	Chain	Res	Type
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
1	D	25	VAL

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Mol	Chain	Res	Type
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
1	M	195	ILE

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Mol	Chain	Res	Type
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
2	k	125	GLY

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Mol	Chain	Res	Type
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
1	D	185	ILE

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Mol	Chain	Res	Type
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 ⓘ

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%)	7	40
1	B	195/224 (87%)	167 (86%)	28 (14%)	5	32
1	C	195/224 (87%)	170 (87%)	25 (13%)	6	38
1	D	195/224 (87%)	170 (87%)	25 (13%)	6	38
1	E	195/224 (87%)	166 (85%)	29 (15%)	4	30
1	F	195/224 (87%)	165 (85%)	30 (15%)	4	28
1	G	195/224 (87%)	166 (85%)	29 (15%)	4	30
1	H	195/224 (87%)	162 (83%)	33 (17%)	3	24
1	I	195/224 (87%)	166 (85%)	29 (15%)	4	30
1	J	195/224 (87%)	170 (87%)	25 (13%)	6	38
1	K	195/224 (87%)	170 (87%)	25 (13%)	6	38
1	L	195/224 (87%)	166 (85%)	29 (15%)	4	30
1	M	195/224 (87%)	169 (87%)	26 (13%)	6	36
1	N	195/224 (87%)	170 (87%)	25 (13%)	6	38
2	a	163/179 (91%)	135 (83%)	28 (17%)	3	22
2	b	163/179 (91%)	126 (77%)	37 (23%)	1	10
2	c	163/179 (91%)	133 (82%)	30 (18%)	2	18
2	d	163/179 (91%)	128 (78%)	35 (22%)	1	11
2	e	163/179 (91%)	129 (79%)	34 (21%)	1	13
2	f	163/179 (91%)	125 (77%)	38 (23%)	1	9
2	g	163/179 (91%)	131 (80%)	32 (20%)	2	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	h	163/179 (91%)	126 (77%)	37 (23%)	1	10
2	i	163/179 (91%)	132 (81%)	31 (19%)	2	16
2	j	163/179 (91%)	126 (77%)	37 (23%)	1	10
2	k	163/179 (91%)	132 (81%)	31 (19%)	2	16
2	l	163/179 (91%)	127 (78%)	36 (22%)	1	11
2	m	163/179 (91%)	124 (76%)	39 (24%)	1	8
2	n	163/179 (91%)	132 (81%)	31 (19%)	2	16
All	All	5012/5642 (89%)	4154 (83%)	858 (17%)	3	23

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
1	B	19	GLU
1	B	36	THR
1	B	45	ASP

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Mol	Chain	Res	Type
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
1	C	121	LYS
1	C	135	VAL
1	C	153	ASP

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Mol	Chain	Res	Type
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
1	E	55	ILE
1	E	58	LYS
1	E	60	VAL

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Mol	Chain	Res	Type
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
1	F	136	SER
1	F	159	ILE
1	F	168	SER

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Mol	Chain	Res	Type
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
2	a	23	ASP
2	a	27	SER
2	a	43	ILE

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Mol	Chain	Res	Type
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
2	b	101	PHE
2	b	102	LEU
2	b	104	GLN

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Mol	Chain	Res	Type
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
2	c	113	LEU
2	c	124	LEU
2	c	154	ASP

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Mol	Chain	Res	Type
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
2	d	199	GLU
2	e	10	VAL
2	e	15	ASP

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Mol	Chain	Res	Type
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
2	f	43	ILE
2	f	45	ASP
2	f	50	THR

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Mol	Chain	Res	Type
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
2	g	80	ILE
2	g	83	LEU
2	g	85	CYS

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Mol	Chain	Res	Type
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
1	H	135	VAL
1	H	153	ASP
1	H	159	ILE

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Mol	Chain	Res	Type
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
1	J	19	GLU
1	J	25	VAL
1	J	36	THR

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Mol	Chain	Res	Type
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
1	K	180	GLU
1	K	205	ILE
1	K	207	PRO

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Mol	Chain	Res	Type
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
1	M	58	LYS
1	M	60	VAL
1	M	68	ILE

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Mol	Chain	Res	Type
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
1	N	211	ASP
1	N	212	VAL
1	N	242	ASN

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Mol	Chain	Res	Type
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
2	i	16	ASP
2	i	23	ASP
2	i	27	SER

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Mol	Chain	Res	Type
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
2	j	83	LEU
2	j	93	LEU
2	j	101	PHE

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Mol	Chain	Res	Type
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
2	k	103	THR
2	k	105	ILE
2	k	107	ILE

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Mol	Chain	Res	Type
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
2	l	155	MET
2	l	184	LEU
2	l	187	ILE

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Mol	Chain	Res	Type
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
2	m	198	GLU
2	m	199	GLU
2	m	202	LYS

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Mol	Chain	Res	Type
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.