



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:22 PM GMT

PDB ID : 4R67
Title : Human constitutive 20S proteasome in complex with carfilzomib
Authors : Sacchettini, J.C.; Harshbarger, W.H.
Deposited on : 2014-08-22
Resolution : 2.89 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

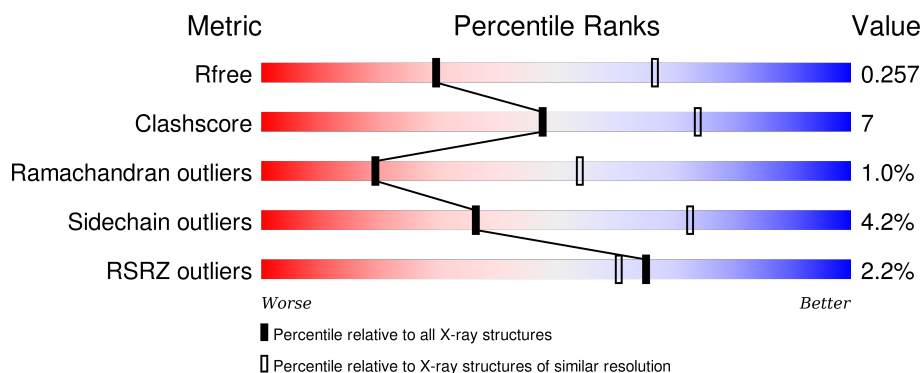
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	244	<div> <div>2%</div> <div>80%</div> <div>18%</div> <div>•</div> </div>
1	O	244	<div> <div>2%</div> <div>82%</div> <div>16%</div> <div>•</div> </div>
1	c	244	<div> <div>3%</div> <div>95%</div> <div>5%</div> </div>
1	q	244	<div> <div>2%</div> <div>94%</div> <div>5%</div> </div>
2	B	233	<div> <div>2%</div> <div>85%</div> <div>15%</div> </div>

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Mol	Chain	Length	Quality of chain
2	P	233	
2	d	233	
2	r	233	
3	C	250	
3	Q	250	
3	e	250	
3	s	250	
4	D	243	
4	R	243	
4	f	243	
4	t	243	
5	E	234	
5	S	234	
5	g	234	
5	u	234	
6	F	238	
6	T	238	
6	h	238	
6	v	238	
7	G	245	
7	U	245	
7	i	245	
7	w	245	
8	H	202	
8	V	202	

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Mol	Chain	Length	Quality of chain
8	j	202	 3% 97%
8	x	202	 2% 97%
9	I	220	 80% 19%
9	W	220	 78% 21%
9	k	220	 97%
9	y	220	 97%
10	J	204	 79% 17%
10	X	204	 78% 19%
10	l	204	 93% 7%
10	z	204	 93% 7%
11	0	199	 2% 84% 14%
11	K	199	 2% 84% 14%
11	Y	199	 2% 84% 13%
11	m	199	 2% 95% 5%
12	3	201	 83% 16%
12	L	201	 83% 16%
12	Z	201	 86% 13%
12	n	201	 96%
13	1	213	 87% 12%
13	M	213	 86% 13%
13	a	213	 97%
13	o	213	 98%
14	2	217	 80% 17%
14	N	217	 78% 19%
14	b	217	 94% 6%

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Mol	Chain	Length	Quality of chain
14	p	217	<div> <div></div> <div>%</div> <div>94%</div> <div>6%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	3BV	3	301	-	-	-	X
15	3BV	H	301	-	-	-	X
15	3BV	I	301	-	-	-	X
15	3BV	V	301	-	-	X	X
15	3BV	W	301	-	-	X	-
15	3BV	j	301	-	-	-	X
15	3BV	k	301	-	-	-	X
15	3BV	y	301	-	-	-	X

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 96005 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 type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	0	0
			1842	1170	309	350	13			
1	O	244	Total	C	N	O	S	0	0	0
			1845	1171	309	352	13			
1	c	244	Total	C	N	O	S	0	0	0
			1842	1170	309	350	13			
1	q	244	Total	C	N	O	S	0	0	0
			1842	1170	309	350	13			

- Molecule 2 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	233	Total	C	N	O	S	0	0	0
			1713	1087	287	334	5			
2	P	233	Total	C	N	O	S	0	0	0
			1712	1085	287	334	6			
2	d	233	Total	C	N	O	S	0	0	0
			1710	1083	287	334	6			
2	r	233	Total	C	N	O	S	0	0	0
			1716	1090	287	334	5			

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	250	Total	C	N	O	S	0	0	0
			1902	1195	329	370	8			
3	Q	250	Total	C	N	O	S	0	0	0
			1902	1195	329	370	8			
3	e	250	Total	C	N	O	S	0	0	0
			1902	1195	329	370	8			
3	s	250	Total	C	N	O	S	0	0	0
			1902	1195	329	370	8			

- Molecule 4 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	243	Total	C	N	O	S	0	0	0
			1684	1041	310	329	4			
4	R	243	Total	C	N	O	S	0	0	0
			1698	1053	312	329	4			
4	f	243	Total	C	N	O	S	0	0	0
			1668	1033	308	323	4			
4	t	243	Total	C	N	O	S	0	0	0
			1672	1035	309	324	4			

- Molecule 5 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	234	Total	C	N	O	S	0	0	0
			1759	1102	290	356	11			
5	S	234	Total	C	N	O	S	0	0	0
			1759	1102	290	356	11			
5	g	234	Total	C	N	O	S	0	0	0
			1759	1102	290	356	11			
5	u	234	Total	C	N	O	S	0	0	0
			1763	1105	291	356	11			

- Molecule 6 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	238	Total	C	N	O	S	0	0	0
			1850	1159	334	346	11			
6	T	238	Total	C	N	O	S	0	0	0
			1850	1159	334	346	11			
6	h	238	Total	C	N	O	S	0	0	0
			1850	1159	334	346	11			
6	v	238	Total	C	N	O	S	0	0	0
			1850	1159	334	346	11			

- Molecule 7 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	245	Total	C	N	O	S	0	0	0
			1885	1195	319	360	11			
7	U	245	Total	C	N	O	S	0	0	0
			1885	1195	319	360	11			
7	i	245	Total	C	N	O	S	0	0	0
			1885	1195	319	360	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	w	245	Total	C	N	O	S	0	0	0
			1885	1195	319	360	11			

- Molecule 8 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	202	Total	C	N	O	S	0	0	0
			1509	945	258	294	12			
8	V	202	Total	C	N	O	S	0	0	0
			1509	945	258	294	12			
8	j	202	Total	C	N	O	S	0	0	0
			1509	945	258	294	12			
8	x	202	Total	C	N	O	S	0	0	0
			1509	945	258	294	12			

- Molecule 9 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	220	Total	C	N	O	S	0	0	0
			1643	1033	280	318	12			
9	W	220	Total	C	N	O	S	0	0	0
			1643	1033	280	318	12			
9	k	220	Total	C	N	O	S	0	0	0
			1643	1033	280	318	12			
9	y	220	Total	C	N	O	S	0	0	0
			1647	1035	280	320	12			

- Molecule 10 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	204	Total	C	N	O	S	0	0	0
			1585	1010	262	294	19			
10	X	204	Total	C	N	O	S	0	0	0
			1585	1010	262	294	19			
10	l	204	Total	C	N	O	S	0	0	0
			1585	1010	262	294	19			
10	z	204	Total	C	N	O	S	0	0	0
			1585	1010	262	294	19			

- Molecule 11 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	199	Total	C	N	O	S	0	0	0
			1570	1006	265	290	9			
11	Y	199	Total	C	N	O	S	0	0	0
			1570	1006	265	290	9			
11	m	199	Total	C	N	O	S	0	0	0
			1570	1006	265	290	9			
11	0	199	Total	C	N	O	S	0	0	0
			1570	1006	265	290	9			

- Molecule 12 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	201	Total	C	N	O	S	0	0	0
			1548	974	273	292	9			
12	Z	201	Total	C	N	O	S	0	0	0
			1551	977	273	292	9			
12	n	201	Total	C	N	O	S	0	0	0
			1548	974	273	292	9			
12	3	201	Total	C	N	O	S	0	0	0
			1551	977	273	292	9			

- Molecule 13 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	213	Total	C	N	O	S	0	0	0
			1641	1036	282	313	10			
13	1	213	Total	C	N	O	S	0	0	0
			1639	1034	282	313	10			
13	o	213	Total	C	N	O	S	0	0	0
			1639	1034	282	313	10			
13	a	213	Total	C	N	O	S	0	0	0
			1639	1034	282	313	10			

- Molecule 14 is a protein called Proteasome subunit beta type-4.

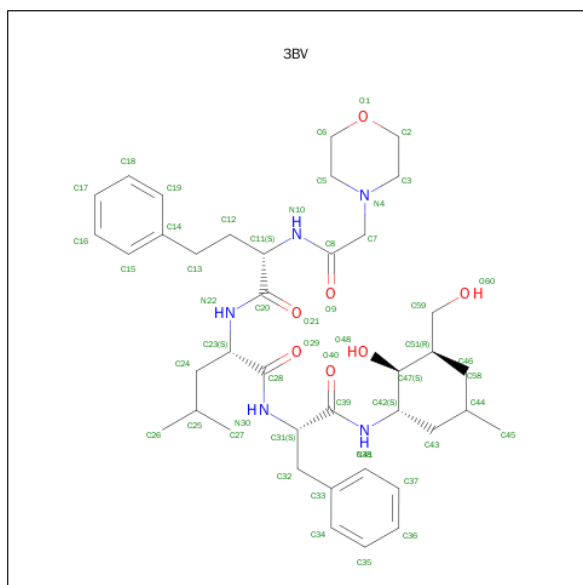
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	217	Total	C	N	O	S	0	0	0
			1676	1057	287	320	12			
14	2	217	Total	C	N	O	S	0	0	0
			1678	1058	290	318	12			
14	p	217	Total	C	N	O	S	0	0	0
			1672	1055	287	318	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	b	217	Total	C	N	O	S	0	0	0
			1669	1055	287	315	12			

- Molecule 15 is N-{(2S)-2-[(MORPHOLIN-4-YLACETYL)AMINO]-4-PHENYLBUTANOYL}-L-LEUCYL-N-[(2R,3S,4S)-1,3-DIHYDROXY-2,6-DIMETHYLHEPTAN-4-YL]-L-PHENYLALANINAMIDE (three-letter code: 3BV) (formula: C₄₀H₆₁N₅O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	H	1	Total	C	N	O	0	0
			52	40	5	7		
15	I	1	Total	C	N	O	0	0
			52	40	5	7		
15	L	1	Total	C	N	O	0	0
			52	40	5	7		
15	V	1	Total	C	N	O	0	0
			52	40	5	7		
15	W	1	Total	C	N	O	0	0
			52	40	5	7		
15	Z	1	Total	C	N	O	0	0
			52	40	5	7		
15	j	1	Total	C	N	O	0	0
			52	40	5	7		
15	k	1	Total	C	N	O	0	0
			52	40	5	7		
15	n	1	Total	C	N	O	0	0
			52	40	5	7		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	y	1	Total	C	N	O	0	0
			52	40	5	7		
15	3	1	Total	C	N	O	0	0
			52	40	5	7		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	H	1	Total	O	0	0
			1	1		
16	I	1	Total	O	0	0
			1	1		
16	L	1	Total	O	0	0
			1	1		
16	V	1	Total	O	0	0
			1	1		
16	W	1	Total	O	0	0
			1	1		
16	Z	1	Total	O	0	0
			1	1		
16	j	1	Total	O	0	0
			1	1		
16	k	1	Total	O	0	0
			1	1		
16	n	1	Total	O	0	0
			1	1		
16	3	1	Total	O	0	0
			1	1		
16	A	1	Total	O	0	0
			1	1		
16	B	4	Total	O	0	0
			4	4		
16	C	2	Total	O	0	0
			2	2		
16	D	1	Total	O	0	0
			1	1		
16	E	2	Total	O	0	0
			2	2		
16	F	4	Total	O	0	0
			4	4		
16	G	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	H	5	Total O 5 5	0	0
16	I	6	Total O 6 6	0	0
16	J	2	Total O 2 2	0	0
16	K	5	Total O 5 5	0	0
16	L	2	Total O 2 2	0	0
16	M	8	Total O 8 8	0	0
16	N	3	Total O 3 3	0	0
16	O	6	Total O 6 6	0	0
16	P	3	Total O 3 3	0	0
16	Q	9	Total O 9 9	0	0
16	R	2	Total O 2 2	0	0
16	S	1	Total O 1 1	0	0
16	U	2	Total O 2 2	0	0
16	V	3	Total O 3 3	0	0
16	W	4	Total O 4 4	0	0
16	X	9	Total O 9 9	0	0
16	Y	8	Total O 8 8	0	0
16	Z	7	Total O 7 7	0	0
16	1	5	Total O 5 5	0	0
16	2	5	Total O 5 5	0	0
16	c	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	d	1	Total O 1 1	0	0
16	e	5	Total O 5 5	0	0
16	f	1	Total O 1 1	0	0
16	h	1	Total O 1 1	0	0
16	i	4	Total O 4 4	0	0
16	j	1	Total O 1 1	0	0
16	k	5	Total O 5 5	0	0
16	l	7	Total O 7 7	0	0
16	m	5	Total O 5 5	0	0
16	n	4	Total O 4 4	0	0
16	o	10	Total O 10 10	0	0
16	p	2	Total O 2 2	0	0
16	q	3	Total O 3 3	0	0
16	r	3	Total O 3 3	0	0
16	s	5	Total O 5 5	0	0
16	u	1	Total O 1 1	0	0
16	v	2	Total O 2 2	0	0
16	w	2	Total O 2 2	0	0
16	x	3	Total O 3 3	0	0
16	y	8	Total O 8 8	0	0
16	z	2	Total O 2 2	0	0

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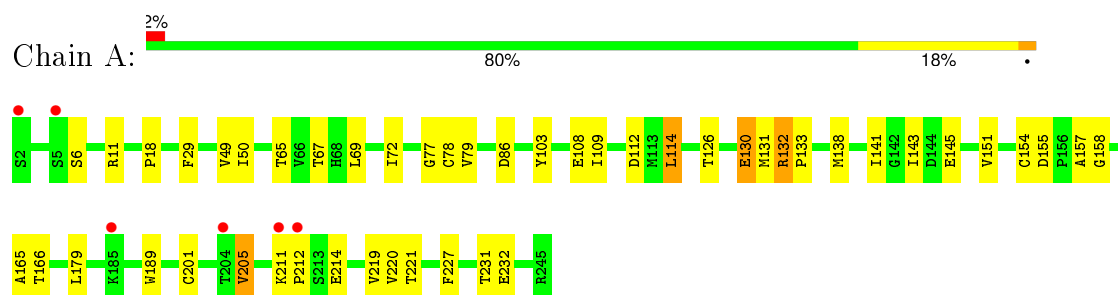
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	0	3	Total 3	O 3	0	0
16	3	6	Total 6	O 6	0	0
16	a	6	Total 6	O 6	0	0
16	b	5	Total 5	O 5	0	0

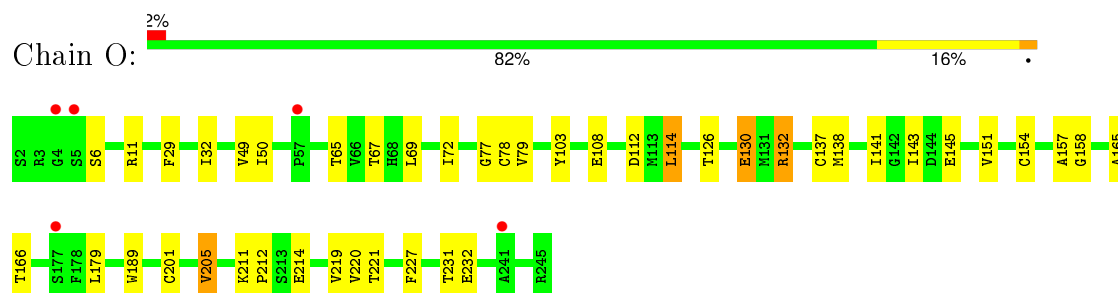
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

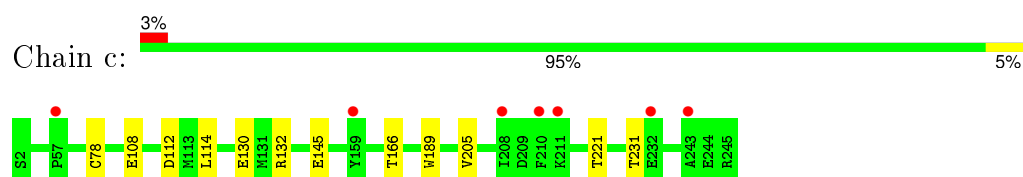
- Molecule 1: Proteasome subunit alpha type-6



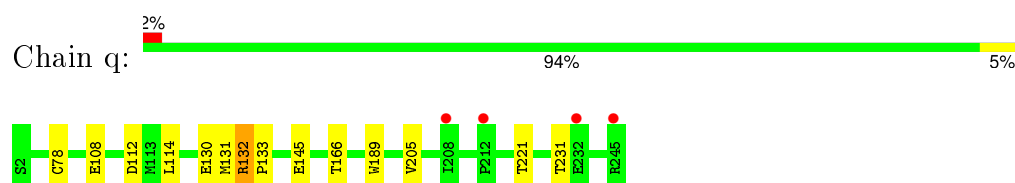
- Molecule 1: Proteasome subunit alpha type-6



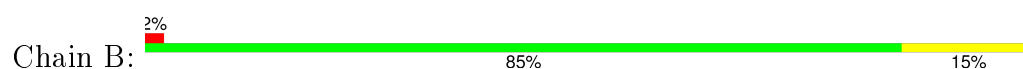
- Molecule 1: Proteasome subunit alpha type-6

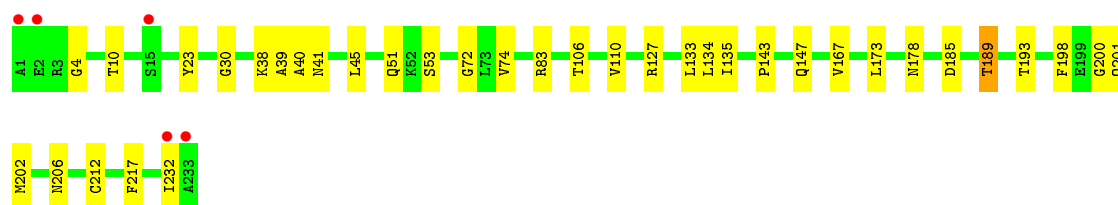


- Molecule 1: Proteasome subunit alpha type-6

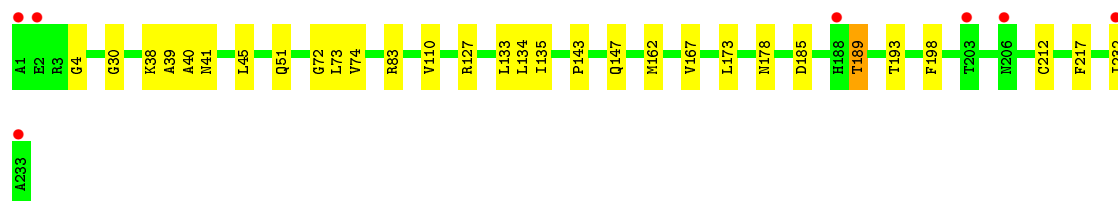
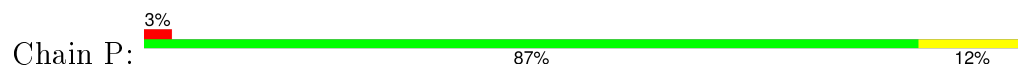


- Molecule 2: Proteasome subunit alpha type-2





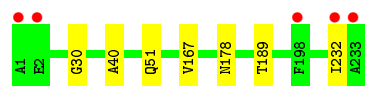
- Molecule 2: Proteasome subunit alpha type-2



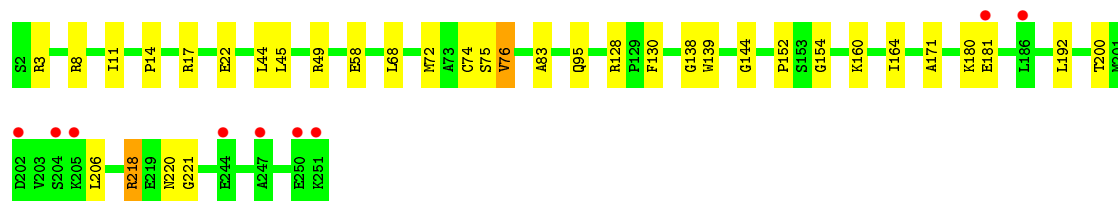
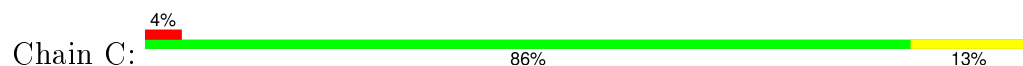
- Molecule 2: Proteasome subunit alpha type-2



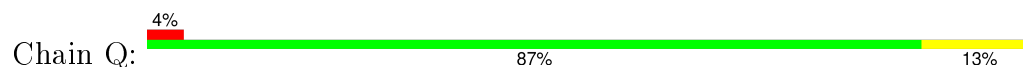
- Molecule 2: Proteasome subunit alpha type-2

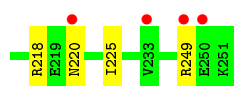


- Molecule 3: Proteasome subunit alpha type-4

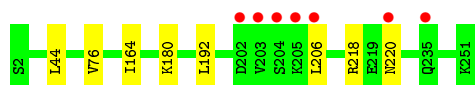


- Molecule 3: Proteasome subunit alpha type-4

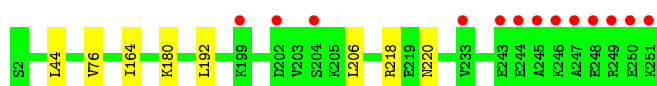




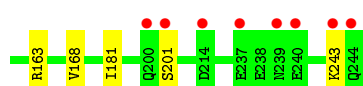
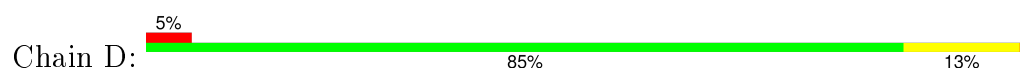
- Molecule 3: Proteasome subunit alpha type-4



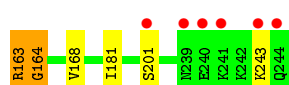
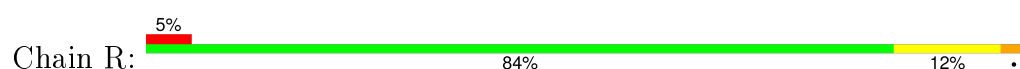
- Molecule 3: Proteasome subunit alpha type-4



- Molecule 4: Proteasome subunit alpha type-7



- Molecule 4: Proteasome subunit alpha type-7



- Molecule 4: Proteasome subunit alpha type-7

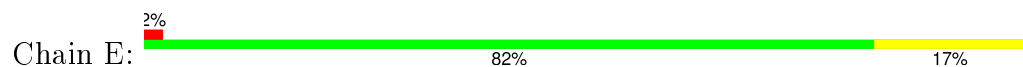


- Molecule 4: Proteasome subunit alpha type-7

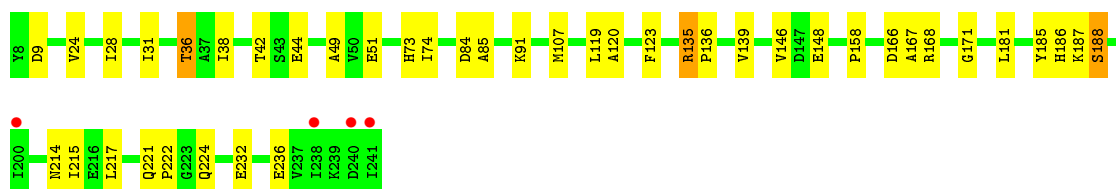
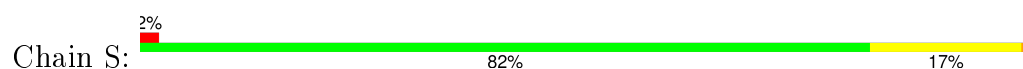




• Molecule 5: Proteasome subunit alpha type-5



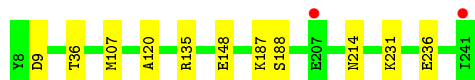
• Molecule 5: Proteasome subunit alpha type-5



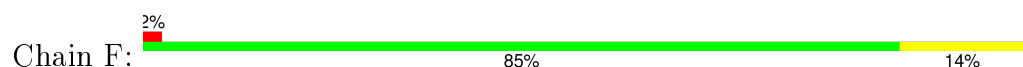
• Molecule 5: Proteasome subunit alpha type-5



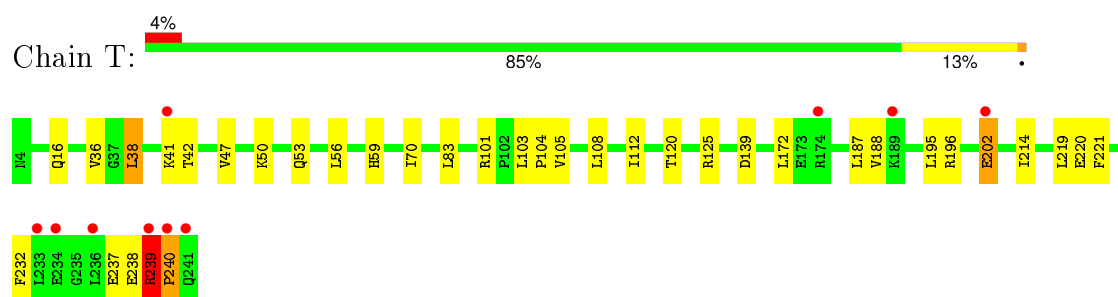
• Molecule 5: Proteasome subunit alpha type-5



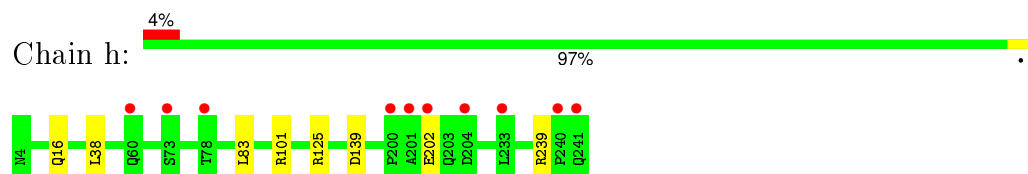
• Molecule 6: Proteasome subunit alpha type-1



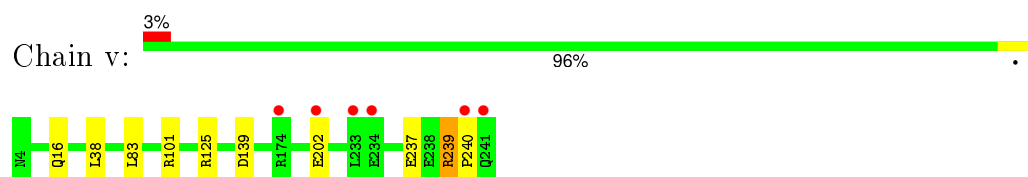
• Molecule 6: Proteasome subunit alpha type-1



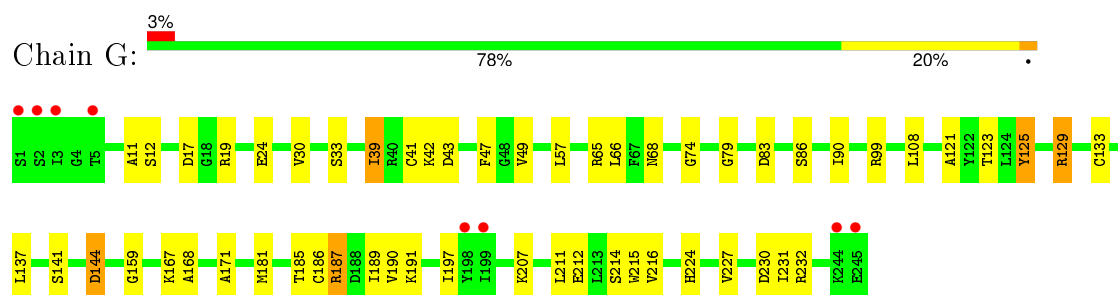
- Molecule 6: Proteasome subunit alpha type-1



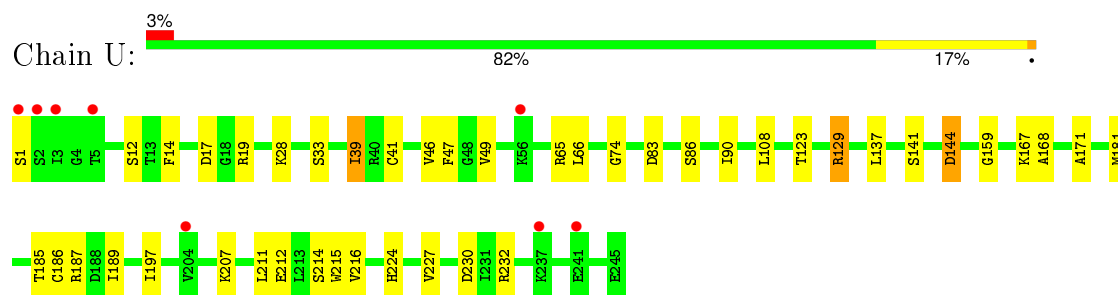
- Molecule 6: Proteasome subunit alpha type-1



- Molecule 7: Proteasome subunit alpha type-3

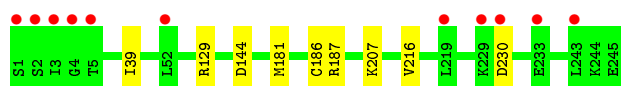


- Molecule 7: Proteasome subunit alpha type-3



- Molecule 7: Proteasome subunit alpha type-3

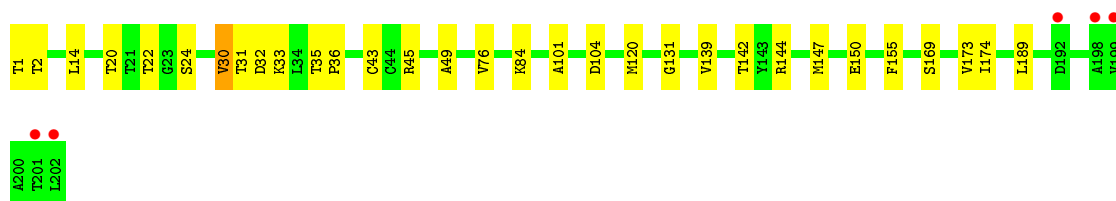
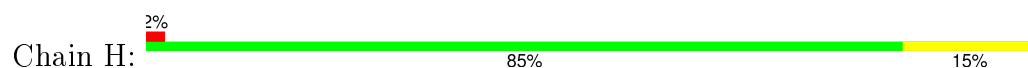




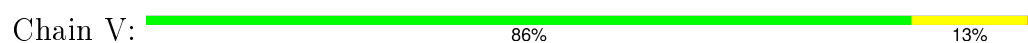
- Molecule 7: Proteasome subunit alpha type-3



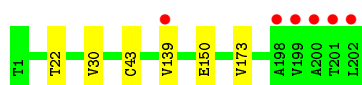
- Molecule 8: Proteasome subunit beta type-6



- Molecule 8: Proteasome subunit beta type-6



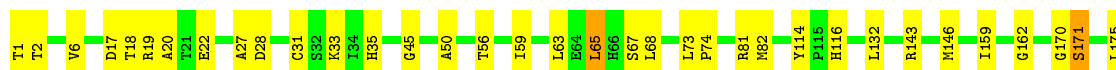
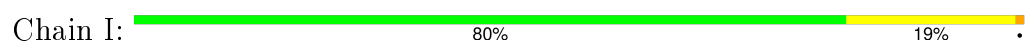
- Molecule 8: Proteasome subunit beta type-6

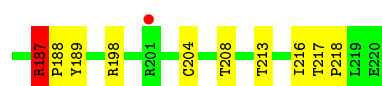


- Molecule 8: Proteasome subunit beta type-6



- Molecule 9: Proteasome subunit beta type-7





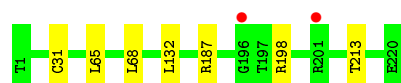
- Molecule 9: Proteasome subunit beta type-7

Chain W: 78% 21% .



- Molecule 9: Proteasome subunit beta type-7

Chain k: 97% .



- Molecule 9: Proteasome subunit beta type-7

Chain y: 97% .



- Molecule 10: Proteasome subunit beta type-3

Chain J: 79% 17% .

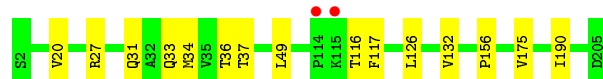
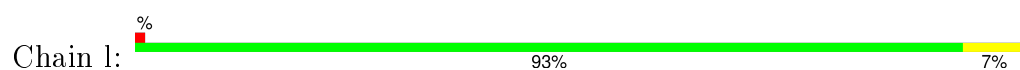


- Molecule 10: Proteasome subunit beta type-3

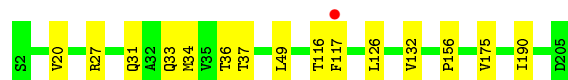
Chain X: 78% 19% .



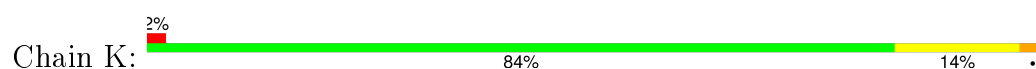
- Molecule 10: Proteasome subunit beta type-3



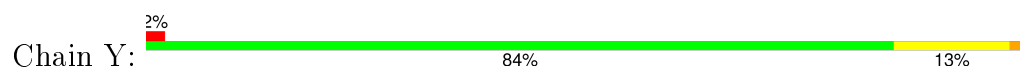
- Molecule 10: Proteasome subunit beta type-3



- Molecule 11: Proteasome subunit beta type-2



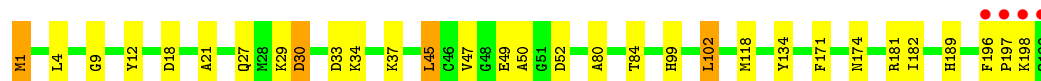
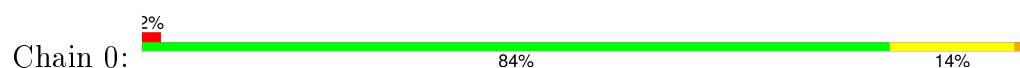
- Molecule 11: Proteasome subunit beta type-2



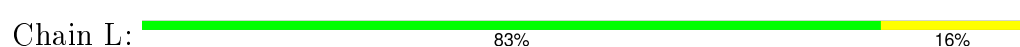
- Molecule 11: Proteasome subunit beta type-2



- Molecule 11: Proteasome subunit beta type-2



- Molecule 12: Proteasome subunit beta type-5





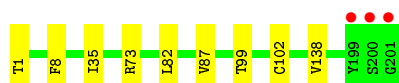
- Molecule 12: Proteasome subunit beta type-5

Chain Z: 86% 13%



- Molecule 12: Proteasome subunit beta type-5

Chain n: 96%



- Molecule 12: Proteasome subunit beta type-5

Chain 3: 83% 16%



- Molecule 13: Proteasome subunit beta type-1

Chain M: 86% 13%



- Molecule 13: Proteasome subunit beta type-1

Chain 1: 87% 12%



- Molecule 13: Proteasome subunit beta type-1

Chain o: 98%

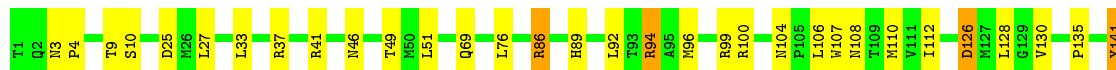
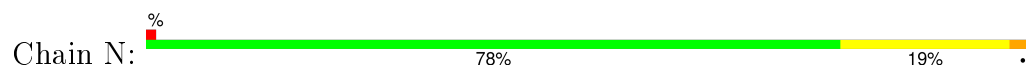


- Molecule 13: Proteasome subunit beta type-1

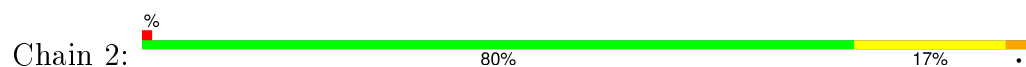
Chain a: 97%



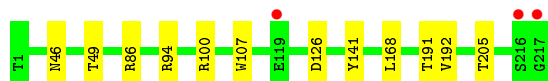
- Molecule 14: Proteasome subunit beta type-4



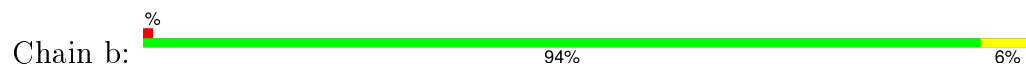
- Molecule 14: Proteasome subunit beta type-4



- Molecule 14: Proteasome subunit beta type-4



- Molecule 14: Proteasome subunit beta type-4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	171.99Å 201.03Å 225.59Å 90.00° 107.93° 90.00°	Depositor
Resolution (Å)	33.51 – 2.89 33.51 – 2.89	Depositor EDS
% Data completeness (in resolution range)	98.6 (33.51-2.89) 98.7 (33.51-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.215 , 0.245 0.229 , 0.257	Depositor DCC
R_{free} test set	16212 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	72.6	Xtriage
Anisotropy	0.471	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 57.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	5 of 321261 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	96005	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 3BV

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	0.26	1/1875 (0.1%)	0.43	0/2545
1	O	0.23	0/1878	0.41	0/2549
1	c	0.23	0/1875	0.41	0/2545
1	q	0.27	1/1875 (0.1%)	0.44	1/2545 (0.0%)
2	B	0.23	0/1749	0.41	0/2381
2	P	0.23	0/1747	0.41	0/2378
2	d	0.24	0/1745	0.41	0/2375
2	r	0.25	0/1752	0.41	0/2385
3	C	0.23	0/1931	0.41	0/2613
3	Q	0.23	0/1931	0.41	0/2613
3	e	0.23	0/1931	0.41	0/2613
3	s	0.23	0/1931	0.41	0/2613
4	D	0.22	0/1707	0.41	0/2335
4	R	0.23	0/1723	0.43	0/2355
4	f	0.22	0/1691	0.41	0/2314
4	t	0.21	0/1695	0.41	0/2319
5	E	0.22	0/1786	0.41	0/2419
5	S	0.22	0/1786	0.41	0/2419
5	g	0.23	0/1786	0.42	0/2419
5	u	0.22	0/1790	0.41	0/2423
6	F	0.24	0/1885	0.42	0/2552
6	T	0.26	1/1885 (0.1%)	0.43	0/2552
6	h	0.23	0/1885	0.43	0/2552
6	v	0.23	0/1885	0.43	0/2552
7	G	0.32	0/1920	0.42	0/2591
7	U	0.22	0/1920	0.39	0/2591
7	i	0.22	0/1920	0.39	0/2591
7	w	0.22	0/1920	0.39	0/2591
8	H	0.27	0/1535	0.43	0/2078
8	V	0.23	0/1535	0.42	0/2078
8	j	0.23	0/1535	0.42	0/2078
8	x	0.23	0/1535	0.42	0/2078

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	I	0.28	0/1670	0.43	0/2265
9	W	0.24	0/1670	0.43	0/2265
9	k	0.23	0/1670	0.43	0/2265
9	y	0.23	0/1674	0.43	0/2270
10	J	0.28	1/1614 (0.1%)	0.42	0/2177
10	X	0.25	0/1614	0.43	0/2177
10	l	0.25	0/1614	0.42	0/2177
10	z	0.32	0/1614	0.44	0/2177
11	0	0.22	0/1603	0.42	0/2174
11	K	0.22	0/1603	0.42	0/2174
11	Y	0.22	0/1603	0.42	0/2174
11	m	0.23	0/1603	0.41	0/2174
12	3	0.23	0/1582	0.44	2/2138 (0.1%)
12	L	0.27	1/1579 (0.1%)	0.44	2/2134 (0.1%)
12	Z	0.23	0/1582	0.40	0/2138
12	n	0.28	0/1579	0.45	2/2134 (0.1%)
13	1	0.24	0/1669	0.43	0/2250
13	M	0.24	0/1671	0.43	0/2253
13	a	0.27	0/1669	0.45	0/2250
13	o	0.32	1/1669 (0.1%)	0.45	0/2250
14	2	0.23	0/1711	0.42	0/2319
14	N	0.23	0/1709	0.42	0/2317
14	b	0.23	0/1702	0.42	0/2306
14	p	0.23	0/1705	0.42	0/2312
All	All	0.24	6/96923 (0.0%)	0.42	7/131312 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	3	THR	C-N	-5.74	1.20	1.34
1	q	133	PRO	N-CD	5.28	1.55	1.47
1	A	133	PRO	N-CD	5.28	1.55	1.47
6	T	240	PRO	N-CD	5.25	1.55	1.47
10	J	173	ASN	CG-ND2	-5.05	1.20	1.32
13	o	75	TYR	CE2-CZ	-5.01	1.32	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	n	73	ARG	NE-CZ-NH2	-5.93	117.34	120.30
12	3	73	ARG	NE-CZ-NH2	-5.89	117.35	120.30
12	L	73	ARG	NE-CZ-NH2	-5.88	117.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	q	132	ARG	C-N-CD	5.59	140.15	128.40
12	L	73	ARG	NE-CZ-NH1	5.58	123.09	120.30
12	3	73	ARG	NE-CZ-NH1	5.46	123.03	120.30
12	n	73	ARG	NE-CZ-NH1	5.42	123.01	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1842	0	1803	29	0
1	O	1845	0	1805	26	0
1	c	1842	0	1803	0	0
1	q	1842	0	1803	0	0
2	B	1713	0	1598	27	0
2	P	1712	0	1605	16	0
2	d	1710	0	1598	0	0
2	r	1716	0	1607	0	0
3	C	1902	0	1835	17	0
3	Q	1902	0	1835	16	0
3	e	1902	0	1835	0	0
3	s	1902	0	1835	0	0
4	D	1684	0	1460	17	0
4	R	1698	0	1474	34	0
4	f	1668	0	1437	0	0
4	t	1672	0	1443	0	0
5	E	1759	0	1707	19	0
5	S	1759	0	1707	20	0
5	g	1759	0	1707	0	0
5	u	1763	0	1718	0	0
6	F	1850	0	1822	29	0
6	T	1850	0	1822	36	0
6	h	1850	0	1822	0	0
6	v	1850	0	1822	0	0
7	G	1885	0	1845	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	U	1885	0	1845	36	0
7	i	1885	0	1845	0	0
7	w	1885	0	1845	0	0
8	H	1509	0	1470	28	0
8	V	1509	0	1470	18	0
8	j	1509	0	1471	0	0
8	x	1509	0	1473	0	0
9	I	1643	0	1642	58	0
9	W	1643	0	1643	64	0
9	k	1643	0	1642	0	0
9	y	1647	0	1645	0	0
10	J	1585	0	1598	28	0
10	X	1585	0	1598	28	0
10	l	1585	0	1598	0	0
10	z	1585	0	1598	0	0
11	0	1570	0	1547	17	0
11	K	1570	0	1547	18	0
11	Y	1570	0	1547	17	0
11	m	1570	0	1547	0	0
12	3	1551	0	1506	34	0
12	L	1548	0	1497	30	0
12	Z	1551	0	1506	23	0
12	n	1548	0	1496	0	0
13	1	1639	0	1611	17	0
13	M	1641	0	1618	16	0
13	a	1639	0	1611	0	0
13	o	1639	0	1611	0	0
14	2	1678	0	1640	23	0
14	N	1676	0	1633	29	0
14	b	1669	0	1629	0	0
14	p	1672	0	1629	0	0
15	3	52	0	58	8	0
15	H	52	0	58	15	0
15	I	52	0	58	12	0
15	L	52	0	58	6	0
15	V	52	0	58	23	0
15	W	52	0	59	25	0
15	Z	52	0	55	9	0
15	j	52	0	58	0	0
15	k	52	0	58	0	0
15	n	52	0	57	0	0
15	y	52	0	57	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	0	3	0	0	1	0
16	1	5	0	0	0	0
16	2	5	0	0	0	0
16	3	7	0	0	2	0
16	A	1	0	0	0	0
16	B	4	0	0	0	0
16	C	2	0	0	0	0
16	D	1	0	0	0	0
16	E	2	0	0	0	0
16	F	4	0	0	0	0
16	G	1	0	0	0	0
16	H	6	0	0	0	0
16	I	7	0	0	1	0
16	J	2	0	0	0	0
16	K	5	0	0	1	0
16	L	3	0	0	1	0
16	M	8	0	0	0	0
16	N	3	0	0	0	0
16	O	6	0	0	0	0
16	P	3	0	0	0	0
16	Q	9	0	0	1	0
16	R	2	0	0	0	0
16	S	1	0	0	0	0
16	U	2	0	0	0	0
16	V	4	0	0	1	0
16	W	5	0	0	0	0
16	X	9	0	0	2	0
16	Y	8	0	0	0	0
16	Z	8	0	0	0	0
16	a	6	0	0	0	0
16	b	5	0	0	0	0
16	c	3	0	0	0	0
16	d	1	0	0	0	0
16	e	5	0	0	0	0
16	f	1	0	0	0	0
16	h	1	0	0	0	0
16	i	4	0	0	0	0
16	j	2	0	0	0	0
16	k	6	0	0	0	0
16	l	7	0	0	0	0
16	m	5	0	0	0	0
16	n	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	o	10	0	0	0	0
16	p	2	0	0	0	0
16	q	3	0	0	0	0
16	r	3	0	0	0	0
16	s	5	0	0	0	0
16	u	1	0	0	0	0
16	v	2	0	0	0	0
16	w	2	0	0	0	0
16	x	3	0	0	0	0
16	y	8	0	0	0	0
16	z	2	0	0	0	0
All	All	96005	0	92940	782	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (782) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:1:THR:N	15:I:301:3BV:C51	1.68	1.50
9:W:1:THR:N	15:W:301:3BV:C51	1.72	1.48
9:I:187:ARG:HB3	9:I:188:PRO:CD	1.61	1.30
9:W:1:THR:CA	15:W:301:3BV:H56	1.59	1.29
8:H:1:THR:HG23	8:H:33:LYS:NZ	1.50	1.26
4:R:46:GLU:CG	4:R:47:LYS:H	1.44	1.26
9:W:1:THR:N	15:W:301:3BV:H56	0.93	1.25
9:I:187:ARG:CB	9:I:188:PRO:HD3	1.70	1.22
9:W:1:THR:HG21	9:W:46:ALA:CB	1.69	1.21
4:R:47:LYS:CB	4:R:163:ARG:HH21	1.54	1.21
9:W:1:THR:H3	15:W:301:3BV:C51	1.42	1.18
6:F:196:ARG:HD3	6:F:239:ARG:CD	1.75	1.17
6:T:239:ARG:HG3	6:T:240:PRO:HD3	1.16	1.14
9:I:187:ARG:CG	9:I:188:PRO:HD3	1.79	1.12
6:T:239:ARG:CG	6:T:240:PRO:HD3	1.80	1.11
6:T:196:ARG:NH2	6:T:239:ARG:HB2	1.67	1.10
6:T:239:ARG:HG3	6:T:240:PRO:CD	1.80	1.10
12:3:2:THR:HG21	12:3:163:ALA:CB	1.82	1.09
7:U:46:VAL:CG2	7:U:186:CYS:SG	2.41	1.09
9:W:2:THR:HG21	9:W:162:GLY:HA3	1.29	1.08
9:W:1:THR:HG21	9:W:46:ALA:HB2	1.09	1.07
15:V:301:3BV:O9	15:V:301:3BV:H9	1.53	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:20:ALA:HB1	15:Z:301:3BV:H14	1.35	1.06
15:V:301:3BV:C39	15:V:301:3BV:H52	1.84	1.06
2:B:198:PHE:CE2	2:B:202:MET:HA	1.91	1.05
7:U:46:VAL:HG22	7:U:186:CYS:SG	1.99	1.03
4:R:46:GLU:HG2	4:R:47:LYS:H	0.88	1.03
9:I:187:ARG:HG3	9:I:188:PRO:HD3	1.41	1.01
4:R:46:GLU:HG2	4:R:47:LYS:N	1.72	1.01
6:F:196:ARG:HD3	6:F:239:ARG:HD2	1.04	1.01
12:3:167:ASP:HB3	12:3:170:SER:OG	1.60	0.99
2:B:198:PHE:CE2	2:B:202:MET:CA	2.46	0.98
9:W:1:THR:H1	15:W:301:3BV:C51	1.48	0.97
9:I:187:ARG:HB3	9:I:188:PRO:HD3	1.26	0.97
9:I:1:THR:H2	15:I:301:3BV:C51	1.76	0.97
6:F:196:ARG:CD	6:F:239:ARG:HD2	1.93	0.96
9:I:187:ARG:HB3	9:I:188:PRO:HD2	1.48	0.95
4:R:47:LYS:CB	4:R:163:ARG:NH2	2.29	0.95
9:W:1:THR:N	15:W:301:3BV:C59	2.30	0.94
8:H:1:THR:HG23	8:H:33:LYS:HZ2	1.14	0.94
15:V:301:3BV:N22	15:V:301:3BV:H32	1.84	0.93
15:V:301:3BV:H32	15:V:301:3BV:H28	1.32	0.93
2:B:198:PHE:CD2	2:B:202:MET:HB2	2.04	0.93
9:W:1:THR:CG2	9:W:46:ALA:HB2	1.97	0.92
12:3:2:THR:HG21	12:3:163:ALA:HB3	1.52	0.91
6:T:196:ARG:CZ	6:T:239:ARG:HB2	1.99	0.91
9:I:187:ARG:CB	9:I:188:PRO:CD	2.31	0.91
6:T:196:ARG:HG3	6:T:239:ARG:HD3	1.51	0.91
9:I:1:THR:N	15:I:301:3BV:C59	2.34	0.89
4:R:46:GLU:CG	4:R:47:LYS:N	2.21	0.89
6:F:196:ARG:CD	6:F:239:ARG:CD	2.50	0.89
8:H:1:THR:HG23	8:H:33:LYS:HZ3	1.32	0.88
12:3:2:THR:O	12:3:160:ILE:HD12	1.74	0.88
8:H:1:THR:CG2	8:H:33:LYS:NZ	2.37	0.87
9:W:1:THR:H3	15:W:301:3BV:C59	1.87	0.86
15:V:301:3BV:H16	15:V:301:3BV:H9	1.56	0.85
12:3:2:THR:HG21	12:3:163:ALA:HB1	1.57	0.83
9:W:2:THR:CG2	9:W:162:GLY:HA3	2.08	0.83
6:T:238:GLU:O	6:T:239:ARG:HB3	1.76	0.83
9:I:204:CYS:SG	16:I:403:HOH:O	2.37	0.83
7:U:186:CYS:SG	7:U:215:TRP:CZ3	2.73	0.82
9:I:1:THR:CA	15:I:301:3BV:C51	2.59	0.81
9:W:1:THR:CG2	9:W:46:ALA:CB	2.57	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:3:2:THR:O	12:3:160:ILE:CD1	2.28	0.81
15:H:301:3BV:H8	9:I:116:HIS:CD2	2.16	0.81
6:F:196:ARG:CZ	6:F:239:ARG:HG3	2.09	0.81
15:I:301:3BV:H1	15:I:301:3BV:H21	1.47	0.80
6:T:239:ARG:CB	6:T:240:PRO:HD3	2.12	0.80
1:A:132:ARG:HG2	7:G:12:SER:HA	1.62	0.80
12:Z:20:ALA:HB1	15:Z:301:3BV:C26	2.13	0.79
9:W:187:ARG:CB	9:W:188:PRO:HD3	2.13	0.78
10:J:173:ASN:ND2	13:1:151:ASN:HB2	1.99	0.78
2:B:110:VAL:HG22	2:B:135:ILE:HD12	1.67	0.77
2:B:198:PHE:CZ	2:B:202:MET:HA	2.19	0.76
9:W:187:ARG:CG	9:W:188:PRO:HD3	2.15	0.76
15:3:301:3BV:C39	15:3:301:3BV:H49	2.16	0.76
7:G:187:ARG:NH1	7:G:231:ILE:HD12	2.01	0.76
5:E:85:ALA:HB2	5:E:139:VAL:HG21	1.66	0.76
8:H:169:SER:O	15:H:301:3BV:H57	1.85	0.76
5:E:42:THR:HG22	5:E:44:GLU:H	1.51	0.76
5:S:42:THR:HG22	5:S:44:GLU:H	1.51	0.76
15:H:301:3BV:C15	9:I:116:HIS:CE1	2.70	0.75
2:P:110:VAL:HG22	2:P:135:ILE:HD12	1.67	0.75
12:3:167:ASP:CB	12:3:170:SER:OG	2.34	0.75
5:S:85:ALA:HB2	5:S:139:VAL:HG21	1.67	0.74
9:W:187:ARG:HB3	9:W:188:PRO:HD3	1.69	0.74
15:V:301:3BV:O9	15:V:301:3BV:C15	2.33	0.74
15:V:301:3BV:O9	15:V:301:3BV:H7	1.87	0.74
9:W:1:THR:H3	15:W:301:3BV:H56	1.01	0.74
8:H:1:THR:CG2	8:H:33:LYS:HZ3	2.01	0.73
9:W:1:THR:H1	15:W:301:3BV:H56	0.97	0.73
7:G:83:ASP:OD2	7:G:129:ARG:NH2	2.22	0.73
15:H:301:3BV:H9	9:I:116:HIS:CE1	2.23	0.73
4:R:31:THR:HB	4:R:46:GLU:HB3	1.68	0.73
7:U:83:ASP:OD2	7:U:129:ARG:NH2	2.21	0.73
9:I:1:THR:HG22	9:I:2:THR:H	1.52	0.73
12:L:2:THR:O	12:L:160:ILE:HD12	1.88	0.73
15:V:301:3BV:C39	15:V:301:3BV:C46	2.67	0.73
1:A:67:THR:HG22	1:A:69:LEU:H	1.55	0.72
9:I:2:THR:HG21	9:I:162:GLY:HA3	1.71	0.71
3:Q:8:ARG:HB3	3:Q:11:ILE:HD12	1.72	0.71
12:3:4:LEU:O	12:3:4:LEU:HD12	1.91	0.71
10:J:173:ASN:HD22	13:1:151:ASN:HB2	1.55	0.71
2:B:198:PHE:CE2	2:B:202:MET:N	2.58	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:33:VAL:HG11	4:R:168:VAL:HG11	1.72	0.71
15:I:301:3BV:H7	10:J:126:LEU:HD11	1.73	0.71
1:O:67:THR:HG22	1:O:69:LEU:H	1.55	0.71
4:R:46:GLU:CD	4:R:47:LYS:N	2.45	0.71
6:F:120:THR:O	7:G:129:ARG:NH1	2.24	0.70
9:W:3:ILE:HD11	9:W:127:MET:HB2	1.74	0.70
5:E:51:GLU:HA	5:E:215:ILE:HG22	1.74	0.70
4:R:46:GLU:CD	4:R:47:LYS:H	1.95	0.69
2:B:198:PHE:HE2	2:B:202:MET:N	1.89	0.69
15:H:301:3BV:C13	9:I:116:HIS:NE2	2.55	0.69
3:C:8:ARG:HB3	3:C:11:ILE:HD12	1.72	0.69
11:K:1:MET:HE1	11:K:134:TYR:H	1.56	0.69
12:L:1:THR:HG22	12:L:2:THR:N	2.08	0.69
6:T:239:ARG:CB	6:T:240:PRO:CD	2.71	0.69
8:H:169:SER:HB3	15:H:301:3BV:H61	1.73	0.69
8:H:1:THR:HG21	8:H:33:LYS:HD3	1.75	0.69
6:F:196:ARG:CZ	6:F:239:ARG:CG	2.71	0.69
12:3:2:THR:CG2	12:3:163:ALA:CB	2.67	0.69
9:W:187:ARG:HB3	9:W:188:PRO:CD	2.22	0.69
10:X:125:ASP:HB2	10:X:129:CYS:H	1.57	0.69
5:S:51:GLU:HA	5:S:215:ILE:HG22	1.74	0.68
9:W:3:ILE:HD12	9:W:99:VAL:HG23	1.76	0.68
14:N:51:LEU:HD13	14:N:112:ILE:HG12	1.75	0.68
7:G:187:ARG:HH12	7:G:231:ILE:HD12	1.59	0.68
5:E:49:ALA:HB2	5:E:217:LEU:HD23	1.76	0.68
15:V:301:3BV:H13	9:W:114:TYR:CD1	2.29	0.68
11:O:1:MET:HE1	11:O:134:TYR:H	1.59	0.68
5:S:49:ALA:HB2	5:S:217:LEU:HD23	1.76	0.68
11:Y:1:MET:HE1	11:Y:134:TYR:H	1.59	0.67
14:2:51:LEU:HD13	14:2:112:ILE:HG12	1.74	0.67
14:2:51:LEU:HD11	14:2:110:MET:HB3	1.77	0.67
11:Y:21:ALA:HB3	11:Y:29:LYS:HB3	1.75	0.67
9:W:187:ARG:HG3	9:W:188:PRO:HD3	1.75	0.67
14:N:51:LEU:HD11	14:N:110:MET:HB3	1.76	0.67
11:O:21:ALA:HB3	11:O:29:LYS:HB3	1.75	0.67
9:I:19:ARG:O	15:I:301:3BV:H58	1.94	0.66
1:A:132:ARG:NH1	7:G:123:THR:O	2.28	0.66
10:J:125:ASP:HB2	10:J:129:CYS:H	1.58	0.66
11:K:21:ALA:HB3	11:K:29:LYS:HB3	1.76	0.66
4:R:33:VAL:HG12	4:R:160:ALA:CB	2.25	0.66
1:A:158:GLY:O	2:B:83:ARG:NH2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:1:THR:HG22	9:I:2:THR:N	2.11	0.66
8:H:1:THR:CG2	8:H:33:LYS:HD3	2.26	0.66
7:U:168:ALA:HB1	7:U:171:ALA:HB3	1.78	0.66
7:G:168:ALA:HB1	7:G:171:ALA:HB3	1.78	0.66
10:X:36:THR:HG23	10:X:38:ASP:H	1.60	0.66
6:T:239:ARG:CG	6:T:240:PRO:CD	2.56	0.65
12:3:33:LYS:HE2	15:3:301:3BV:H45	1.79	0.65
9:W:3:ILE:CD1	9:W:99:VAL:HG23	2.25	0.65
12:L:2:THR:HG21	12:L:163:ALA:CB	2.27	0.65
12:3:4:LEU:C	12:3:4:LEU:HD12	2.17	0.65
10:J:34:MET:O	12:Z:166:ARG:NH1	2.28	0.65
15:V:301:3BV:C8	15:V:301:3BV:H9	2.25	0.65
15:H:301:3BV:C13	9:I:116:HIS:CD2	2.79	0.65
12:3:2:THR:CG2	12:3:163:ALA:HB1	2.27	0.65
10:J:36:THR:HG23	10:J:38:ASP:H	1.60	0.65
15:I:301:3BV:C5	15:I:301:3BV:H21	2.10	0.64
6:T:239:ARG:HB3	6:T:240:PRO:HD3	1.78	0.64
15:3:301:3BV:H49	15:3:301:3BV:O40	1.97	0.64
10:J:53:LEU:HB2	10:J:60:VAL:HG13	1.80	0.64
12:L:166:ARG:NH1	10:X:34:MET:O	2.27	0.64
9:W:1:THR:H3	15:W:301:3BV:C47	2.08	0.64
9:I:45:GLY:O	15:I:301:3BV:H52	1.98	0.64
15:V:301:3BV:N41	15:V:301:3BV:H52	2.11	0.63
10:X:53:LEU:HB2	10:X:60:VAL:HG13	1.80	0.63
6:F:196:ARG:CD	6:F:239:ARG:HD3	2.29	0.63
15:H:301:3BV:H8	9:I:116:HIS:NE2	2.13	0.63
1:O:158:GLY:O	2:P:83:ARG:NH2	2.31	0.63
5:S:84:ASP:OD2	5:S:135:ARG:NH2	2.31	0.63
9:W:3:ILE:HD12	9:W:99:VAL:CG2	2.29	0.63
12:3:45:MET:HG2	15:3:301:3BV:H53	1.79	0.63
12:L:1:THR:HG22	12:L:2:THR:H	1.63	0.62
4:R:29:GLY:O	4:R:163:ARG:HB2	2.00	0.62
9:W:187:ARG:CB	9:W:188:PRO:CD	2.76	0.62
2:P:39:ALA:O	2:P:41:ASN:N	2.31	0.62
12:3:167:ASP:HB3	12:3:170:SER:HG	1.61	0.62
9:W:1:THR:CA	15:W:301:3BV:C51	2.54	0.62
12:3:45:MET:HG2	15:3:301:3BV:C46	2.30	0.62
1:A:49:VAL:HG22	1:A:219:VAL:HG23	1.81	0.62
5:E:84:ASP:OD2	5:E:135:ARG:NH2	2.32	0.62
10:J:189:ILE:HG23	10:J:196:THR:HB	1.82	0.61
1:O:49:VAL:HG22	1:O:219:VAL:HG23	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:1:THR:H1	15:W:301:3BV:C58	2.09	0.61
2:B:39:ALA:O	2:B:41:ASN:N	2.31	0.61
15:V:301:3BV:O9	15:V:301:3BV:C13	2.48	0.61
12:3:167:ASP:CB	12:3:170:SER:HG	2.13	0.61
4:R:33:VAL:HG12	4:R:160:ALA:HB2	1.82	0.61
1:O:132:ARG:HB3	7:U:12:SER:O	2.01	0.61
11:K:4:LEU:HD22	11:K:45:LEU:HD12	1.82	0.61
12:Z:4:LEU:HD12	12:Z:4:LEU:C	2.22	0.61
15:L:301:3BV:H49	15:L:301:3BV:C39	2.30	0.60
6:T:239:ARG:HB3	6:T:240:PRO:CD	2.30	0.60
15:W:301:3BV:H52	15:W:301:3BV:C39	2.31	0.60
14:N:9:THR:O	14:N:41:ARG:NH2	2.34	0.60
11:K:33:ASP:OD2	11:K:181:ARG:NH2	2.35	0.60
9:W:1:THR:HG21	9:W:46:ALA:HB1	1.80	0.60
12:3:167:ASP:CG	12:3:170:SER:HG	2.04	0.60
4:D:100:ASP:OD1	12:L:107:ARG:NH2	2.31	0.60
6:T:196:ARG:CG	6:T:239:ARG:HD3	2.28	0.60
15:V:301:3BV:H16	15:V:301:3BV:O9	2.00	0.59
11:Y:33:ASP:OD2	11:Y:181:ARG:NH2	2.35	0.59
11:O:33:ASP:OD2	11:O:181:ARG:NH2	2.35	0.59
11:O:4:LEU:HD22	11:O:45:LEU:HD12	1.84	0.59
10:J:14:MET:HB3	10:J:163:LEU:HD11	1.82	0.59
9:W:1:THR:HA	15:W:301:3BV:H56	1.76	0.59
3:C:49:ARG:NH2	3:C:58:GLU:OE2	2.35	0.59
10:X:189:ILE:HG23	10:X:196:THR:HB	1.84	0.59
8:H:49:ALA:HB2	15:H:301:3BV:H51	1.84	0.59
10:X:14:MET:HB3	10:X:163:LEU:HD11	1.83	0.59
4:D:38:ARG:NE	4:D:181:ILE:O	2.35	0.59
6:T:120:THR:O	7:U:129:ARG:NH1	2.36	0.59
9:I:1:THR:HG23	9:I:33:LYS:HD3	1.84	0.59
14:2:9:THR:O	14:2:41:ARG:NH2	2.35	0.59
11:Y:4:LEU:HD22	11:Y:45:LEU:HD12	1.83	0.59
3:Q:49:ARG:NH2	3:Q:58:GLU:OE2	2.35	0.59
1:A:130:GLU:HG2	2:B:4:GLY:HA2	1.84	0.58
12:L:1:THR:O	12:L:2:THR:OG1	2.20	0.58
1:O:132:ARG:HG2	7:U:12:SER:HA	1.86	0.58
9:I:170:GLY:O	9:I:171:SER:HB2	2.04	0.58
9:W:204:CYS:HB3	9:W:208:THR:HG21	1.86	0.58
12:L:2:THR:O	12:L:160:ILE:CD1	2.51	0.58
9:W:163:ILE:HG23	9:W:170:GLY:HA2	1.86	0.58
13:M:63:THR:OG1	14:N:94:ARG:NH2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:1:THR:H3	15:W:301:3BV:H60	1.68	0.58
9:I:204:CYS:HB3	9:I:208:THR:HG21	1.86	0.58
1:O:132:ARG:NH1	7:U:123:THR:O	2.37	0.58
9:I:175:LEU:HD12	9:I:189:TYR:CD2	2.39	0.58
4:R:38:ARG:NE	4:R:181:ILE:O	2.35	0.58
1:A:126:THR:HG22	2:B:127:ARG:HH21	1.68	0.58
11:Y:37:LYS:H	11:Y:37:LYS:HD2	1.69	0.58
2:B:198:PHE:CE2	2:B:202:MET:CB	2.86	0.57
12:L:4:LEU:C	12:L:4:LEU:HD12	2.24	0.57
9:W:1:THR:O	9:W:128:GLY:HA3	2.05	0.57
15:V:301:3BV:H13	9:W:114:TYR:CG	2.39	0.57
11:O:37:LYS:H	11:O:37:LYS:HD2	1.70	0.57
12:3:38:ASN:HB2	12:3:41:LEU:HB2	1.86	0.57
7:U:186:CYS:SG	7:U:215:TRP:CE3	2.91	0.57
15:L:301:3BV:H49	15:L:301:3BV:O40	2.05	0.57
9:W:1:THR:H1	15:W:301:3BV:C59	2.07	0.56
7:U:141:SER:HB3	7:U:144:ASP:HB2	1.87	0.56
9:I:1:THR:HG23	9:I:33:LYS:NZ	2.21	0.56
8:H:1:THR:HG22	8:H:2:THR:H	1.69	0.56
8:H:1:THR:CG2	8:H:33:LYS:HZ2	2.03	0.56
7:U:46:VAL:HG21	7:U:186:CYS:SG	2.41	0.56
7:U:186:CYS:SG	7:U:215:TRP:HZ3	2.27	0.56
15:V:301:3BV:C27	15:V:301:3BV:N22	2.56	0.56
14:N:9:THR:OG1	14:N:10:SER:N	2.38	0.56
6:F:103:LEU:HD12	6:F:104:PRO:HD2	1.86	0.56
4:D:79:ASP:OD2	4:D:125:ARG:NH2	2.39	0.56
15:Z:301:3BV:H21	15:Z:301:3BV:H2	1.71	0.56
12:L:38:ASN:HB2	12:L:41:LEU:HB2	1.86	0.56
4:D:36:ARG:HA	4:D:41:VAL:HG12	1.86	0.56
8:H:2:THR:OG1	8:H:131:GLY:HA3	2.04	0.56
4:R:31:THR:N	4:R:46:GLU:OE2	2.37	0.56
14:2:9:THR:OG1	14:2:10:SER:N	2.38	0.56
4:R:36:ARG:HA	4:R:41:VAL:HG12	1.86	0.56
11:K:37:LYS:HD2	11:K:37:LYS:H	1.70	0.56
13:1:99:ARG:NH1	13:1:102:PHE:O	2.39	0.56
4:R:136:PHE:CZ	4:R:142:PRO:HB3	2.41	0.56
13:M:151:ASN:HD22	10:X:173:ASN:ND2	2.03	0.56
14:N:192:VAL:HG13	14:N:197:VAL:HG22	1.88	0.56
6:T:103:LEU:HD12	6:T:104:PRO:HD2	1.87	0.56
15:V:301:3BV:O40	15:V:301:3BV:H52	2.04	0.56
12:Z:38:ASN:HB2	12:Z:41:LEU:HB2	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:3:1:THR:CG2	12:3:3:THR:HG23	2.37	0.55
7:U:227:VAL:O	7:U:232:ARG:NH1	2.38	0.55
4:R:29:GLY:O	4:R:163:ARG:N	2.29	0.55
12:3:2:THR:HG22	12:3:2:THR:O	2.06	0.55
15:V:301:3BV:C46	15:V:301:3BV:O40	2.54	0.55
2:B:198:PHE:CE2	2:B:202:MET:HB2	2.40	0.55
7:G:227:VAL:O	7:G:232:ARG:NH1	2.39	0.55
1:O:103:TYR:O	9:W:81:ARG:NH1	2.40	0.55
9:I:1:THR:CG2	9:I:33:LYS:HD3	2.36	0.55
7:G:141:SER:HB3	7:G:144:ASP:HB2	1.87	0.55
9:W:50:ALA:HB2	10:X:129:CYS:HB2	1.89	0.55
9:I:175:LEU:HD12	9:I:189:TYR:CE2	2.41	0.55
13:M:145:LEU:HD22	13:M:178:VAL:HB	1.87	0.55
14:2:192:VAL:HG13	14:2:197:VAL:HG22	1.89	0.55
13:1:137:ALA:H	13:1:146:GLN:HE21	1.54	0.55
13:1:145:LEU:HD22	13:1:178:VAL:HB	1.87	0.55
1:O:141:ILE:HD12	1:O:220:VAL:HG12	1.89	0.55
8:V:1:THR:HG23	8:V:33:LYS:HD3	1.89	0.55
6:F:47:VAL:HG12	6:F:195:LEU:HD22	1.88	0.55
1:A:141:ILE:HD12	1:A:220:VAL:HG12	1.89	0.55
4:R:79:ASP:OD2	4:R:125:ARG:NH2	2.39	0.55
11:K:30:ASP:N	11:K:30:ASP:OD1	2.40	0.55
9:W:2:THR:O	9:W:159:ILE:HD12	2.07	0.54
13:M:99:ARG:NH1	13:M:102:PHE:O	2.38	0.54
8:V:14:LEU:HD21	8:V:101:ALA:HB3	1.89	0.54
11:Y:80:ALA:O	11:Y:84:THR:HG23	2.07	0.54
5:S:167:ALA:HB3	6:T:56:LEU:HD13	1.90	0.54
11:0:30:ASP:N	11:0:30:ASP:OD1	2.41	0.54
12:3:1:THR:HG22	12:3:2:THR:N	2.22	0.54
9:I:1:THR:N	15:I:301:3BV:C47	2.62	0.54
7:U:47:PHE:HB2	7:U:214:SER:HB2	1.90	0.54
8:H:14:LEU:HD21	8:H:101:ALA:HB3	1.88	0.54
1:A:103:TYR:O	9:I:81:ARG:NH1	2.40	0.54
6:T:50:LYS:HB3	6:T:59:HIS:HB3	1.90	0.54
3:C:154:GLY:O	4:D:81:ARG:NH2	2.34	0.54
12:3:115:ASP:HB2	12:3:119:ASN:HB2	1.90	0.54
6:T:47:VAL:HG12	6:T:195:LEU:HD22	1.90	0.54
7:G:47:PHE:HB2	7:G:214:SER:HB2	1.90	0.54
11:Y:49:GLU:HB3	11:Y:52:ASP:HB2	1.90	0.54
13:1:63:THR:OG1	14:2:94:ARG:NH2	2.41	0.54
13:M:137:ALA:H	13:M:146:GLN:HE21	1.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:3:7:LYS:HB3	12:3:12:VAL:HG22	1.90	0.54
6:F:50:LYS:HB3	6:F:59:HIS:HB3	1.89	0.54
2:B:198:PHE:CZ	2:B:206:ASN:HB3	2.43	0.53
10:J:107:PRO:HG2	10:J:124:LEU:HB2	1.90	0.53
12:L:7:LYS:HB3	12:L:12:VAL:HG22	1.90	0.53
12:Z:115:ASP:HB2	12:Z:119:ASN:HB2	1.89	0.53
11:K:49:GLU:HB3	11:K:52:ASP:HB2	1.90	0.53
3:Q:154:GLY:O	4:R:81:ARG:NH2	2.32	0.53
9:I:1:THR:HG23	9:I:33:LYS:CD	2.38	0.53
15:H:301:3BV:H3	15:H:301:3BV:O9	2.08	0.53
12:L:115:ASP:HB2	12:L:119:ASN:HB2	1.90	0.53
11:K:80:ALA:O	11:K:84:THR:HG23	2.08	0.53
6:T:196:ARG:HG3	6:T:239:ARG:CD	2.33	0.53
11:O:49:GLU:HB3	11:O:52:ASP:HB2	1.90	0.53
6:F:196:ARG:NE	6:F:239:ARG:HG3	2.23	0.53
7:U:41:CYS:HB3	7:U:189:ILE:HG13	1.89	0.53
9:W:168:GLY:O	15:W:301:3BV:H57	2.09	0.53
9:W:2:THR:HG22	9:W:2:THR:O	2.08	0.53
12:Z:2:THR:HG21	12:Z:163:ALA:HB1	1.90	0.53
15:W:301:3BV:H21	15:W:301:3BV:C5	2.22	0.53
4:R:30:SER:HB3	4:R:46:GLU:OE2	2.09	0.53
12:L:2:THR:HG22	12:L:2:THR:O	2.08	0.52
15:I:301:3BV:N10	15:I:301:3BV:C5	2.73	0.52
3:C:45:LEU:HD13	3:C:75:SER:HB2	1.92	0.52
11:O:80:ALA:O	11:O:84:THR:HG23	2.09	0.52
8:V:49:ALA:HB2	15:V:301:3BV:H51	1.90	0.52
6:T:38:LEU:HD13	6:T:187:LEU:HG	1.91	0.52
6:F:41:LYS:HG3	6:F:42:THR:HG23	1.90	0.52
9:W:22:GLU:HG2	9:W:27:ALA:HB2	1.92	0.52
10:X:107:PRO:HG2	10:X:124:LEU:HB2	1.92	0.52
6:F:38:LEU:HD13	6:F:187:LEU:HG	1.91	0.52
6:T:41:LYS:HG3	6:T:42:THR:HG23	1.90	0.52
14:2:27:LEU:HD22	14:2:184:TYR:HB2	1.92	0.52
8:V:169:SER:O	15:V:301:3BV:H57	2.09	0.52
13:1:136:LYS:HA	13:1:146:GLN:NE2	2.25	0.52
9:I:22:GLU:HG2	9:I:27:ALA:HB2	1.92	0.52
3:Q:45:LEU:HD13	3:Q:75:SER:HB2	1.91	0.52
10:J:116:THR:O	10:J:192:LYS:NZ	2.43	0.52
9:I:17:ASP:N	9:I:17:ASP:OD1	2.91	0.52
1:O:126:THR:HG22	2:P:127:ARG:HH21	1.75	0.51
13:M:198:VAL:HG22	13:M:203:ILE:HG12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:7:LYS:HB3	12:Z:12:VAL:HG22	1.91	0.51
7:U:17:ASP:OD1	7:U:17:ASP:N	2.40	0.51
12:Z:1:THR:HG23	12:Z:33:LYS:HD3	1.90	0.51
13:M:136:LYS:HA	13:M:146:GLN:NE2	2.26	0.51
9:W:17:ASP:OD1	9:W:17:ASP:N	2.92	0.51
12:L:2:THR:HG21	12:L:163:ALA:HB3	1.91	0.51
13:1:198:VAL:HG22	13:1:203:ILE:HG12	1.92	0.51
1:A:132:ARG:HB3	7:G:12:SER:O	2.10	0.51
2:P:185:ASP:O	2:P:189:THR:HG22	2.11	0.51
13:M:12:ILE:HD12	13:M:55:SER:HB2	1.92	0.51
7:U:49:VAL:HG11	7:U:65:ARG:HB2	1.93	0.51
13:M:28:ARG:NE	13:M:191:ASP:OD2	2.41	0.51
12:3:87:VAL:HG11	12:3:116:SER:HA	1.92	0.51
13:1:28:ARG:NE	13:1:191:ASP:OD2	2.42	0.51
2:B:185:ASP:O	2:B:189:THR:HG22	2.11	0.51
1:A:65:THR:HG21	7:G:159:GLY:HA3	1.92	0.51
6:T:239:ARG:HG3	6:T:240:PRO:N	2.25	0.51
13:1:12:ILE:HD12	13:1:55:SER:HB2	1.93	0.51
4:D:66:ASP:OD1	4:D:67:ASP:N	2.41	0.51
9:I:2:THR:O	9:I:159:ILE:HD12	2.11	0.50
14:N:27:LEU:HD22	14:N:184:TYR:HB2	1.93	0.50
12:L:97:MET:HB3	12:L:116:SER:HB3	1.93	0.50
12:Z:97:MET:HB3	12:Z:116:SER:HB3	1.93	0.50
1:A:6:SER:HB2	1:A:11:ARG:HH11	1.75	0.50
10:X:116:THR:O	10:X:192:LYS:NZ	2.43	0.50
9:I:19:ARG:CZ	9:I:170:GLY:HA3	2.41	0.50
12:L:87:VAL:HG11	12:L:116:SER:HA	1.92	0.50
7:G:49:VAL:HG11	7:G:65:ARG:HB2	1.93	0.50
1:O:6:SER:HB2	1:O:11:ARG:HH11	1.75	0.50
5:S:168:ARG:NH1	6:T:53:GLN:OE1	2.43	0.50
12:L:1:THR:CG2	12:L:2:THR:N	2.75	0.50
12:Z:87:VAL:HG11	12:Z:116:SER:HA	1.92	0.50
7:U:41:CYS:SG	7:U:186:CYS:HB2	2.52	0.50
9:W:18:THR:HB	9:W:31:CYS:H	1.77	0.50
12:L:49:ALA:HB3	16:L:402:HOH:O	2.11	0.50
9:W:1:THR:CG2	9:W:46:ALA:HB1	2.41	0.49
12:3:167:ASP:CG	12:3:170:SER:OG	2.50	0.49
8:V:76:VAL:HG23	8:V:104:ASP:HB2	1.94	0.49
5:E:221:GLN:HG3	5:E:224:GLN:HB3	1.94	0.49
15:I:301:3BV:H5	10:J:106:GLU:OE2	2.12	0.49
2:B:198:PHE:HE2	2:B:201:GLN:C	2.14	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:17:ASP:N	7:G:17:ASP:OD1	2.40	0.49
11:Y:30:ASP:N	11:Y:30:ASP:OD1	2.41	0.49
6:F:196:ARG:HD3	6:F:239:ARG:HD3	1.79	0.49
6:T:238:GLU:O	6:T:240:PRO:HD2	2.13	0.49
2:P:147:GLN:HE21	2:P:162:MET:HE2	1.75	0.49
5:S:221:GLN:HG3	5:S:224:GLN:HB3	1.95	0.49
9:I:50:ALA:HB2	10:J:129:CYS:HB2	1.94	0.49
10:J:37:THR:HG22	10:J:183:MET:HB3	1.94	0.49
6:F:196:ARG:NE	6:F:239:ARG:CD	2.76	0.49
6:T:196:ARG:NE	6:T:239:ARG:CD	2.75	0.49
12:L:20:ALA:HB1	15:L:301:3BV:H14	1.95	0.49
13:I:16:ALA:HB2	13:I:121:VAL:HG23	1.95	0.49
5:E:146:VAL:HG11	5:E:222:PRO:HA	1.95	0.49
8:H:76:VAL:HG23	8:H:104:ASP:HB2	1.95	0.49
13:M:16:ALA:HB2	13:M:121:VAL:HG23	1.95	0.49
7:U:1:SER:HA	7:U:19:ARG:HH12	1.78	0.49
12:3:97:MET:HB3	12:3:116:SER:HB3	1.95	0.48
7:G:197:ILE:HG21	7:G:211:LEU:HD13	1.94	0.48
10:X:37:THR:HG22	10:X:183:MET:HB3	1.94	0.48
5:S:146:VAL:HG11	5:S:222:PRO:HA	1.95	0.48
9:I:18:THR:HB	9:I:31:CYS:H	1.77	0.48
9:W:20:ALA:HB3	9:W:28:ASP:HB3	1.95	0.48
12:L:45:MET:HG2	15:L:301:3BV:C46	2.43	0.48
2:P:212:CYS:HB2	2:P:217:PHE:HD1	1.79	0.48
9:W:33:LYS:HZ3	15:W:301:3BV:H58	1.77	0.48
4:R:31:THR:HB	4:R:46:GLU:CB	2.38	0.48
2:B:198:PHE:CD2	2:B:200:GLY:O	2.67	0.48
5:E:38:ILE:HG23	5:E:181:LEU:HD11	1.96	0.48
8:H:30:VAL:HG21	14:2:212:ALA:HA	1.94	0.48
7:U:46:VAL:HG23	7:U:186:CYS:SG	2.45	0.48
10:X:12:MET:HG3	10:X:138:VAL:HG12	1.94	0.48
1:O:130:GLU:HG2	2:P:4:GLY:HA2	1.94	0.48
5:E:123:PHE:CE1	5:E:136:PRO:HG3	2.49	0.48
15:V:301:3BV:O48	16:V:302:HOH:O	2.20	0.48
15:H:301:3BV:C14	9:I:116:HIS:NE2	2.77	0.48
12:Z:1:THR:HG22	12:Z:2:THR:N	2.28	0.48
5:E:186:HIS:O	5:E:188:SER:N	2.44	0.48
13:M:17:GLY:HA3	13:M:20:PHE:CE1	2.49	0.48
7:G:186:CYS:O	7:G:190:VAL:HG23	2.14	0.48
7:U:197:ILE:HG21	7:U:211:LEU:HD13	1.94	0.48
11:O:99:HIS:HB3	16:O:203:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:1:THR:CG2	12:L:2:THR:H	2.27	0.48
1:O:65:THR:HG21	7:U:159:GLY:HA3	1.96	0.48
2:B:212:CYS:HB2	2:B:217:PHE:HD1	1.79	0.47
14:2:106:LEU:O	14:2:108:ASN:N	2.47	0.47
8:H:1:THR:HG22	8:H:2:THR:N	2.29	0.47
10:J:12:MET:HG3	10:J:138:VAL:HG12	1.95	0.47
14:N:106:LEU:O	14:N:108:ASN:N	2.47	0.47
15:W:301:3BV:N10	15:W:301:3BV:C5	2.77	0.47
1:O:141:ILE:HG22	1:O:151:VAL:HG22	1.95	0.47
9:I:20:ALA:HB3	9:I:28:ASP:HB3	1.96	0.47
3:Q:76:VAL:HG21	3:Q:83:ALA:HB1	1.96	0.47
12:L:113:TYR:O	12:L:120:ARG:HA	2.15	0.47
1:A:132:ARG:HD3	7:G:11:ALA:O	2.14	0.47
10:X:15:LYS:NZ	10:X:134:ASP:OD1	2.47	0.47
9:I:213:THR:HB	10:J:199:THR:OG1	2.15	0.47
13:1:17:GLY:HA3	13:1:20:PHE:CE1	2.49	0.47
7:G:187:ARG:HD2	7:G:187:ARG:HA	1.70	0.47
1:A:141:ILE:HG22	1:A:151:VAL:HG22	1.96	0.47
1:O:211:LYS:HB2	1:O:214:GLU:HG3	1.97	0.47
12:Z:3:THR:HG22	12:Z:16:ALA:CB	2.45	0.47
15:W:301:3BV:H21	15:W:301:3BV:H1	1.80	0.47
6:T:239:ARG:CG	6:T:240:PRO:N	2.78	0.47
1:A:211:LYS:HB2	1:A:214:GLU:HG3	1.97	0.47
4:D:94:HIS:ND1	4:D:101:PRO:O	2.46	0.47
14:2:99:ARG:NH1	14:2:104:ASN:O	2.46	0.47
7:G:121:ALA:O	7:G:125:TYR:HE1	1.98	0.47
12:Z:8:PHE:H	12:Z:8:PHE:HD1	1.62	0.47
3:Q:160:LYS:NZ	3:Q:181:GLU:OE1	2.48	0.47
10:X:47:ASP:HA	16:X:301:HOH:O	2.14	0.47
11:K:24:ASN:HB3	16:K:203:HOH:O	2.15	0.47
10:J:66:ARG:O	10:J:69:PHE:HB3	2.15	0.47
3:C:171:ALA:HB2	3:C:200:THR:HG21	1.97	0.47
7:U:39:ILE:HD11	7:U:189:ILE:HD12	1.97	0.47
7:G:43:ASP:OD1	7:G:186:CYS:SG	2.73	0.47
1:O:212:PRO:HB2	1:O:232:GLU:HG3	1.96	0.47
7:G:39:ILE:HD11	7:G:189:ILE:HD12	1.96	0.47
8:V:142:THR:HB	8:V:155:PHE:HE1	1.80	0.47
3:Q:171:ALA:HB2	3:Q:200:THR:HG21	1.97	0.47
5:E:91:LYS:HG3	5:E:119:LEU:HD11	1.97	0.47
10:J:15:LYS:NZ	10:J:134:ASP:OD1	2.47	0.47
12:3:8:PHE:HD1	12:3:8:PHE:H	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:8:PHE:HD1	12:L:8:PHE:H	1.63	0.47
12:Z:4:LEU:HD12	12:Z:4:LEU:O	2.14	0.46
10:X:53:LEU:HD23	10:X:107:PRO:HB3	1.95	0.46
11:O:102:LEU:HG	11:O:118:MET:HB2	1.96	0.46
9:I:2:THR:HG22	9:I:2:THR:O	2.14	0.46
11:K:102:LEU:HG	11:K:118:MET:HB2	1.97	0.46
9:I:67:SER:HB3	9:I:74:PRO:HG3	1.97	0.46
10:X:66:ARG:NH1	16:X:304:HOH:O	2.47	0.46
7:G:108:LEU:HD11	7:G:137:LEU:HB3	1.97	0.46
15:W:301:3BV:N10	15:W:301:3BV:H1	2.30	0.46
12:L:2:THR:HG21	12:L:163:ALA:HB1	1.96	0.46
1:A:212:PRO:HB2	1:A:232:GLU:HG3	1.96	0.46
14:N:135:PRO:HB2	14:N:154:LEU:HD13	1.97	0.46
14:N:212:ALA:HA	8:V:30:VAL:HG21	1.97	0.46
1:A:138:MET:HB3	1:A:154:CYS:SG	2.55	0.46
12:Z:45:MET:HG2	15:Z:301:3BV:C46	2.46	0.46
11:Y:18:ASP:OD2	11:Y:34:LYS:NZ	2.48	0.46
9:I:187:ARG:HA	9:I:187:ARG:HD2	1.63	0.46
14:N:126:ASP:HB2	14:N:130:VAL:HB	1.96	0.46
7:G:99:ARG:HD2	14:N:69:GLN:OE1	2.16	0.46
3:C:76:VAL:HG21	3:C:83:ALA:HB1	1.96	0.46
8:H:142:THR:HB	8:H:155:PHE:HE1	1.81	0.46
1:O:138:MET:HB3	1:O:154:CYS:SG	2.55	0.46
7:U:108:LEU:HD11	7:U:137:LEU:HB3	1.96	0.46
4:D:101:PRO:HB2	4:D:102:VAL:H	1.60	0.46
3:C:160:LYS:NZ	3:C:181:GLU:OE1	2.48	0.46
5:S:123:PHE:CE1	5:S:136:PRO:HG3	2.51	0.46
11:Y:182:ILE:HG22	11:Y:189:HIS:HB2	1.97	0.46
7:G:86:SER:O	7:G:90:ILE:HD12	2.15	0.46
5:S:38:ILE:HG23	5:S:181:LEU:HD11	1.97	0.46
11:Y:102:LEU:HG	11:Y:118:MET:HB2	1.97	0.46
14:2:135:PRO:HB2	14:2:154:LEU:HD13	1.98	0.46
14:2:142:GLY:HA2	14:2:176:LEU:HD21	1.96	0.46
13:1:24:ALA:HB1	13:1:193:LEU:HD11	1.97	0.46
3:Q:8:ARG:NH1	4:R:5:ARG:HD3	2.31	0.46
7:G:215:TRP:CD1	7:G:227:VAL:HA	2.51	0.46
10:J:53:LEU:HD23	10:J:107:PRO:HB3	1.97	0.46
4:D:31:THR:OG1	4:D:163:ARG:O	2.30	0.46
15:V:301:3BV:H16	15:V:301:3BV:C15	2.37	0.46
7:G:33:SER:HB2	7:G:79:GLY:HA2	1.97	0.46
11:K:18:ASP:OD2	11:K:34:LYS:NZ	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:66:ARG:O	10:X:69:PHE:HB3	2.16	0.46
12:Z:113:TYR:O	12:Z:120:ARG:HA	2.16	0.46
14:N:37:ARG:HD2	8:V:166:ARG:NH1	2.30	0.46
11:O:18:ASP:OD2	11:O:34:LYS:NZ	2.49	0.46
5:S:31:ILE:HD11	5:S:158:PRO:HD2	1.98	0.45
9:W:67:SER:HB3	9:W:74:PRO:HG3	1.98	0.45
4:R:66:ASP:OD1	4:R:67:ASP:N	2.41	0.45
12:3:113:TYR:O	12:3:120:ARG:HA	2.16	0.45
8:H:20:THR:HG23	15:H:301:3BV:H52	1.98	0.45
10:J:173:ASN:ND2	13:1:151:ASN:CB	2.76	0.45
14:N:142:GLY:HA2	14:N:176:LEU:HD21	1.97	0.45
9:W:35:HIS:CG	9:W:56:THR:HG21	2.51	0.45
13:M:24:ALA:HB1	13:M:193:LEU:HD11	1.98	0.45
6:F:158:ALA:HB3	7:G:57:LEU:HD22	1.97	0.45
6:T:196:ARG:CZ	6:T:239:ARG:CB	2.85	0.45
15:Z:301:3BV:H21	15:Z:301:3BV:C5	2.27	0.45
15:H:301:3BV:H31	9:I:114:TYR:CE2	2.51	0.45
11:O:118:MET:HE2	11:O:118:MET:HB3	1.75	0.45
5:E:31:ILE:HD11	5:E:158:PRO:HD2	1.98	0.45
2:B:173:LEU:HD21	2:B:193:THR:HG21	1.99	0.45
4:R:46:GLU:OE2	4:R:47:LYS:N	2.49	0.45
15:3:301:3BV:O48	16:3:302:HOH:O	2.21	0.45
11:O:182:ILE:HG22	11:O:189:HIS:HB2	1.98	0.45
7:U:215:TRP:CD1	7:U:227:VAL:HA	2.52	0.45
6:F:11:THR:O	7:G:129:ARG:HB3	2.17	0.45
1:A:18:PRO:HA	2:B:23:TYR:CE1	2.51	0.45
15:W:301:3BV:H52	15:W:301:3BV:O40	2.16	0.45
8:V:84:LYS:HG3	8:V:120:MET:HB2	1.99	0.45
9:I:59:ILE:HD12	9:I:82:MET:HB3	1.99	0.45
4:R:94:HIS:ND1	4:R:101:PRO:O	2.46	0.45
1:A:201:CYS:O	1:A:205:VAL:HB	2.17	0.45
2:P:173:LEU:HD21	2:P:193:THR:HG21	1.98	0.45
9:W:33:LYS:NZ	15:W:301:3BV:H58	2.31	0.45
5:E:166:ASP:HB3	5:E:185:TYR:CZ	2.52	0.45
14:2:126:ASP:HB2	14:2:130:VAL:HB	1.97	0.45
7:G:187:ARG:HH21	7:G:191:LYS:HZ3	1.65	0.45
1:A:77:GLY:HA3	1:A:227:PHE:CD1	2.52	0.45
11:K:182:ILE:HG22	11:K:189:HIS:HB2	1.98	0.45
8:H:31:THR:HG22	8:H:32:ASP:N	2.31	0.45
15:Z:301:3BV:C5	15:Z:301:3BV:N10	2.80	0.45
8:H:84:LYS:HG3	8:H:120:MET:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:0:1:MET:CE	11:0:134:TYR:H	2.29	0.45
1:O:132:ARG:HD2	7:U:14:PHE:CE2	2.51	0.45
12:Z:2:THR:HG21	12:Z:163:ALA:CB	2.46	0.45
4:D:116:GLN:HG3	5:E:83:ALA:HB1	1.99	0.45
7:U:86:SER:O	7:U:90:ILE:HD12	2.16	0.45
14:2:25:ASP:OD1	14:2:41:ARG:NH1	2.51	0.44
7:G:66:LEU:HD13	7:G:214:SER:OG	2.18	0.44
9:I:65:LEU:HD12	9:I:65:LEU:HA	1.80	0.44
7:G:74:GLY:HA3	7:G:224:HIS:CD2	2.52	0.44
8:H:35:THR:HA	8:H:36:PRO:HD3	1.86	0.44
9:I:35:HIS:CG	9:I:56:THR:HG21	2.51	0.44
10:J:4:MET:HG3	10:J:127:ILE:HG22	11.33	0.44
7:G:33:SER:O	7:G:167:LYS:HG3	2.18	0.44
14:N:126:ASP:HB3	14:N:128:LEU:H	1.83	0.44
5:S:166:ASP:HB3	5:S:185:TYR:CZ	2.52	0.44
9:W:63:LEU:HD23	9:W:63:LEU:HA	1.77	0.44
7:U:66:LEU:HD12	7:U:212:GLU:HB3	2.00	0.44
9:W:59:ILE:HD12	9:W:82:MET:HB3	2.00	0.44
14:N:215:ILE:HD11	8:V:175:ARG:NH1	2.32	0.44
14:N:99:ARG:NH1	14:N:104:ASN:O	2.45	0.44
9:I:216:ILE:HD13	10:J:196:THR:HG23	2.00	0.44
7:U:74:GLY:HA3	7:U:224:HIS:CD2	2.52	0.44
1:O:201:CYS:O	1:O:205:VAL:HB	2.17	0.44
6:T:202:GLU:H	6:T:202:GLU:HG3	1.55	0.44
7:U:215:TRP:CD1	7:U:227:VAL:HG22	2.53	0.44
14:N:25:ASP:HA	14:N:187:PHE:HA	1.99	0.44
9:W:65:LEU:HD12	9:W:65:LEU:HA	1.81	0.44
5:S:221:GLN:NE2	5:S:224:GLN:OE1	2.49	0.44
14:2:126:ASP:HB3	14:2:128:LEU:H	1.83	0.44
1:A:165:ALA:HB1	1:A:179:LEU:HD13	2.00	0.44
5:S:186:HIS:O	5:S:188:SER:N	2.45	0.44
5:E:24:VAL:O	5:E:28:ILE:HG12	2.17	0.44
12:3:1:THR:CG2	12:3:2:THR:N	2.81	0.44
8:V:84:LYS:HE3	8:V:84:LYS:HB3	1.81	0.44
1:O:77:GLY:HA3	1:O:227:PHE:CD1	2.53	0.44
13:M:184:GLU:OE2	13:M:211:ARG:NH1	2.44	0.44
7:G:215:TRP:CD1	7:G:227:VAL:HG22	2.53	0.44
4:R:100:ASP:OD1	12:Z:107:ARG:NH2	2.37	0.44
6:F:36:VAL:HG13	6:F:172:LEU:HD11	2.00	0.44
7:U:66:LEU:HD13	7:U:214:SER:OG	2.18	0.44
7:G:66:LEU:HD12	7:G:212:GLU:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:196:ARG:O	6:T:239:ARG:NH1	2.51	0.43
15:Z:301:3BV:H25	15:Z:301:3BV:H24	1.75	0.43
11:O:1:MET:HE2	11:O:134:TYR:CD2	2.52	0.43
4:D:137:ASP:OD2	4:D:143:ARG:NH1	2.51	0.43
11:O:9:GLY:HA3	11:O:12:TYR:CE1	2.53	0.43
7:U:33:SER:O	7:U:167:LYS:HG3	2.17	0.43
12:Z:45:MET:HG3	12:Z:52:CYS:CB	2.49	0.43
11:K:196:PHE:O	11:K:198:LYS:N	2.51	0.43
5:S:91:LYS:HG3	5:S:119:LEU:HD11	1.99	0.43
11:K:1:MET:HE2	11:K:134:TYR:CD2	2.52	0.43
5:S:73:HIS:CD2	5:S:74:ILE:HG13	2.54	0.43
3:Q:17:ARG:HD2	3:Q:22:GLU:OE2	2.18	0.43
9:I:1:THR:CG2	9:I:2:THR:H	2.26	0.43
11:Y:9:GLY:HA3	11:Y:12:TYR:CE1	2.53	0.43
3:C:17:ARG:HD2	3:C:22:GLU:OE2	2.18	0.43
13:1:40:SER:O	13:1:42:LYS:HE3	2.19	0.43
11:K:9:GLY:HA3	11:K:12:TYR:CE1	2.53	0.43
12:3:169:TYR:O	15:3:301:3BV:H57	2.19	0.43
14:2:25:ASP:HA	14:2:187:PHE:HA	1.99	0.43
13:M:40:SER:O	13:M:42:LYS:HE3	2.19	0.43
8:H:174:ILE:HB	8:H:189:LEU:HB2	2.00	0.43
2:B:38:LYS:HE3	2:B:143:PRO:HG2	2.01	0.43
5:E:167:ALA:HB3	6:F:56:LEU:HD13	2.00	0.43
9:W:1:THR:CB	9:W:46:ALA:HB1	2.48	0.43
15:V:301:3BV:C46	15:V:301:3BV:N41	2.77	0.43
10:X:125:ASP:HB3	10:X:127:ILE:H	1.84	0.43
6:T:36:VAL:HG13	6:T:172:LEU:HD11	2.01	0.43
8:V:174:ILE:HB	8:V:189:LEU:HB2	1.99	0.43
9:W:143:ARG:O	9:W:146:MET:HG3	2.18	0.43
9:I:1:THR:CG2	9:I:2:THR:N	2.80	0.43
1:O:143:ILE:HG12	1:O:220:VAL:HG22	2.00	0.43
10:J:116:THR:HG22	10:J:117:PHE:CD1	2.53	0.43
10:X:65:GLN:OE1	11:Y:86:ARG:NH2	2.51	0.43
10:J:125:ASP:HB3	10:J:127:ILE:H	1.84	0.43
12:L:1:THR:HG21	12:L:46:ALA:HB2	2.01	0.43
6:T:214:ILE:O	6:T:221:PHE:HA	2.19	0.43
3:C:95:GLN:HG3	10:J:73:LEU:HG	2.00	0.43
1:O:165:ALA:HB1	1:O:179:LEU:HD13	2.01	0.43
12:3:3:THR:HG22	12:3:16:ALA:CB	2.49	0.43
11:Y:1:MET:HE2	11:Y:134:TYR:CD2	2.54	0.42
3:Q:249:ARG:NH2	16:Q:306:HOH:O	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ILE:HG23	1:A:109:ILE:HD13	3.00	0.42
9:I:143:ARG:O	9:I:146:MET:HG3	2.18	0.42
14:2:150:LEU:HD23	14:2:168:LEU:HD22	2.01	0.42
13:1:46:LEU:HB3	13:1:72:LEU:HD11	2.01	0.42
11:Y:1:MET:CE	11:Y:134:TYR:H	2.29	0.42
15:H:301:3BV:H31	9:I:114:TYR:CD2	2.54	0.42
9:W:217:THR:HA	9:W:218:PRO:HD3	1.88	0.42
6:F:108:LEU:O	6:F:112:ILE:HG13	2.19	0.42
4:D:13:ASP:N	4:D:13:ASP:OD1	2.50	0.42
12:3:45:MET:HG3	12:3:52:CYS:CB	2.49	0.42
10:X:116:THR:HG22	10:X:117:PHE:CD1	2.54	0.42
6:F:158:ALA:O	7:G:57:LEU:HB3	2.19	0.42
1:A:72:ILE:HG21	1:A:114:LEU:HD11	2.01	0.42
2:B:45:LEU:HD13	2:B:74:VAL:HG22	2.01	0.42
4:D:33:VAL:HG11	4:D:168:VAL:HG11	2.01	0.42
14:N:3:ASN:HA	14:N:4:PRO:HD2	1.94	0.42
14:N:141:TYR:CE2	8:V:24:SER:HB2	2.53	0.42
14:N:150:LEU:HD23	14:N:168:LEU:HD22	2.02	0.42
11:Y:196:PHE:O	11:Y:198:LYS:N	2.51	0.42
5:E:73:HIS:CD2	5:E:74:ILE:HG13	2.54	0.42
4:R:31:THR:H	4:R:46:GLU:CD	2.23	0.42
1:A:86:ASP:OD2	1:A:132:ARG:NH2	2.52	0.42
12:L:1:THR:HA	12:L:33:LYS:HZ3	1.84	0.42
8:H:24:SER:HB2	14:2:141:TYR:CE2	2.54	0.42
6:T:219:LEU:HG	6:T:220:GLU:O	2.19	0.42
2:P:38:LYS:HE3	2:P:143:PRO:HG2	2.02	0.42
4:R:46:GLU:CD	4:R:47:LYS:CB	2.88	0.42
12:Z:3:THR:HG22	12:Z:16:ALA:HB1	2.02	0.42
6:F:219:LEU:HG	6:F:220:GLU:O	2.20	0.42
11:O:196:PHE:O	11:O:198:LYS:N	2.51	0.42
4:R:13:ASP:OD1	4:R:13:ASP:N	2.49	0.42
12:L:45:MET:HG2	15:L:301:3BV:H53	2.00	0.42
9:W:216:ILE:HD13	10:X:196:THR:HG23	2.02	0.42
11:K:60:ILE:HG21	11:K:84:THR:HG22	2.01	0.42
10:X:171:MET:O	10:X:175:VAL:HB	2.19	0.42
2:P:45:LEU:HD13	2:P:74:VAL:HG22	2.02	0.42
9:W:3:ILE:HD11	9:W:99:VAL:HG23	1.98	0.42
8:H:33:LYS:HA	8:H:45:ARG:NH1	2.35	0.42
12:3:1:THR:HG22	12:3:3:THR:HG23	2.01	0.42
12:Z:20:ALA:CB	15:Z:301:3BV:C26	2.91	0.42
8:H:169:SER:O	15:H:301:3BV:C58	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:W:301:3BV:H25	15:W:301:3BV:H24	1.85	0.42
14:N:25:ASP:OD1	14:N:41:ARG:NH1	2.53	0.42
7:U:28:LYS:HB2	7:U:28:LYS:HE3	1.84	0.42
1:O:72:ILE:HG21	1:O:114:LEU:HD11	2.01	0.42
4:D:80:ALA:HA	4:D:129:ILE:HD13	2.02	0.42
15:3:301:3BV:H60	16:3:302:HOH:O	2.20	0.41
1:A:143:ILE:HG12	1:A:220:VAL:HG22	2.01	0.41
9:W:204:CYS:SG	10:X:169:GLN:HG3	2.60	0.41
9:W:141:LYS:NZ	9:W:157:GLU:OE2	2.38	0.41
1:A:29:PHE:HE2	1:A:157:ALA:HB2	1.85	0.41
9:W:187:ARG:HA	9:W:187:ARG:HD2	2.04	0.41
14:2:89:HIS:HA	14:2:112:ILE:HD12	2.02	0.41
8:V:104:ASP:HA	8:V:105:PRO:HD3	1.95	0.41
1:O:50:ILE:HG21	1:O:79:VAL:HB	2.02	0.41
12:L:45:MET:HG3	12:L:52:CYS:CB	2.49	0.41
9:W:213:THR:HB	10:X:199:THR:OG1	2.19	0.41
6:F:71:GLY:HA3	6:F:221:PHE:CE1	2.56	0.41
6:T:108:LEU:O	6:T:112:ILE:HG13	2.20	0.41
6:F:62:LYS:HB3	6:F:62:LYS:HE3	1.89	0.41
7:G:185:THR:O	7:G:187:ARG:N	2.53	0.41
6:F:11:THR:HA	7:G:129:ARG:HG2	2.03	0.41
2:P:133:LEU:O	2:P:147:GLN:HA	2.21	0.41
3:C:14:PRO:HA	4:D:21:TYR:CE1	2.55	0.41
1:A:50:ILE:HG21	1:A:79:VAL:HB	2.02	0.41
5:S:24:VAL:O	5:S:28:ILE:HG12	2.19	0.41
3:Q:68:LEU:HD11	3:Q:74:CYS:HB3	2.03	0.41
8:V:22:THR:HB	15:V:301:3BV:H33	2.01	0.41
1:A:6:SER:HB2	1:A:11:ARG:NH1	2.36	0.41
11:K:196:PHE:HA	11:K:197:PRO:HD3	1.85	0.41
5:E:168:ARG:NH1	6:F:53:GLN:OE1	2.49	0.41
4:D:138:PHE:O	4:D:139:ASP:HB3	2.20	0.41
14:N:177:TYR:CZ	14:N:185:ASN:HB2	2.56	0.41
3:C:130:PHE:O	3:C:152:PRO:HB3	2.20	0.41
8:V:35:THR:HA	8:V:36:PRO:HD3	1.85	0.41
14:2:86:ARG:HB3	14:2:86:ARG:HH11	1.86	0.41
14:N:89:HIS:HA	14:N:112:ILE:HD12	2.02	0.41
13:M:157:ASN:OD1	10:X:172:LEU:HB3	2.20	0.41
4:R:138:PHE:O	4:R:139:ASP:HB3	2.20	0.41
7:U:185:THR:O	7:U:189:ILE:HG12	2.21	0.41
8:H:84:LYS:HE3	8:H:84:LYS:HB3	1.82	0.41
13:M:46:LEU:HB3	13:M:72:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:29:PHE:HE2	1:O:157:ALA:HB2	1.86	0.41
7:G:68:ASN:HB3	14:N:76:LEU:HD22	2.02	0.41
9:I:170:GLY:O	9:I:171:SER:CB	2.68	0.41
14:N:33:LEU:HD13	8:V:134:TYR:CE1	2.56	0.41
3:C:3:ARG:HG2	3:C:8:ARG:NH2	2.36	0.41
12:L:27:ALA:HB3	15:L:301:3BV:H13	2.03	0.41
7:G:19:ARG:NH2	7:G:24:GLU:OE1	2.46	0.41
2:B:72:GLY:HA3	2:B:217:PHE:CE1	2.56	0.41
9:I:73:LEU:HA	9:I:74:PRO:HD3	1.91	0.41
2:B:74:VAL:HG23	2:B:134:LEU:HB2	2.03	0.41
3:Q:14:PRO:HA	4:R:21:TYR:CE1	2.56	0.41
7:G:30:VAL:HG22	7:G:133:CYS:HA	2.01	0.41
14:2:122:LEU:HG	14:2:137:LEU:HD12	2.03	0.41
3:Q:139:TRP:HA	3:Q:144:GLY:O	2.21	0.41
12:3:17:ASP:HB2	12:3:171:GLY:O	2.21	0.41
3:C:68:LEU:HD11	3:C:74:CYS:HB3	2.03	0.41
3:C:139:TRP:HA	3:C:144:GLY:O	2.21	0.41
10:J:171:MET:O	10:J:175:VAL:HB	2.21	0.41
3:Q:187:LYS:HD2	3:Q:187:LYS:HA	1.88	0.41
6:T:70:ILE:HD11	6:T:105:VAL:HG22	2.03	0.41
12:Z:45:MET:HG2	15:Z:301:3BV:H52	2.03	0.41
1:O:32:ILE:HD13	1:O:137:CYS:HB2	2.03	0.41
3:Q:130:PHE:O	3:Q:152:PRO:HB3	2.20	0.41
12:L:134:TYR:OH	10:X:33:GLN:HB2	2.21	0.41
2:P:74:VAL:HG23	2:P:134:LEU:HB2	2.03	0.41
14:2:177:TYR:CZ	14:2:185:ASN:HB2	2.56	0.41
2:B:133:LEU:O	2:B:147:GLN:HA	2.21	0.41
3:C:218:ARG:NH2	3:C:221:GLY:O	2.54	0.41
4:R:80:ALA:HA	4:R:129:ILE:HD13	2.03	0.41
10:X:115:LYS:HD2	10:X:115:LYS:HA	1.78	0.41
6:F:239:ARG:HE	6:F:240:PRO:HD2	1.86	0.40
6:T:196:ARG:NE	6:T:239:ARG:HD3	2.36	0.40
2:P:72:GLY:HA3	2:P:217:PHE:CE1	2.57	0.40
13:1:72:LEU:HD23	13:1:83:MET:SD	2.62	0.40
1:A:29:PHE:CZ	1:A:155:ASP:HB3	2.56	0.40
8:V:4:MET:HG3	8:V:127:ILE:HG22	2.03	0.40
6:F:188:VAL:HG11	6:F:232:PHE:CD1	2.56	0.40
6:T:188:VAL:HG11	6:T:232:PHE:CD1	2.56	0.40
14:N:86:ARG:HH11	14:N:86:ARG:HB3	1.85	0.40
10:J:4:MET:HE2	10:J:126:LEU:HD23	2.03	0.40
3:C:72:MET:HG3	3:C:138:GLY:HA3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:73:ALA:HB2	3:Q:225:ILE:HD13	2.03	0.40
9:I:63:LEU:HA	9:I:63:LEU:HD23	1.76	0.40
2:P:73:LEU:HA	2:P:73:LEU:HD23	1.90	0.40
4:R:163:ARG:O	4:R:164:GLY:C	2.59	0.40
2:B:106:THR:O	2:B:110:VAL:HG23	2.21	0.40
2:B:10:THR:O	3:C:128:ARG:HD3	2.20	0.40
1:O:6:SER:HB2	1:O:11:ARG:NH1	2.36	0.40
2:P:147:GLN:HE21	2:P:162:MET:CE	2.35	0.40
5:S:232:GLU:N	5:S:232:GLU:OE2	2.54	0.40
4:D:119:THR:O	5:E:135:ARG:NH1	2.54	0.40
14:N:25:ASP:O	14:N:41:ARG:HD3	2.22	0.40
9:I:217:THR:HA	9:I:218:PRO:HD3	1.88	0.40
8:H:144:ARG:O	8:H:147:MET:HG3	2.22	0.40
10:X:112:LEU:HD23	10:X:119:PRO:HA	2.03	0.40
14:2:92:LEU:O	14:2:96:MET:HG2	2.22	0.40
9:W:3:ILE:O	9:W:4:ALA:HB2	2.21	0.40
11:K:1:MET:CE	11:K:134:TYR:H	2.29	0.40
5:S:36:THR:HA	5:S:171:GLY:HA3	2.03	0.40
11:Y:196:PHE:HA	11:Y:197:PRO:HD3	1.86	0.40
14:N:92:LEU:O	14:N:96:MET:HG2	2.21	0.40
10:J:112:LEU:HD23	10:J:119:PRO:HA	2.04	0.40
7:U:187:ARG:HD2	7:U:187:ARG:HA	1.84	0.40

There are no symmetry-related clashes.

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	242/244 (99%)	229 (95%)	12 (5%)	1 (0%)	39	74
1	O	242/244 (99%)	228 (94%)	13 (5%)	1 (0%)	39	74
1	c	242/244 (99%)	229 (95%)	12 (5%)	1 (0%)	39	74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	q	242/244 (99%)	229 (95%)	12 (5%)	1 (0%)	39	74
2	B	231/233 (99%)	209 (90%)	17 (7%)	5 (2%)	8	31
2	P	231/233 (99%)	208 (90%)	18 (8%)	5 (2%)	8	31
2	d	231/233 (99%)	209 (90%)	17 (7%)	5 (2%)	8	31
2	r	231/233 (99%)	208 (90%)	19 (8%)	4 (2%)	11	38
3	C	248/250 (99%)	236 (95%)	11 (4%)	1 (0%)	39	74
3	Q	248/250 (99%)	236 (95%)	11 (4%)	1 (0%)	39	74
3	e	248/250 (99%)	236 (95%)	11 (4%)	1 (0%)	39	74
3	s	248/250 (99%)	236 (95%)	11 (4%)	1 (0%)	39	74
4	D	241/243 (99%)	225 (93%)	10 (4%)	6 (2%)	7	27
4	R	241/243 (99%)	222 (92%)	13 (5%)	6 (2%)	7	27
4	f	241/243 (99%)	225 (93%)	10 (4%)	6 (2%)	7	27
4	t	241/243 (99%)	225 (93%)	10 (4%)	6 (2%)	7	27
5	E	232/234 (99%)	220 (95%)	9 (4%)	3 (1%)	15	46
5	S	232/234 (99%)	220 (95%)	9 (4%)	3 (1%)	15	46
5	g	232/234 (99%)	219 (94%)	10 (4%)	3 (1%)	15	46
5	u	232/234 (99%)	220 (95%)	9 (4%)	3 (1%)	15	46
6	F	236/238 (99%)	227 (96%)	9 (4%)	0	100	100
6	T	236/238 (99%)	228 (97%)	6 (2%)	2 (1%)	24	60
6	h	236/238 (99%)	229 (97%)	6 (2%)	1 (0%)	39	74
6	v	236/238 (99%)	227 (96%)	6 (2%)	3 (1%)	15	46
7	G	243/245 (99%)	229 (94%)	12 (5%)	2 (1%)	24	60
7	U	243/245 (99%)	230 (95%)	11 (4%)	2 (1%)	24	60
7	i	243/245 (99%)	229 (94%)	12 (5%)	2 (1%)	24	60
7	w	243/245 (99%)	231 (95%)	9 (4%)	3 (1%)	16	48
8	H	200/202 (99%)	194 (97%)	5 (2%)	1 (0%)	34	71
8	V	200/202 (99%)	194 (97%)	5 (2%)	1 (0%)	34	71
8	j	200/202 (99%)	192 (96%)	7 (4%)	1 (0%)	34	71
8	x	200/202 (99%)	194 (97%)	5 (2%)	1 (0%)	34	71
9	I	218/220 (99%)	205 (94%)	11 (5%)	2 (1%)	21	57
9	W	218/220 (99%)	204 (94%)	13 (6%)	1 (0%)	34	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	k	218/220 (99%)	206 (94%)	11 (5%)	1 (0%)	34	71
9	y	218/220 (99%)	206 (94%)	11 (5%)	1 (0%)	34	71
10	J	202/204 (99%)	191 (95%)	7 (4%)	4 (2%)	9	33
10	X	202/204 (99%)	191 (95%)	7 (4%)	4 (2%)	9	33
10	l	202/204 (99%)	191 (95%)	7 (4%)	4 (2%)	9	33
10	z	202/204 (99%)	190 (94%)	8 (4%)	4 (2%)	9	33
11	0	197/199 (99%)	187 (95%)	7 (4%)	3 (2%)	13	42
11	K	197/199 (99%)	187 (95%)	7 (4%)	3 (2%)	13	42
11	Y	197/199 (99%)	187 (95%)	7 (4%)	3 (2%)	13	42
11	m	197/199 (99%)	187 (95%)	7 (4%)	3 (2%)	13	42
12	3	199/201 (99%)	185 (93%)	14 (7%)	0	100	100
12	L	199/201 (99%)	186 (94%)	12 (6%)	1 (0%)	34	71
12	Z	199/201 (99%)	186 (94%)	13 (6%)	0	100	100
12	n	199/201 (99%)	184 (92%)	15 (8%)	0	100	100
13	1	211/213 (99%)	207 (98%)	4 (2%)	0	100	100
13	M	211/213 (99%)	206 (98%)	5 (2%)	0	100	100
13	a	211/213 (99%)	207 (98%)	4 (2%)	0	100	100
13	o	211/213 (99%)	206 (98%)	5 (2%)	0	100	100
14	2	215/217 (99%)	199 (93%)	13 (6%)	3 (1%)	14	44
14	N	215/217 (99%)	199 (93%)	14 (6%)	2 (1%)	21	57
14	b	215/217 (99%)	199 (93%)	13 (6%)	3 (1%)	14	44
14	p	215/217 (99%)	199 (93%)	14 (6%)	2 (1%)	21	57
All	All	12460/12572 (99%)	11768 (94%)	566 (4%)	126 (1%)	19	54

All (126) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	232	ILE
4	D	47	LYS
9	I	187	ARG
10	J	117	PHE
10	J	156	PRO
2	P	232	ILE
4	R	47	LYS

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Mol	Chain	Res	Type
6	T	237	GLU
6	T	239	ARG
10	X	117	PHE
10	X	156	PRO
2	d	232	ILE
4	f	47	LYS
10	l	117	PHE
10	l	156	PRO
2	r	232	ILE
4	t	47	LYS
6	v	237	GLU
6	v	239	ARG
10	z	117	PHE
10	z	156	PRO
2	B	51	GLN
4	D	101	PRO
5	E	120	ALA
9	I	171	SER
4	R	101	PRO
5	S	120	ALA
4	f	101	PRO
5	g	120	ALA
4	t	101	PRO
5	u	120	ALA
6	v	240	PRO
7	w	2	SER
2	B	30	GLY
4	D	46	GLU
4	D	139	ASP
4	D	201	SER
10	J	116	THR
11	K	50	ALA
12	L	2	THR
14	N	46	ASN
2	P	30	GLY
2	P	51	GLN
2	P	198	PHE
4	R	139	ASP
4	R	164	GLY
4	R	201	SER
10	X	116	THR
11	Y	50	ALA

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Mol	Chain	Res	Type
14	2	46	ASN
2	d	30	GLY
2	d	198	PHE
4	f	46	GLU
4	f	139	ASP
4	f	201	SER
10	l	116	THR
11	m	50	ALA
14	p	46	ASN
2	r	30	GLY
4	t	46	GLU
4	t	139	ASP
4	t	201	SER
10	z	116	THR
11	0	50	ALA
14	b	46	ASN
2	B	40	ALA
3	C	206	LEU
5	E	187	LYS
5	E	188	SER
7	G	207	LYS
11	K	174	ASN
14	N	107	TRP
2	P	40	ALA
3	Q	206	LEU
5	S	187	LYS
7	U	207	LYS
11	Y	174	ASN
14	2	107	TRP
2	d	40	ALA
2	d	51	GLN
3	e	206	LEU
5	g	187	LYS
5	g	188	SER
6	h	239	ARG
7	i	207	LYS
14	p	107	TRP
2	r	51	GLN
3	s	206	LEU
5	u	187	LYS
5	u	188	SER
7	w	207	LYS

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Mol	Chain	Res	Type
11	0	174	ASN
14	b	107	TRP
1	A	189	TRP
2	B	53	SER
10	J	31	GLN
1	O	189	TRP
4	R	243	LYS
5	S	188	SER
9	W	187	ARG
10	X	31	GLN
1	c	189	TRP
9	k	187	ARG
10	l	31	GLN
11	m	174	ASN
1	q	189	TRP
2	r	40	ALA
9	y	187	ARG
10	z	31	GLN
4	D	243	LYS
11	Y	197	PRO
14	2	216	SER
4	f	243	LYS
4	t	243	LYS
11	0	197	PRO
14	b	216	SER
11	K	197	PRO
11	m	197	PRO
8	j	30	VAL
8	H	30	VAL
8	V	30	VAL
8	x	30	VAL
7	G	216	VAL
7	U	216	VAL
7	i	216	VAL
7	w	216	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	192/208 (92%)	180 (94%)	12 (6%)	22	54
1	O	193/208 (93%)	182 (94%)	11 (6%)	25	59
1	c	192/208 (92%)	181 (94%)	11 (6%)	25	59
1	q	192/208 (92%)	180 (94%)	12 (6%)	22	54
2	B	164/190 (86%)	161 (98%)	3 (2%)	66	90
2	P	165/190 (87%)	162 (98%)	3 (2%)	66	90
2	d	164/190 (86%)	161 (98%)	3 (2%)	66	90
2	r	165/190 (87%)	162 (98%)	3 (2%)	66	90
3	C	191/210 (91%)	184 (96%)	7 (4%)	41	77
3	Q	191/210 (91%)	184 (96%)	7 (4%)	41	77
3	e	191/210 (91%)	184 (96%)	7 (4%)	41	77
3	s	191/210 (91%)	184 (96%)	7 (4%)	41	77
4	D	142/207 (69%)	132 (93%)	10 (7%)	19	47
4	R	143/207 (69%)	132 (92%)	11 (8%)	16	42
4	f	137/207 (66%)	131 (96%)	6 (4%)	35	70
4	t	138/207 (67%)	130 (94%)	8 (6%)	25	58
5	E	189/196 (96%)	182 (96%)	7 (4%)	41	77
5	S	189/196 (96%)	182 (96%)	7 (4%)	41	77
5	g	189/196 (96%)	181 (96%)	8 (4%)	36	73
5	u	190/196 (97%)	182 (96%)	8 (4%)	36	73
6	F	198/204 (97%)	190 (96%)	8 (4%)	38	74
6	T	198/204 (97%)	190 (96%)	8 (4%)	38	74
6	h	198/204 (97%)	191 (96%)	7 (4%)	43	78
6	v	198/204 (97%)	190 (96%)	8 (4%)	38	74
7	G	195/202 (96%)	186 (95%)	9 (5%)	33	69
7	U	195/202 (96%)	190 (97%)	5 (3%)	54	85
7	i	195/202 (96%)	188 (96%)	7 (4%)	42	78
7	w	195/202 (96%)	190 (97%)	5 (3%)	54	85
8	H	155/157 (99%)	150 (97%)	5 (3%)	46	81
8	V	155/157 (99%)	150 (97%)	5 (3%)	46	81
8	j	155/157 (99%)	150 (97%)	5 (3%)	46	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	x	155/157 (99%)	150 (97%)	5 (3%)	46	81
9	I	177/181 (98%)	171 (97%)	6 (3%)	44	79
9	W	177/181 (98%)	171 (97%)	6 (3%)	44	79
9	k	177/181 (98%)	171 (97%)	6 (3%)	44	79
9	y	178/181 (98%)	173 (97%)	5 (3%)	51	84
10	J	172/173 (99%)	161 (94%)	11 (6%)	22	53
10	X	172/173 (99%)	161 (94%)	11 (6%)	22	53
10	l	172/173 (99%)	161 (94%)	11 (6%)	22	53
10	z	172/173 (99%)	161 (94%)	11 (6%)	22	53
11	0	164/170 (96%)	157 (96%)	7 (4%)	35	71
11	K	164/170 (96%)	157 (96%)	7 (4%)	35	71
11	Y	164/170 (96%)	157 (96%)	7 (4%)	35	71
11	m	164/170 (96%)	157 (96%)	7 (4%)	35	71
12	3	154/156 (99%)	146 (95%)	8 (5%)	29	64
12	L	153/156 (98%)	147 (96%)	6 (4%)	39	75
12	Z	154/156 (99%)	147 (96%)	7 (4%)	34	70
12	n	153/156 (98%)	145 (95%)	8 (5%)	29	64
13	1	173/178 (97%)	169 (98%)	4 (2%)	58	87
13	M	174/178 (98%)	170 (98%)	4 (2%)	58	87
13	a	173/178 (97%)	167 (96%)	6 (4%)	43	78
13	o	173/178 (97%)	169 (98%)	4 (2%)	58	87
14	2	175/179 (98%)	165 (94%)	10 (6%)	25	59
14	N	175/179 (98%)	165 (94%)	10 (6%)	25	59
14	b	174/179 (97%)	164 (94%)	10 (6%)	25	59
14	p	174/179 (97%)	164 (94%)	10 (6%)	25	59
All	All	9758/10444 (93%)	9348 (96%)	410 (4%)	36	73

All (410) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	CYS
1	A	108	GLU
1	A	112	ASP

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Mol	Chain	Res	Type
1	A	114	LEU
1	A	130	GLU
1	A	131	MET
1	A	132	ARG
1	A	145	GLU
1	A	166	THR
1	A	205	VAL
1	A	221	THR
1	A	231	THR
2	B	167	VAL
2	B	178	ASN
2	B	189	THR
3	C	44	LEU
3	C	76	VAL
3	C	164	ILE
3	C	180	LYS
3	C	192	LEU
3	C	218	ARG
3	C	220	ASN
4	D	5	ARG
4	D	38	ARG
4	D	41	VAL
4	D	70	CYS
4	D	99	GLU
4	D	103	THR
4	D	105	GLU
4	D	137	ASP
4	D	139	ASP
4	D	146	GLN
5	E	9	ASP
5	E	36	THR
5	E	107	MET
5	E	135	ARG
5	E	148	GLU
5	E	214	ASN
5	E	236	GLU
6	F	16	GLN
6	F	38	LEU
6	F	83	LEU
6	F	101	ARG
6	F	125	ARG
6	F	139	ASP

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Mol	Chain	Res	Type
6	F	202	GLU
6	F	239	ARG
7	G	39	ILE
7	G	41	CYS
7	G	42	LYS
7	G	125	TYR
7	G	129	ARG
7	G	144	ASP
7	G	181	MET
7	G	187	ARG
7	G	230	ASP
8	H	22	THR
8	H	43	CYS
8	H	139	VAL
8	H	150	GLU
8	H	173	VAL
9	I	6	VAL
9	I	65	LEU
9	I	68	LEU
9	I	132	LEU
9	I	187	ARG
9	I	198	ARG
10	J	20	VAL
10	J	27	ARG
10	J	33	GLN
10	J	34	MET
10	J	36	THR
10	J	37	THR
10	J	49	LEU
10	J	126	LEU
10	J	132	VAL
10	J	175	VAL
10	J	190	ILE
11	K	1	MET
11	K	27	GLN
11	K	30	ASP
11	K	45	LEU
11	K	47	VAL
11	K	102	LEU
11	K	171	PHE
12	L	8	PHE
12	L	35	ILE

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Mol	Chain	Res	Type
12	L	82	LEU
12	L	99	THR
12	L	102	CYS
12	L	138	VAL
13	M	1	ARG
13	M	12	ILE
13	M	84	THR
13	M	99	ARG
14	N	49	THR
14	N	86	ARG
14	N	94	ARG
14	N	100	ARG
14	N	126	ASP
14	N	141	TYR
14	N	168	LEU
14	N	191	THR
14	N	192	VAL
14	N	205	THR
1	O	78	CYS
1	O	108	GLU
1	O	112	ASP
1	O	114	LEU
1	O	130	GLU
1	O	132	ARG
1	O	145	GLU
1	O	166	THR
1	O	205	VAL
1	O	221	THR
1	O	231	THR
2	P	167	VAL
2	P	178	ASN
2	P	189	THR
3	Q	44	LEU
3	Q	76	VAL
3	Q	164	ILE
3	Q	180	LYS
3	Q	192	LEU
3	Q	218	ARG
3	Q	220	ASN
4	R	5	ARG
4	R	38	ARG
4	R	41	VAL

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Mol	Chain	Res	Type
4	R	46	GLU
4	R	70	CYS
4	R	99	GLU
4	R	103	THR
4	R	105	GLU
4	R	139	ASP
4	R	146	GLN
4	R	163	ARG
5	S	9	ASP
5	S	36	THR
5	S	107	MET
5	S	135	ARG
5	S	148	GLU
5	S	214	ASN
5	S	236	GLU
6	T	16	GLN
6	T	38	LEU
6	T	83	LEU
6	T	101	ARG
6	T	125	ARG
6	T	139	ASP
6	T	202	GLU
6	T	239	ARG
7	U	39	ILE
7	U	129	ARG
7	U	144	ASP
7	U	181	MET
7	U	230	ASP
8	V	22	THR
8	V	43	CYS
8	V	139	VAL
8	V	150	GLU
8	V	173	VAL
9	W	6	VAL
9	W	65	LEU
9	W	68	LEU
9	W	132	LEU
9	W	169	SER
9	W	198	ARG
10	X	20	VAL
10	X	27	ARG
10	X	33	GLN

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Mol	Chain	Res	Type
10	X	34	MET
10	X	36	THR
10	X	37	THR
10	X	49	LEU
10	X	126	LEU
10	X	132	VAL
10	X	175	VAL
10	X	190	ILE
11	Y	1	MET
11	Y	27	GLN
11	Y	30	ASP
11	Y	45	LEU
11	Y	47	VAL
11	Y	102	LEU
11	Y	171	PHE
12	Z	8	PHE
12	Z	35	ILE
12	Z	82	LEU
12	Z	87	VAL
12	Z	99	THR
12	Z	102	CYS
12	Z	138	VAL
13	1	1	ARG
13	1	12	ILE
13	1	84	THR
13	1	99	ARG
14	2	49	THR
14	2	86	ARG
14	2	94	ARG
14	2	100	ARG
14	2	126	ASP
14	2	141	TYR
14	2	168	LEU
14	2	191	THR
14	2	192	VAL
14	2	205	THR
1	c	78	CYS
1	c	108	GLU
1	c	112	ASP
1	c	114	LEU
1	c	130	GLU
1	c	132	ARG

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Mol	Chain	Res	Type
1	c	145	GLU
1	c	166	THR
1	c	205	VAL
1	c	221	THR
1	c	231	THR
2	d	167	VAL
2	d	178	ASN
2	d	189	THR
3	e	44	LEU
3	e	76	VAL
3	e	164	ILE
3	e	180	LYS
3	e	192	LEU
3	e	218	ARG
3	e	220	ASN
4	f	5	ARG
4	f	38	ARG
4	f	41	VAL
4	f	70	CYS
4	f	99	GLU
4	f	105	GLU
5	g	9	ASP
5	g	36	THR
5	g	107	MET
5	g	135	ARG
5	g	148	GLU
5	g	168	ARG
5	g	214	ASN
5	g	236	GLU
6	h	16	GLN
6	h	38	LEU
6	h	83	LEU
6	h	101	ARG
6	h	125	ARG
6	h	139	ASP
6	h	202	GLU
7	i	39	ILE
7	i	129	ARG
7	i	144	ASP
7	i	181	MET
7	i	186	CYS
7	i	187	ARG

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Mol	Chain	Res	Type
7	i	230	ASP
8	j	22	THR
8	j	43	CYS
8	j	139	VAL
8	j	150	GLU
8	j	173	VAL
9	k	31	CYS
9	k	65	LEU
9	k	68	LEU
9	k	132	LEU
9	k	198	ARG
9	k	213	THR
10	l	20	VAL
10	l	27	ARG
10	l	33	GLN
10	l	34	MET
10	l	36	THR
10	l	37	THR
10	l	49	LEU
10	l	126	LEU
10	l	132	VAL
10	l	175	VAL
10	l	190	ILE
11	m	1	MET
11	m	27	GLN
11	m	30	ASP
11	m	45	LEU
11	m	47	VAL
11	m	102	LEU
11	m	171	PHE
12	n	1	THR
12	n	8	PHE
12	n	35	ILE
12	n	82	LEU
12	n	87	VAL
12	n	99	THR
12	n	102	CYS
12	n	138	VAL
13	o	1	ARG
13	o	12	ILE
13	o	84	THR
13	o	99	ARG

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Mol	Chain	Res	Type
14	p	49	THR
14	p	86	ARG
14	p	94	ARG
14	p	100	ARG
14	p	126	ASP
14	p	141	TYR
14	p	168	LEU
14	p	191	THR
14	p	192	VAL
14	p	205	THR
1	q	78	CYS
1	q	108	GLU
1	q	112	ASP
1	q	114	LEU
1	q	130	GLU
1	q	131	MET
1	q	132	ARG
1	q	145	GLU
1	q	166	THR
1	q	205	VAL
1	q	221	THR
1	q	231	THR
2	r	167	VAL
2	r	178	ASN
2	r	189	THR
3	s	44	LEU
3	s	76	VAL
3	s	164	ILE
3	s	180	LYS
3	s	192	LEU
3	s	218	ARG
3	s	220	ASN
4	t	5	ARG
4	t	38	ARG
4	t	41	VAL
4	t	70	CYS
4	t	99	GLU
4	t	103	THR
4	t	105	GLU
4	t	146	GLN
5	u	9	ASP
5	u	36	THR

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Mol	Chain	Res	Type
5	u	107	MET
5	u	135	ARG
5	u	148	GLU
5	u	214	ASN
5	u	231	LYS
5	u	236	GLU
6	v	16	GLN
6	v	38	LEU
6	v	83	LEU
6	v	101	ARG
6	v	125	ARG
6	v	139	ASP
6	v	202	GLU
6	v	239	ARG
7	w	39	ILE
7	w	129	ARG
7	w	144	ASP
7	w	181	MET
7	w	230	ASP
8	x	22	THR
8	x	43	CYS
8	x	139	VAL
8	x	150	GLU
8	x	173	VAL
9	y	6	VAL
9	y	65	LEU
9	y	68	LEU
9	y	132	LEU
9	y	198	ARG
10	z	20	VAL
10	z	27	ARG
10	z	33	GLN
10	z	34	MET
10	z	36	THR
10	z	37	THR
10	z	49	LEU
10	z	126	LEU
10	z	132	VAL
10	z	175	VAL
10	z	190	ILE
11	0	1	MET
11	0	27	GLN

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Mol	Chain	Res	Type
11	0	30	ASP
11	0	45	LEU
11	0	47	VAL
11	0	102	LEU
11	0	171	PHE
12	3	8	PHE
12	3	35	ILE
12	3	82	LEU
12	3	99	THR
12	3	102	CYS
12	3	138	VAL
12	3	170	SER
12	3	185	ILE
13	a	1	ARG
13	a	12	ILE
13	a	84	THR
13	a	99	ARG
13	a	108	ASN
13	a	109	ILE
14	b	49	THR
14	b	86	ARG
14	b	94	ARG
14	b	100	ARG
14	b	126	ASP
14	b	141	TYR
14	b	168	LEU
14	b	191	THR
14	b	192	VAL
14	b	205	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	206	ASN
5	E	152	GLN
13	M	146	GLN
2	P	147	GLN
10	X	173	ASN
13	1	146	GLN
2	d	206	ASN
10	l	173	ASN
13	o	146	GLN

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Mol	Chain	Res	Type
13	o	152	GLN
5	u	152	GLN
10	z	173	ASN
13	a	146	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

11 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	3BV	3	301	12	53,54,54	2.38	11 (20%)	67,71,71	1.51	9 (13%)
15	3BV	H	301	8	53,54,54	2.62	11 (20%)	67,71,71	1.52	9 (13%)
15	3BV	I	301	-	53,54,54	2.67	12 (22%)	67,71,71	2.09	15 (22%)
15	3BV	L	301	-	53,54,54	2.39	12 (22%)	67,71,71	1.97	15 (22%)
15	3BV	V	301	8	53,54,54	2.37	11 (20%)	67,71,71	1.55	9 (13%)
15	3BV	W	301	-	53,54,54	2.39	11 (20%)	67,71,71	1.83	19 (28%)
15	3BV	Z	301	12	53,54,54	2.89	14 (26%)	67,71,71	2.94	22 (32%)
15	3BV	j	301	8	53,54,54	2.41	10 (18%)	67,71,71	2.32	19 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	3BV	k	301	9	53,54,54	2.52	11 (20%)	67,71,71	1.79	17 (25%)
15	3BV	n	301	12	53,54,54	2.61	10 (18%)	67,71,71	2.07	21 (31%)
15	3BV	y	301	9	53,54,54	2.71	13 (24%)	67,71,71	1.87	10 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	3BV	3	301	12	-	0/59/67/67	0/3/3/3
15	3BV	H	301	8	-	0/59/67/67	0/3/3/3
15	3BV	I	301	-	-	0/59/67/67	0/3/3/3
15	3BV	L	301	-	-	0/59/67/67	0/3/3/3
15	3BV	V	301	8	-	0/59/67/67	0/3/3/3
15	3BV	W	301	-	-	0/59/67/67	0/3/3/3
15	3BV	Z	301	12	-	0/59/67/67	0/3/3/3
15	3BV	j	301	8	-	0/59/67/67	0/3/3/3
15	3BV	k	301	9	-	0/59/67/67	0/3/3/3
15	3BV	n	301	12	-	0/59/67/67	0/3/3/3
15	3BV	y	301	9	-	0/59/67/67	0/3/3/3

All (126) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	I	301	3BV	O48-C47	-12.75	1.12	1.43
15	n	301	3BV	O48-C47	-11.82	1.14	1.43
15	Z	301	3BV	O48-C47	-10.79	1.17	1.43
15	k	301	3BV	O48-C47	-10.42	1.18	1.43
15	Z	301	3BV	C43-C42	-10.01	1.37	1.53
15	H	301	3BV	O48-C47	-9.82	1.19	1.43
15	W	301	3BV	O48-C47	-9.53	1.20	1.43
15	y	301	3BV	O48-C47	-8.93	1.21	1.43
15	L	301	3BV	O48-C47	-8.68	1.22	1.43
15	j	301	3BV	O48-C47	-8.39	1.22	1.43
15	y	301	3BV	C59-C51	-6.03	1.45	1.52
15	3	301	3BV	O48-C47	-5.55	1.29	1.43
15	V	301	3BV	O48-C47	-5.28	1.30	1.43
15	Z	301	3BV	C43-C44	-5.23	1.28	1.52
15	Z	301	3BV	O40-C39	-4.77	1.14	1.23
15	L	301	3BV	O40-C39	-4.50	1.14	1.23
15	n	301	3BV	O40-C39	-4.26	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	I	301	3BV	O40-C39	-4.25	1.15	1.23
15	L	301	3BV	O29-C28	-4.02	1.15	1.23
15	k	301	3BV	O40-C39	-3.94	1.15	1.23
15	Z	301	3BV	O29-C28	-3.73	1.16	1.23
15	n	301	3BV	C43-C42	-3.68	1.47	1.53
15	n	301	3BV	O29-C28	-3.67	1.16	1.23
15	I	301	3BV	C43-C42	-3.60	1.47	1.53
15	W	301	3BV	O40-C39	-3.58	1.16	1.23
15	I	301	3BV	O29-C28	-3.52	1.16	1.23
15	j	301	3BV	O40-C39	-3.48	1.16	1.23
15	L	301	3BV	C43-C42	-3.43	1.47	1.53
15	W	301	3BV	O29-C28	-3.43	1.16	1.23
15	W	301	3BV	C43-C42	-3.17	1.48	1.53
15	k	301	3BV	O29-C28	-3.15	1.17	1.23
15	j	301	3BV	O29-C28	-3.08	1.17	1.23
15	k	301	3BV	C43-C42	-2.90	1.48	1.53
15	Z	301	3BV	C42-N41	-2.81	1.41	1.46
15	j	301	3BV	C43-C42	-2.77	1.48	1.53
15	Z	301	3BV	C23-N22	-2.68	1.39	1.45
15	Z	301	3BV	C46-C44	-2.52	1.36	1.51
15	Z	301	3BV	C35-C34	-2.44	1.33	1.38
15	Z	301	3BV	C23-C28	-2.33	1.46	1.52
15	y	301	3BV	O40-C39	-2.31	1.18	1.23
15	3	301	3BV	O40-C39	-2.26	1.19	1.23
15	V	301	3BV	O40-C39	-2.25	1.19	1.23
15	W	301	3BV	C35-C34	-2.25	1.34	1.38
15	L	301	3BV	C23-C28	-2.25	1.46	1.52
15	H	301	3BV	O40-C39	-2.22	1.19	1.23
15	V	301	3BV	C43-C42	-2.21	1.49	1.53
15	3	301	3BV	C43-C42	-2.21	1.49	1.53
15	L	301	3BV	O21-C20	-2.16	1.19	1.23
15	H	301	3BV	C43-C42	-2.15	1.49	1.53
15	y	301	3BV	C43-C42	-2.15	1.49	1.53
15	L	301	3BV	C23-N22	-2.15	1.41	1.45
15	I	301	3BV	C23-N22	-2.12	1.41	1.45
15	3	301	3BV	O29-C28	-2.11	1.19	1.23
15	k	301	3BV	C35-C34	-2.11	1.34	1.38
15	I	301	3BV	C42-N41	-2.11	1.42	1.46
15	L	301	3BV	C42-N41	-2.10	1.42	1.46
15	H	301	3BV	O29-C28	-2.09	1.19	1.23
15	y	301	3BV	O60-C59	-2.07	1.33	1.42
15	V	301	3BV	O29-C28	-2.07	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	y	301	3BV	O29-C28	-2.06	1.19	1.23
15	n	301	3BV	C35-C34	-2.06	1.34	1.38
15	I	301	3BV	O21-C20	-2.01	1.19	1.23
15	n	301	3BV	C31-C39	2.04	1.58	1.52
15	I	301	3BV	C16-C15	2.07	1.43	1.38
15	W	301	3BV	C20-N22	2.11	1.38	1.34
15	W	301	3BV	C31-C39	2.19	1.58	1.52
15	k	301	3BV	C20-N22	2.23	1.39	1.34
15	k	301	3BV	C31-C39	2.24	1.59	1.52
15	j	301	3BV	C16-C15	2.32	1.43	1.38
15	V	301	3BV	C16-C15	2.73	1.44	1.38
15	H	301	3BV	C16-C15	2.74	1.44	1.38
15	3	301	3BV	C16-C15	2.74	1.44	1.38
15	y	301	3BV	C16-C15	2.74	1.44	1.38
15	j	301	3BV	C31-C39	2.80	1.60	1.52
15	3	301	3BV	C20-N22	3.09	1.41	1.34
15	V	301	3BV	C20-N22	3.10	1.41	1.34
15	H	301	3BV	C20-N22	3.10	1.41	1.34
15	y	301	3BV	C20-N22	3.12	1.41	1.34
15	Z	301	3BV	C28-N30	3.16	1.41	1.34
15	H	301	3BV	C31-C39	3.44	1.62	1.52
15	V	301	3BV	C31-C39	3.45	1.62	1.52
15	3	301	3BV	C31-C39	3.45	1.62	1.52
15	y	301	3BV	C31-C39	3.47	1.62	1.52
15	n	301	3BV	C28-N30	3.69	1.42	1.34
15	I	301	3BV	C28-N30	3.74	1.42	1.34
15	Z	301	3BV	C31-N30	3.82	1.54	1.45
15	L	301	3BV	C28-N30	4.17	1.43	1.34
15	W	301	3BV	C28-N30	4.23	1.43	1.34
15	n	301	3BV	C31-N30	4.50	1.56	1.45
15	j	301	3BV	C28-N30	4.50	1.44	1.34
15	I	301	3BV	C31-N30	4.54	1.56	1.45
15	k	301	3BV	C28-N30	4.55	1.44	1.34
15	Z	301	3BV	C39-N41	4.60	1.44	1.34
15	W	301	3BV	C31-N30	4.83	1.56	1.45
15	L	301	3BV	C31-N30	4.86	1.56	1.45
15	L	301	3BV	C39-N41	4.89	1.45	1.34
15	I	301	3BV	C39-N41	5.07	1.45	1.34
15	n	301	3BV	C39-N41	5.09	1.45	1.34
15	k	301	3BV	C31-N30	5.26	1.57	1.45
15	y	301	3BV	C28-N30	5.31	1.46	1.34
15	H	301	3BV	C28-N30	5.35	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	3	301	3BV	C28-N30	5.35	1.46	1.34
15	V	301	3BV	C28-N30	5.37	1.46	1.34
15	j	301	3BV	C31-N30	5.40	1.58	1.45
15	k	301	3BV	C39-N41	5.56	1.46	1.34
15	W	301	3BV	C39-N41	5.86	1.47	1.34
15	V	301	3BV	C31-N30	6.15	1.59	1.45
15	H	301	3BV	C31-N30	6.15	1.59	1.45
15	3	301	3BV	C31-N30	6.18	1.59	1.45
15	y	301	3BV	C31-N30	6.19	1.59	1.45
15	j	301	3BV	C39-N41	6.27	1.48	1.34
15	Z	301	3BV	C8-N10	6.73	1.47	1.34
15	H	301	3BV	C39-N41	7.06	1.50	1.34
15	V	301	3BV	C39-N41	7.06	1.50	1.34
15	3	301	3BV	C39-N41	7.08	1.50	1.34
15	y	301	3BV	C39-N41	7.08	1.50	1.34
15	W	301	3BV	C8-N10	7.19	1.48	1.34
15	L	301	3BV	C8-N10	7.29	1.48	1.34
15	n	301	3BV	C8-N10	7.41	1.49	1.34
15	I	301	3BV	C8-N10	7.46	1.49	1.34
15	k	301	3BV	C8-N10	8.14	1.50	1.34
15	j	301	3BV	C8-N10	8.21	1.50	1.34
15	V	301	3BV	C8-N10	8.73	1.51	1.34
15	3	301	3BV	C8-N10	8.76	1.51	1.34
15	y	301	3BV	C8-N10	8.77	1.51	1.34
15	H	301	3BV	C8-N10	8.77	1.51	1.34

All (165) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	j	301	3BV	O48-C47-C51	-9.82	90.93	109.83
15	Z	301	3BV	C58-C51-C59	-9.50	97.33	109.86
15	L	301	3BV	C58-C51-C59	-8.26	98.97	109.86
15	I	301	3BV	C58-C51-C59	-8.14	99.12	109.86
15	n	301	3BV	C58-C51-C59	-7.52	99.95	109.86
15	Z	301	3BV	C43-C42-N41	-7.46	100.11	110.15
15	Z	301	3BV	C20-C11-N10	-6.59	92.68	111.26
15	Z	301	3BV	C47-C42-N41	-6.10	98.20	110.31
15	W	301	3BV	C58-C51-C59	-5.27	102.91	109.86
15	k	301	3BV	C58-C51-C59	-4.64	103.74	109.86
15	j	301	3BV	C43-C42-N41	-4.40	104.24	110.15
15	j	301	3BV	C58-C51-C59	-4.37	104.09	109.86
15	L	301	3BV	C47-C42-N41	-4.09	102.20	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Z	301	3BV	C42-N41-C39	-3.93	115.83	123.13
15	Z	301	3BV	O48-C47-C51	-3.87	102.38	109.83
15	W	301	3BV	C47-C42-N41	-3.54	103.28	110.31
15	I	301	3BV	C47-C42-N41	-3.46	103.44	110.31
15	j	301	3BV	C20-C11-N10	-3.17	102.34	111.26
15	n	301	3BV	C39-C31-N30	-3.13	102.44	111.26
15	Z	301	3BV	C39-C31-N30	-3.07	102.62	111.26
15	n	301	3BV	O9-C8-N10	-3.02	117.88	123.01
15	W	301	3BV	O48-C47-C51	-2.99	104.08	109.83
15	3	301	3BV	C58-C51-C59	-2.93	105.99	109.86
15	Z	301	3BV	C37-C38-C33	-2.92	116.01	120.65
15	H	301	3BV	C58-C51-C59	-2.90	106.03	109.86
15	V	301	3BV	C58-C51-C59	-2.89	106.05	109.86
15	W	301	3BV	O9-C8-N10	-2.81	118.24	123.01
15	j	301	3BV	C42-N41-C39	-2.81	117.91	123.13
15	L	301	3BV	O9-C8-N10	-2.78	118.30	123.01
15	y	301	3BV	C58-C51-C59	-2.77	106.20	109.86
15	I	301	3BV	C43-C42-N41	-2.65	106.58	110.15
15	j	301	3BV	O9-C8-N10	-2.63	118.54	123.01
15	Z	301	3BV	C36-C35-C34	-2.56	116.44	120.19
15	Z	301	3BV	O9-C8-N10	-2.54	118.70	123.01
15	n	301	3BV	C42-N41-C39	-2.52	118.45	123.13
15	I	301	3BV	O9-C8-N10	-2.51	118.74	123.01
15	L	301	3BV	C42-N41-C39	-2.46	118.56	123.13
15	I	301	3BV	C39-C31-N30	-2.44	104.40	111.26
15	n	301	3BV	C20-C11-N10	-2.40	104.49	111.26
15	k	301	3BV	C47-C42-N41	-2.38	105.59	110.31
15	I	301	3BV	C42-N41-C39	-2.37	118.71	123.13
15	k	301	3BV	C12-C11-C20	-2.33	104.64	110.32
15	n	301	3BV	C47-C42-N41	-2.32	105.70	110.31
15	j	301	3BV	C39-C31-N30	-2.30	104.77	111.26
15	L	301	3BV	O1-C6-C5	-2.25	106.68	111.84
15	W	301	3BV	C20-C11-N10	-2.14	105.24	111.26
15	Z	301	3BV	C23-C28-N30	-2.07	112.01	116.78
15	n	301	3BV	C35-C34-C33	-2.07	117.36	120.65
15	H	301	3BV	O9-C8-N10	-2.05	119.54	123.01
15	3	301	3BV	O9-C8-N10	-2.04	119.55	123.01
15	I	301	3BV	C24-C23-C28	-2.03	105.32	110.60
15	n	301	3BV	C12-C11-N10	-2.03	107.01	110.87
15	y	301	3BV	O9-C8-N10	-2.02	119.58	123.01
15	V	301	3BV	O9-C8-N10	-2.01	119.59	123.01
15	I	301	3BV	C25-C24-C23	2.05	121.57	115.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	W	301	3BV	C8-C7-N4	2.08	118.44	113.20
15	n	301	3BV	C2-O1-C6	2.10	116.97	109.89
15	j	301	3BV	C2-O1-C6	2.11	116.99	109.89
15	j	301	3BV	C33-C32-C31	2.12	119.57	113.41
15	k	301	3BV	C38-C33-C34	2.12	121.53	118.13
15	W	301	3BV	C15-C14-C19	2.16	121.59	118.13
15	L	301	3BV	C15-C14-C19	2.16	121.59	118.13
15	L	301	3BV	C2-O1-C6	2.17	117.19	109.89
15	W	301	3BV	C2-C3-N4	2.19	113.44	110.12
15	k	301	3BV	C2-O1-C6	2.26	117.49	109.89
15	k	301	3BV	C15-C14-C19	2.29	121.80	118.13
15	L	301	3BV	C8-C7-N4	2.29	118.98	113.20
15	W	301	3BV	C58-C51-C47	2.33	115.97	111.42
15	W	301	3BV	C32-C31-C39	2.36	117.07	110.20
15	n	301	3BV	C38-C33-C34	2.40	121.97	118.13
15	n	301	3BV	C15-C14-C19	2.41	121.99	118.13
15	L	301	3BV	C32-C31-C39	2.45	117.33	110.20
15	W	301	3BV	C7-N4-C3	2.46	114.70	111.07
15	W	301	3BV	C13-C12-C11	2.46	120.65	113.12
15	I	301	3BV	C32-C31-C39	2.49	117.44	110.20
15	n	301	3BV	C32-C31-C39	2.49	117.44	110.20
15	Z	301	3BV	C7-C8-N10	2.49	119.96	115.04
15	n	301	3BV	C7-N4-C3	2.50	114.77	111.07
15	j	301	3BV	C7-C8-N10	2.52	120.02	115.04
15	k	301	3BV	C13-C12-C11	2.56	120.95	113.12
15	3	301	3BV	C7-C8-N10	2.56	120.11	115.04
15	V	301	3BV	C7-C8-N10	2.56	120.11	115.04
15	H	301	3BV	C7-C8-N10	2.57	120.11	115.04
15	y	301	3BV	C7-C8-N10	2.57	120.12	115.04
15	W	301	3BV	C11-C20-N22	2.58	122.73	116.78
15	k	301	3BV	C23-N22-C20	2.58	127.41	121.62
15	3	301	3BV	C8-C7-N4	2.61	119.78	113.20
15	y	301	3BV	C8-C7-N4	2.62	119.80	113.20
15	V	301	3BV	C8-C7-N4	2.62	119.80	113.20
15	H	301	3BV	C8-C7-N4	2.62	119.81	113.20
15	j	301	3BV	C44-C43-C42	2.64	121.34	115.51
15	j	301	3BV	C3-N4-C5	2.65	114.65	108.90
15	Z	301	3BV	C58-C51-C47	2.66	116.60	111.42
15	Z	301	3BV	C2-O1-C6	2.66	118.86	109.89
15	L	301	3BV	C38-C33-C34	2.68	122.42	118.13
15	j	301	3BV	C7-N4-C3	2.68	115.02	111.07
15	n	301	3BV	C8-C7-N4	2.69	119.98	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	I	301	3BV	O60-C59-C51	2.70	117.06	111.34
15	W	301	3BV	C7-C8-N10	2.80	120.57	115.04
15	j	301	3BV	C24-C23-N22	2.83	117.56	110.49
15	k	301	3BV	C32-C31-C39	2.85	118.50	110.20
15	Z	301	3BV	C13-C12-C11	2.88	121.91	113.12
15	I	301	3BV	C7-C8-N10	2.93	120.83	115.04
15	W	301	3BV	C38-C33-C34	2.94	122.84	118.13
15	L	301	3BV	C7-N4-C3	2.94	115.42	111.07
15	3	301	3BV	O60-C59-C51	2.98	117.65	111.34
15	n	301	3BV	C58-C51-C47	2.98	117.23	111.42
15	V	301	3BV	O60-C59-C51	2.99	117.67	111.34
15	H	301	3BV	O60-C59-C51	3.00	117.68	111.34
15	j	301	3BV	C32-C31-N30	3.03	117.14	110.80
15	k	301	3BV	C44-C43-C42	3.13	122.42	115.51
15	3	301	3BV	C3-N4-C5	3.14	115.69	108.90
15	y	301	3BV	C3-N4-C5	3.15	115.73	108.90
15	H	301	3BV	C3-N4-C5	3.16	115.75	108.90
15	Z	301	3BV	C38-C33-C34	3.18	123.23	118.13
15	k	301	3BV	O60-C59-C51	3.19	118.10	111.34
15	W	301	3BV	C7-N4-C5	3.20	115.79	111.07
15	y	301	3BV	O60-C59-C51	3.22	118.15	111.34
15	Z	301	3BV	C7-N4-C3	3.22	115.82	111.07
15	W	301	3BV	O60-C59-C51	3.23	118.18	111.34
15	k	301	3BV	C8-C7-N4	3.25	121.40	113.20
15	Z	301	3BV	O60-C59-C51	3.31	118.36	111.34
15	k	301	3BV	C7-N4-C3	3.32	115.97	111.07
15	k	301	3BV	C7-C8-N10	3.36	121.68	115.04
15	Z	301	3BV	C3-N4-C5	3.38	116.21	108.90
15	j	301	3BV	O60-C59-C51	3.46	118.67	111.34
15	k	301	3BV	C3-N4-C5	3.54	116.57	108.90
15	L	301	3BV	O60-C59-C51	3.57	118.89	111.34
15	W	301	3BV	C3-N4-C5	3.68	116.87	108.90
15	n	301	3BV	O60-C59-C51	3.69	119.15	111.34
15	W	301	3BV	C12-C11-C20	3.74	119.42	110.32
15	n	301	3BV	C24-C23-C28	3.81	120.53	110.60
15	k	301	3BV	C7-N4-C5	3.82	116.72	111.07
15	k	301	3BV	O48-C47-C51	3.84	117.23	109.83
15	n	301	3BV	C7-C8-N10	3.87	122.69	115.04
15	H	301	3BV	C32-C31-C39	4.02	121.90	110.20
15	L	301	3BV	C3-N4-C5	4.03	117.62	108.90
15	y	301	3BV	C32-C31-C39	4.03	121.94	110.20
15	V	301	3BV	C32-C31-C39	4.03	121.94	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	3	301	3BV	C32-C31-C39	4.04	121.96	110.20
15	V	301	3BV	O48-C47-C51	4.07	117.66	109.83
15	n	301	3BV	C7-N4-C5	4.10	117.13	111.07
15	n	301	3BV	C24-C23-N22	4.16	120.88	110.49
15	y	301	3BV	C7-N4-C3	4.17	117.23	111.07
15	I	301	3BV	C3-N4-C5	4.17	117.93	108.90
15	H	301	3BV	C7-N4-C3	4.18	117.25	111.07
15	V	301	3BV	C7-N4-C3	4.19	117.26	111.07
15	3	301	3BV	C7-N4-C3	4.19	117.26	111.07
15	n	301	3BV	C3-N4-C5	4.31	118.23	108.90
15	L	301	3BV	C7-C8-N10	4.33	123.59	115.04
15	j	301	3BV	C8-C7-N4	4.39	124.28	113.20
15	I	301	3BV	C7-N4-C3	4.42	117.60	111.07
15	L	301	3BV	C7-N4-C5	4.67	117.98	111.07
15	j	301	3BV	C32-C31-C39	4.77	124.08	110.20
15	I	301	3BV	C7-N4-C5	4.91	118.33	111.07
15	H	301	3BV	C7-N4-C5	5.39	119.04	111.07
15	y	301	3BV	C7-N4-C5	5.41	119.06	111.07
15	V	301	3BV	C7-N4-C5	5.41	119.07	111.07
15	3	301	3BV	C7-N4-C5	5.42	119.08	111.07
15	Z	301	3BV	C7-N4-C5	6.02	119.96	111.07
15	j	301	3BV	C7-N4-C5	6.29	120.36	111.07
15	I	301	3BV	O48-C47-C51	7.21	123.72	109.83
15	Z	301	3BV	C46-C44-C43	7.46	138.80	111.11
15	y	301	3BV	O48-C47-C51	9.02	127.20	109.83
15	Z	301	3BV	C44-C43-C42	9.46	136.42	115.51

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 98 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	3	301	3BV	8	0
15	H	301	3BV	15	0
15	I	301	3BV	12	0
15	L	301	3BV	6	0
15	V	301	3BV	23	0
15	W	301	3BV	25	0
15	Z	301	3BV	9	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	244/244 (100%)	0.04	6 (2%) 61 55	48, 84, 133, 170	0
1	O	244/244 (100%)	0.02	5 (2%) 68 64	48, 80, 118, 153	0
1	c	244/244 (100%)	-0.00	7 (2%) 55 49	52, 89, 131, 180	0
1	q	244/244 (100%)	0.05	4 (1%) 74 72	55, 87, 130, 178	0
2	B	233/233 (100%)	-0.02	5 (2%) 67 62	48, 72, 123, 252	0
2	P	233/233 (100%)	-0.05	7 (3%) 54 47	47, 77, 121, 237	0
2	d	233/233 (100%)	-0.14	5 (2%) 67 62	46, 77, 120, 234	0
2	r	233/233 (100%)	-0.02	5 (2%) 67 62	50, 76, 119, 248	0
3	C	250/250 (100%)	-0.09	9 (3%) 46 38	50, 79, 135, 232	0
3	Q	250/250 (100%)	0.06	9 (3%) 46 38	48, 77, 127, 221	0
3	e	250/250 (100%)	0.00	7 (2%) 56 50	32, 77, 124, 193	0
3	s	250/250 (100%)	0.18	13 (5%) 31 24	55, 86, 152, 251	0
4	D	243/243 (100%)	0.12	12 (4%) 33 27	53, 94, 180, 223	0
4	R	243/243 (100%)	0.17	11 (4%) 37 31	42, 86, 174, 239	0
4	f	243/243 (100%)	0.08	8 (3%) 50 42	51, 91, 162, 233	0
4	t	243/243 (100%)	0.18	16 (6%) 22 16	54, 95, 184, 221	0
5	E	234/234 (100%)	-0.18	4 (1%) 73 70	49, 83, 118, 173	0
5	S	234/234 (100%)	-0.03	4 (1%) 73 70	50, 86, 127, 169	0
5	g	234/234 (100%)	-0.07	0 100 100	49, 88, 127, 163	0
5	u	234/234 (100%)	-0.08	2 (0%) 85 84	59, 87, 126, 164	0
6	F	238/238 (100%)	-0.11	5 (2%) 67 62	46, 73, 125, 231	0
6	T	238/238 (100%)	0.11	10 (4%) 40 33	46, 81, 135, 205	0
6	h	238/238 (100%)	0.20	10 (4%) 40 33	48, 83, 135, 225	0
6	v	238/238 (100%)	0.03	6 (2%) 61 55	53, 80, 135, 208	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
7	G	245/245 (100%)	0.10	8 (3%)	50	42	48, 82, 133, 254	0
7	U	245/245 (100%)	0.07	8 (3%)	50	42	44, 83, 139, 261	0
7	i	245/245 (100%)	0.10	11 (4%)	37	31	57, 87, 133, 235	0
7	w	245/245 (100%)	0.28	12 (4%)	33	27	57, 87, 131, 274	0
8	H	202/202 (100%)	-0.13	5 (2%)	61	55	43, 65, 114, 206	0
8	V	202/202 (100%)	-0.22	1 (0%)	91	90	46, 69, 111, 177	0
8	j	202/202 (100%)	-0.02	6 (2%)	54	47	48, 74, 116, 186	0
8	x	202/202 (100%)	-0.04	5 (2%)	61	55	43, 72, 115, 193	0
9	I	220/220 (100%)	-0.38	1 (0%)	91	90	44, 61, 92, 139	0
9	W	220/220 (100%)	-0.20	0	100	100	40, 63, 98, 134	0
9	k	220/220 (100%)	-0.15	2 (0%)	85	84	45, 65, 98, 126	0
9	y	220/220 (100%)	-0.21	1 (0%)	91	90	45, 69, 99, 139	0
10	J	204/204 (100%)	-0.22	0	100	100	42, 64, 93, 156	0
10	X	204/204 (100%)	-0.13	2 (0%)	84	82	41, 64, 99, 150	0
10	l	204/204 (100%)	-0.24	2 (0%)	84	82	42, 66, 90, 143	0
10	z	204/204 (100%)	-0.27	1 (0%)	91	90	42, 68, 93, 148	0
11	0	199/199 (100%)	-0.24	4 (2%)	68	64	50, 71, 111, 201	0
11	K	199/199 (100%)	-0.24	3 (1%)	76	74	50, 70, 106, 194	0
11	Y	199/199 (100%)	-0.18	4 (2%)	68	64	40, 70, 102, 218	0
11	m	199/199 (100%)	-0.26	4 (2%)	68	64	41, 71, 100, 184	0
12	3	201/201 (100%)	-0.12	1 (0%)	91	90	38, 68, 103, 134	0
12	L	201/201 (100%)	-0.14	1 (0%)	91	90	45, 67, 106, 158	0
12	Z	201/201 (100%)	-0.13	1 (0%)	91	90	45, 68, 98, 164	0
12	n	201/201 (100%)	-0.09	3 (1%)	76	74	44, 69, 97, 158	0
13	1	213/213 (100%)	-0.25	3 (1%)	78	76	38, 60, 94, 181	0
13	M	213/213 (100%)	-0.34	2 (0%)	85	84	37, 58, 91, 180	0
13	a	213/213 (100%)	-0.27	1 (0%)	91	90	41, 63, 98, 161	0
13	o	213/213 (100%)	-0.14	2 (0%)	85	84	37, 67, 98, 145	0
14	2	217/217 (100%)	-0.30	3 (1%)	78	76	36, 63, 100, 177	0
14	N	217/217 (100%)	-0.24	2 (0%)	85	84	39, 62, 102, 159	0
14	b	217/217 (100%)	-0.20	2 (0%)	85	84	45, 68, 104, 189	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
14	p	217/217 (100%)	-0.09	3 (1%) 78 76	45, 70, 99, 172	0
All	All	12572/12572 (100%)	-0.07	274 (2%) 65 60	32, 75, 126, 274	0

All (274) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	Y	199	GLN	20.6
7	w	1	SER	18.8
2	B	233	ALA	17.9
2	P	233	ALA	15.4
2	B	232	ILE	14.7
7	G	2	SER	13.2
7	w	2	SER	12.8
4	R	244	GLN	12.8
3	s	249	ARG	12.2
2	r	233	ALA	12.1
3	s	247	ALA	11.9
3	s	250	GLU	11.4
11	m	199	GLN	11.2
2	r	232	ILE	10.8
3	s	251	LYS	10.8
7	U	2	SER	10.6
11	0	199	GLN	10.5
11	K	199	GLN	10.0
7	G	1	SER	9.7
4	D	244	GLN	9.7
7	w	3	ILE	9.3
3	Q	204	SER	8.5
14	p	217	GLY	8.2
14	b	217	GLY	8.2
6	v	241	GLN	7.7
3	s	248	GLU	7.5
14	2	217	GLY	7.2
7	i	1	SER	6.8
4	f	242	LYS	6.8
6	h	241	GLN	6.7
11	0	198	LYS	6.7
8	j	202	LEU	6.5
8	x	201	THR	6.4
4	R	243	LYS	6.3
2	d	232	ILE	6.3
2	d	233	ALA	6.1

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Mol	Chain	Res	Type	RSRZ
4	t	243	LYS	6.1
7	i	2	SER	6.1
4	t	244	GLN	5.8
4	f	241	LYS	5.7
7	U	5	THR	5.7
8	x	202	LEU	5.7
2	P	232	ILE	5.7
4	t	240	GLU	5.6
8	V	202	LEU	5.5
7	U	1	SER	5.3
3	e	204	SER	5.3
3	s	243	GLU	5.3
4	t	239	ASN	5.2
11	K	198	LYS	5.1
4	t	242	LYS	5.1
3	Q	205	LYS	5.0
8	j	200	ALA	5.0
6	T	241	GLN	4.9
4	D	243	LYS	4.9
10	X	114	PRO	4.8
3	s	244	GLU	4.8
7	i	3	ILE	4.8
6	h	201	ALA	4.7
4	D	52	LYS	4.7
11	m	198	LYS	4.6
7	G	3	ILE	4.6
8	j	201	THR	4.6
11	0	197	PRO	4.6
14	p	216	SER	4.6
5	E	241	ILE	4.5
2	B	2	GLU	4.5
6	v	240	PRO	4.4
3	e	203	VAL	4.4
4	R	240	GLU	4.4
3	Q	203	VAL	4.3
4	D	50	VAL	4.3
13	M	1	ARG	4.3
8	H	201	THR	4.3
4	D	49	SER	4.2
12	L	201	GLY	4.2
7	i	5	THR	4.1
10	X	115	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
4	f	237	GLU	4.1
4	D	200	GLN	4.1
3	C	205	LYS	4.0
4	t	201	SER	4.0
8	x	198	ALA	3.9
6	F	241	GLN	3.9
11	m	197	PRO	3.8
5	u	241	ILE	3.8
4	t	52	LYS	3.8
12	n	200	SER	3.8
2	P	2	GLU	3.7
6	F	239	ARG	3.7
8	H	198	ALA	3.7
10	l	115	LYS	3.7
1	O	57	PRO	3.6
4	R	241	LYS	3.6
13	a	1	ARG	3.6
4	f	219	ILE	3.6
2	r	2	GLU	3.6
8	x	200	ALA	3.6
4	R	38	ARG	3.5
12	n	199	TYR	3.5
6	T	240	PRO	3.4
2	d	3	ARG	3.4
7	U	241	GLU	3.4
3	s	246	LYS	3.4
7	w	243	LEU	3.4
3	s	245	ALA	3.4
5	E	186	HIS	3.4
5	S	240	ASP	3.3
4	D	47	LYS	3.3
1	q	208	ILE	3.3
6	h	200	PRO	3.3
14	2	216	SER	3.3
4	f	239	ASN	3.3
1	A	212	PRO	3.3
7	i	4	GLY	3.3
4	f	220	LEU	3.3
7	w	5	THR	3.2
6	T	202	GLU	3.2
12	3	201	GLY	3.2
3	Q	202	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
14	b	216	SER	3.1
4	t	200	GLN	3.1
7	G	198	TYR	3.1
8	H	199	VAL	3.1
6	T	234	GLU	3.1
1	c	210	PHE	3.1
6	h	204	ASP	3.1
7	w	239	ALA	3.1
14	2	215	ILE	3.1
7	U	3	ILE	3.0
4	D	239	ASN	3.0
12	n	201	GLY	3.0
3	e	220	ASN	3.0
7	G	199	ILE	3.0
8	x	199	VAL	3.0
5	S	241	ILE	3.0
7	i	229	LYS	2.9
7	w	4	GLY	2.9
3	e	202	ASP	2.9
1	c	57	PRO	2.8
3	C	181	GLU	2.8
4	D	201	SER	2.8
11	K	197	PRO	2.8
4	D	240	GLU	2.8
11	Y	198	LYS	2.8
9	y	201	ARG	2.8
3	s	202	ASP	2.8
3	C	251	LYS	2.8
7	G	244	LYS	2.8
13	l	160	ASN	2.7
4	t	38	ARG	2.7
4	t	241	LYS	2.7
6	v	174	ARG	2.7
3	C	202	ASP	2.7
2	P	1	ALA	2.7
2	d	1	ALA	2.7
7	w	245	GLU	2.7
14	N	216	SER	2.7
6	h	233	LEU	2.7
4	D	237	GLU	2.7
6	T	239	ARG	2.7
8	j	198	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	c	211	LYS	2.7
5	S	200	ILE	2.7
2	d	2	GLU	2.7
6	T	189	LYS	2.6
5	S	238	ILE	2.6
7	G	5	THR	2.6
14	p	119	GLU	2.6
5	E	130	PRO	2.6
9	k	201	ARG	2.6
3	Q	19	TYR	2.6
1	q	232	GLU	2.6
3	Q	233	VAL	2.6
8	j	199	VAL	2.6
3	e	205	LYS	2.6
2	B	1	ALA	2.6
7	w	204	VAL	2.6
6	h	240	PRO	2.6
1	A	211	LYS	2.6
3	s	199	LYS	2.6
1	A	204	THR	2.6
6	F	5	GLN	2.6
7	G	245	GLU	2.5
6	v	233	LEU	2.5
2	r	198	PHE	2.5
4	t	237	GLU	2.5
6	F	193	ARG	2.5
8	H	192	ASP	2.5
2	P	206	ASN	2.5
1	c	159	TYR	2.5
1	c	232	GLU	2.5
6	h	202	GLU	2.5
9	I	201	ARG	2.4
4	R	201	SER	2.4
11	m	110	HIS	2.4
4	D	214	ASP	2.4
1	A	2	SER	2.4
4	R	52	LYS	2.4
3	e	206	LEU	2.4
1	O	5	SER	2.4
3	C	204	SER	2.4
5	E	213	THR	2.4
1	q	245	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	5	SER	2.4
1	O	177	SER	2.3
6	T	236	LEU	2.3
4	t	238	GLU	2.3
6	T	174	ARG	2.3
7	i	230	ASP	2.3
3	e	235	GLN	2.3
3	Q	249	ARG	2.3
6	F	240	PRO	2.3
2	r	1	ALA	2.3
12	Z	197	GLU	2.3
6	v	234	GLU	2.3
7	i	243	LEU	2.3
6	T	41	LYS	2.3
7	i	219	LEU	2.3
7	U	237	LYS	2.3
10	l	114	PRO	2.3
9	k	196	GLY	2.3
7	w	7	TYR	2.3
10	z	117	PHE	2.3
4	f	202	GLY	2.3
4	t	139	ASP	2.2
7	i	233	GLU	2.2
1	A	185	LYS	2.2
4	R	48	LYS	2.2
7	U	204	VAL	2.2
4	t	179	GLU	2.2
11	Y	197	PRO	2.2
4	R	136	PHE	2.2
6	v	202	GLU	2.2
13	l	48	ASP	2.2
1	q	212	PRO	2.2
1	c	208	ILE	2.2
13	M	162	GLU	2.2
2	P	188	HIS	2.2
4	f	100	ASP	2.2
3	Q	250	GLU	2.2
7	i	52	LEU	2.2
3	C	250	GLU	2.1
4	R	46	GLU	2.1
8	j	139	VAL	2.1
3	C	247	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
13	o	1	ARG	2.1
13	l	162	GLU	2.1
4	t	202	GLY	2.1
7	U	56	LYS	2.1
5	u	207	GLU	2.1
13	o	116	GLU	2.1
2	P	203	THR	2.1
7	w	56	LYS	2.1
14	N	217	GLY	2.1
3	C	186	LEU	2.1
6	T	233	LEU	2.1
1	c	243	ALA	2.1
3	Q	220	ASN	2.1
2	B	15	SER	2.1
7	w	230	ASP	2.1
4	t	47	LYS	2.0
3	C	244	GLU	2.0
3	s	233	VAL	2.0
6	h	73	SER	2.0
6	h	60	GLN	2.0
6	h	78	THR	2.0
8	H	202	LEU	2.0
1	O	4	GLY	2.0
1	O	241	ALA	2.0
3	s	204	SER	2.0
11	Y	110	HIS	2.0
4	R	239	ASN	2.0
11	0	196	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
15	3BV	V	301	52/52	0.76	0.40	10.02	67,120,158,160	0
15	3BV	H	301	52/52	0.70	0.47	9.21	55,115,155,162	0
15	3BV	j	301	52/52	0.80	0.36	4.93	43,141,173,181	0
15	3BV	y	301	52/52	0.89	0.27	2.64	55,81,141,146	0
15	3BV	3	301	52/52	0.85	0.27	2.21	42,72,95,102	0
15	3BV	I	301	52/52	0.91	0.24	2.19	51,80,119,132	0
15	3BV	k	301	52/52	0.91	0.24	2.09	39,88,123,130	0
15	3BV	Z	301	52/52	0.90	0.23	1.78	45,62,91,103	0
15	3BV	W	301	52/52	0.91	0.24	1.76	44,78,127,140	0
15	3BV	n	301	52/52	0.88	0.23	1.40	41,72,103,124	0
15	3BV	L	301	52/52	0.92	0.19	0.90	33,63,97,106	0

6.5 Other polymers

There are no such residues in this entry.