



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:32 AM UTC

PDB ID : 3UNB / pdb_00003unb
Title : Mouse constitutive 20S proteasome in complex with PR-957
Authors : Huber, E.; Basler, M.; Schwab, R.; Heinemeyer, W.; Kirk, C.; Groettrup, M.; Groll, M.
Deposited on : 2011-11-15
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

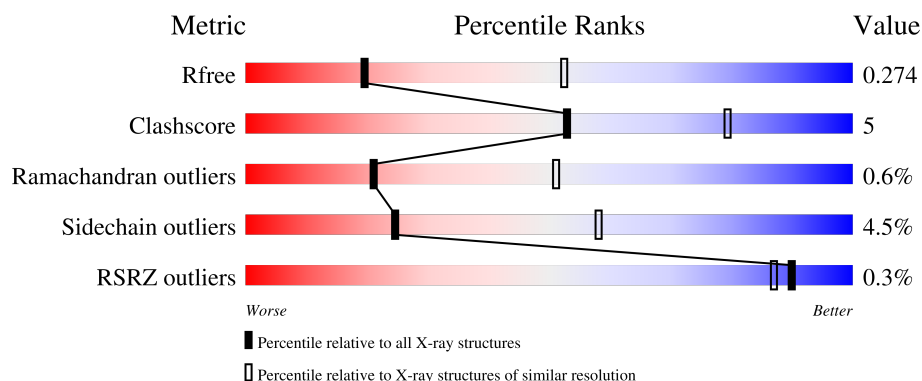
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	234	
1	O	234	
1	c	234	
1	q	234	
2	B	261	

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Mol	Chain	Length	Quality of chain
2	P	261	 83% 11% • 5%
2	d	261	 80% 14% • 5%
2	r	261	 80% 15% • 5%
3	C	248	 80% 15% • •
3	Q	248	 81% 14% • •
3	e	248	 81% 14% • •
3	s	248	 79% 16% • •
4	D	241	 83% 13% •
4	R	241	 79% 17% • •
4	f	241	 84% 12% •
4	t	241	 79% 16% • •
5	E	263	 73% 16% • 10%
5	S	263	 71% 18% • 10%
5	g	263	 73% 14% • 10%
5	u	263	 75% 15% 10%
6	F	255	 80% 14% • •
6	T	255	 81% 15% •
6	h	255	 79% 15% • •
6	v	255	 79% 16% •
7	G	246	 85% 12% • •
7	U	246	 86% 12% • •
7	i	246	 86% 11% • •
7	w	246	 82% 15% • •
8	H	234	 76% 16% • 6%
8	V	234	 80% 13% • 6%

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Mol	Chain	Length	Quality of chain
8	j	234	 3% 73% 18% 6%
8	x	234	 77% 15% 6%
9	I	205	 85% 14%
9	W	205	 87% 12%
9	k	205	 78% 20%
9	y	205	 2% 77% 21%
10	J	201	 84% 13%
10	X	201	 86% 10%
10	l	201	 84% 12%
10	z	201	 83% 12%
11	1	205	 81% 17%
11	K	205	 84% 13%
11	Y	205	 83% 14%
11	m	205	 86% 11%
12	2	213	 86% 13%
12	L	213	 91% 8%
12	Z	213	 88% 11%
12	n	213	 88% 11%
13	3	219	 81% 16%
13	M	219	 88% 10%
13	a	219	 88% 10%
13	o	219	 87% 11%
14	4	205	 91% 7%
14	N	205	 88% 9%
14	b	205	 89% 9%

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Mol	Chain	Length	Quality of chain
14	p	205	 88% 8% ..

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 99236 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-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	0	0
			1806	1153	309	338	6			
1	O	231	Total	C	N	O	S	0	0	0
			1806	1153	309	338	6			
1	c	231	Total	C	N	O	S	0	0	0
			1806	1153	309	338	6			
1	q	231	Total	C	N	O	S	0	0	0
			1806	1153	309	338	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	LYS	GLU	conflict	UNP P49722
O	2	LYS	GLU	conflict	UNP P49722
c	2	LYS	GLU	conflict	UNP P49722
q	2	LYS	GLU	conflict	UNP P49722

- Molecule 2 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	248	Total	C	N	O	S	0	0	0
			1950	1232	335	373	10			
2	P	248	Total	C	N	O	S	0	0	0
			1950	1232	335	373	10			
2	d	248	Total	C	N	O	S	0	0	0
			1950	1232	335	373	10			
2	r	248	Total	C	N	O	S	0	0	0
			1950	1232	335	373	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	239	Total 1881	C 1182	N 332	O 362	S 5	0	0	0
3	Q	239	Total 1881	C 1182	N 332	O 362	S 5	0	0	0
3	e	239	Total 1881	C 1182	N 332	O 362	S 5	0	0	0
3	s	239	Total 1881	C 1182	N 332	O 362	S 5	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	45	ALA	GLU	conflict	UNP Q9Z2U0
Q	45	ALA	GLU	conflict	UNP Q9Z2U0
e	45	ALA	GLU	conflict	UNP Q9Z2U0
s	45	ALA	GLU	conflict	UNP Q9Z2U0

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	233	Total 1778	C 1116	N 294	O 357	S 11	0	0	0
4	R	233	Total 1778	C 1116	N 294	O 357	S 11	0	0	0
4	f	233	Total 1778	C 1116	N 294	O 357	S 11	0	0	0
4	t	233	Total 1778	C 1116	N 294	O 357	S 11	0	0	0

- Molecule 5 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	238	Total 1872	C 1171	N 336	O 354	S 11	0	0	0
5	S	238	Total 1872	C 1171	N 336	O 354	S 11	0	0	0
5	g	238	Total 1872	C 1171	N 336	O 354	S 11	0	0	0
5	u	238	Total 1872	C 1171	N 336	O 354	S 11	0	0	0

- Molecule 6 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	244	Total	C	N	O	S	0	0	0
			1903	1206	325	361	11			
6	T	244	Total	C	N	O	S	0	0	0
			1903	1206	325	361	11			
6	h	244	Total	C	N	O	S	0	0	0
			1903	1206	325	361	11			
6	v	244	Total	C	N	O	S	0	0	0
			1903	1206	325	361	11			

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	243	Total	C	N	O	S	0	0	0
			1890	1199	315	363	13			
7	U	243	Total	C	N	O	S	0	0	0
			1890	1199	315	363	13			
7	i	243	Total	C	N	O	S	0	0	0
			1890	1199	315	363	13			
7	w	243	Total	C	N	O	S	0	0	0
			1890	1199	315	363	13			

- Molecule 8 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	220	Total	C	N	O	S	0	0	0
			1656	1044	282	318	12			
8	V	220	Total	C	N	O	S	0	0	0
			1656	1044	282	318	12			
8	j	220	Total	C	N	O	S	0	0	0
			1656	1044	282	318	12			
8	x	220	Total	C	N	O	S	0	0	0
			1656	1044	282	318	12			

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	204	Total	C	N	O	S	0	0	0
			1592	1013	265	295	19			
9	W	204	Total	C	N	O	S	0	0	0
			1592	1013	265	295	19			
9	k	204	Total	C	N	O	S	0	0	0
			1592	1013	265	295	19			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	y	204	Total	C	N	O	S	0	0	0
			1592	1013	265	295	19			

- Molecule 10 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	196	Total	C	N	O	S	0	0	0
			1570	1006	267	288	9			
10	X	196	Total	C	N	O	S	0	0	0
			1570	1006	267	288	9			
10	l	196	Total	C	N	O	S	0	0	0
			1570	1006	267	288	9			
10	z	196	Total	C	N	O	S	0	0	0
			1570	1006	267	288	9			

- Molecule 11 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	201	Total	C	N	O	S	0	0	0
			1557	983	271	294	9			
11	Y	201	Total	C	N	O	S	0	0	0
			1557	983	271	294	9			
11	m	201	Total	C	N	O	S	0	0	0
			1557	983	271	294	9			
11	1	201	Total	C	N	O	S	0	0	0
			1557	983	271	294	9			

- Molecule 12 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	213	Total	C	N	O	S	0	0	0
			1654	1047	284	313	10			
12	Z	213	Total	C	N	O	S	0	0	0
			1654	1047	284	313	10			
12	n	213	Total	C	N	O	S	0	0	0
			1654	1047	284	313	10			
12	2	213	Total	C	N	O	S	0	0	0
			1654	1047	284	313	10			

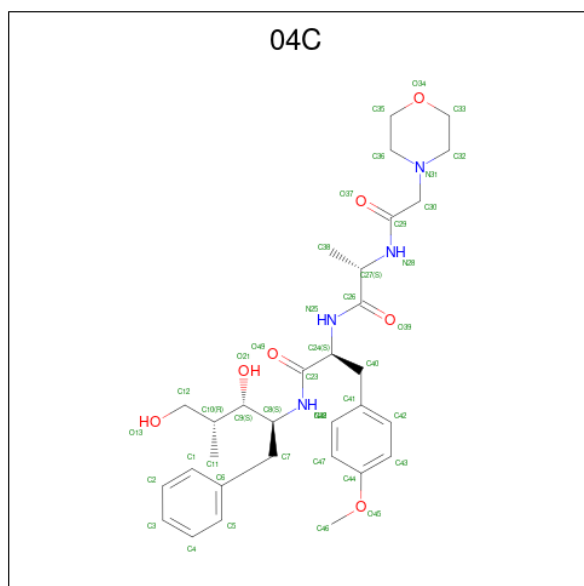
- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	216	Total	C	N	O	S	0	0	0
			1685	1063	291	319	12			
13	a	216	Total	C	N	O	S	0	0	0
			1685	1063	291	319	12			
13	o	216	Total	C	N	O	S	0	0	0
			1685	1063	291	319	12			
13	3	216	Total	C	N	O	S	0	0	0
			1685	1063	291	319	12			

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	202	Total	C	N	O	S	0	0	0
			1519	952	259	296	12			
14	b	202	Total	C	N	O	S	0	0	0
			1519	952	259	296	12			
14	p	202	Total	C	N	O	S	0	0	0
			1519	952	259	296	12			
14	4	202	Total	C	N	O	S	0	0	0
			1519	952	259	296	12			

- Molecule 15 is 1,2,4-trideoxy-4-methyl-2-{[N-(morpholin-4-ylacetyl)-L-alanyl-O-methyl-L-tyrosyl]amino}-1-phenyl-D-xylitol (CCD ID: 04C) (formula: C₃₁H₄₄N₄O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	H	1	Total	C	N	O	0	0
			42	31	4	7		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	K	1	Total	C	N	O	0	0
			42	31	4	7		
15	N	1	Total	C	N	O	0	0
			42	31	4	7		
15	V	1	Total	C	N	O	0	0
			42	31	4	7		
15	Y	1	Total	C	N	O	0	0
			42	31	4	7		
15	b	1	Total	C	N	O	0	0
			42	31	4	7		
15	j	1	Total	C	N	O	0	0
			42	31	4	7		
15	m	1	Total	C	N	O	0	0
			42	31	4	7		
15	p	1	Total	C	N	O	0	0
			42	31	4	7		
15	x	1	Total	C	N	O	0	0
			42	31	4	7		
15	1	1	Total	C	N	O	0	0
			42	31	4	7		
15	4	1	Total	C	N	O	0	0
			42	31	4	7		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	19	Total	O	0	0
			19	19		
16	B	24	Total	O	0	0
			24	24		
16	C	13	Total	O	0	0
			13	13		
16	D	16	Total	O	0	0
			16	16		
16	E	21	Total	O	0	0
			21	21		
16	F	20	Total	O	0	0
			20	20		
16	G	22	Total	O	0	0
			22	22		
16	H	31	Total	O	0	0
			31	31		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	I	32	Total O 32 32	0	0
16	J	25	Total O 25 25	0	0
16	K	28	Total O 28 28	0	0
16	L	23	Total O 23 23	0	0
16	M	27	Total O 27 27	0	0
16	N	33	Total O 33 33	0	0
16	O	33	Total O 33 33	0	0
16	P	38	Total O 38 38	0	0
16	Q	16	Total O 16 16	0	0
16	R	19	Total O 19 19	0	0
16	S	25	Total O 25 25	0	0
16	T	25	Total O 25 25	0	0
16	U	37	Total O 37 37	0	0
16	V	35	Total O 35 35	0	0
16	W	37	Total O 37 37	0	0
16	X	33	Total O 33 33	0	0
16	Y	16	Total O 16 16	0	0
16	Z	32	Total O 32 32	0	0
16	a	33	Total O 33 33	0	0
16	b	40	Total O 40 40	0	0
16	c	21	Total O 21 21	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	d	19	Total O 19 19	0	0
16	e	14	Total O 14 14	0	0
16	f	13	Total O 13 13	0	0
16	g	15	Total O 15 15	0	0
16	h	19	Total O 19 19	0	0
16	i	29	Total O 29 29	0	0
16	j	25	Total O 25 25	0	0
16	k	30	Total O 30 30	0	0
16	l	22	Total O 22 22	0	0
16	m	20	Total O 20 20	0	0
16	n	29	Total O 29 29	0	0
16	o	27	Total O 27 27	0	0
16	p	32	Total O 32 32	0	0
16	q	26	Total O 26 26	0	0
16	r	34	Total O 34 34	0	0
16	s	19	Total O 19 19	0	0
16	t	17	Total O 17 17	0	0
16	u	27	Total O 27 27	0	0
16	v	31	Total O 31 31	0	0
16	w	27	Total O 27 27	0	0
16	x	34	Total O 34 34	0	0

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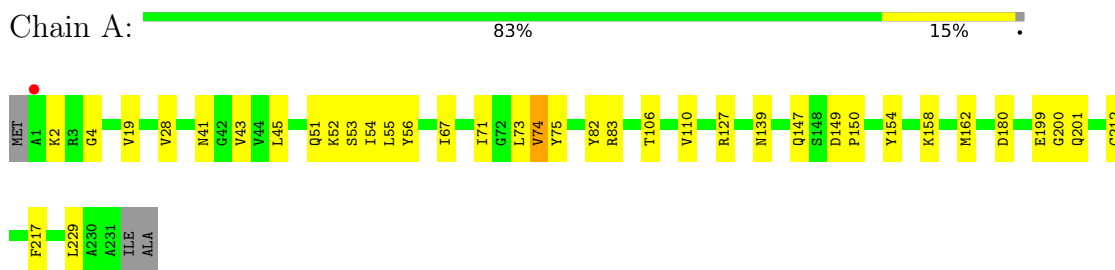
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	y	32	Total 32	O 32	0	0
16	z	38	Total 38	O 38	0	0
16	1	27	Total 27	O 27	0	0
16	2	33	Total 33	O 33	0	0
16	3	37	Total 37	O 37	0	0
16	4	30	Total 30	O 30	0	0

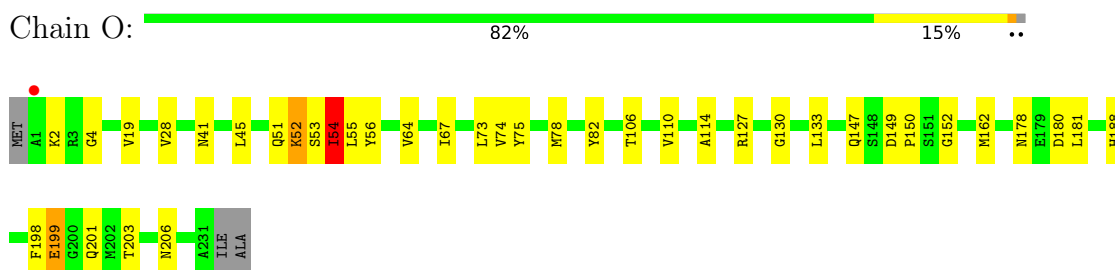
3 Residue-property plots [i](#)

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

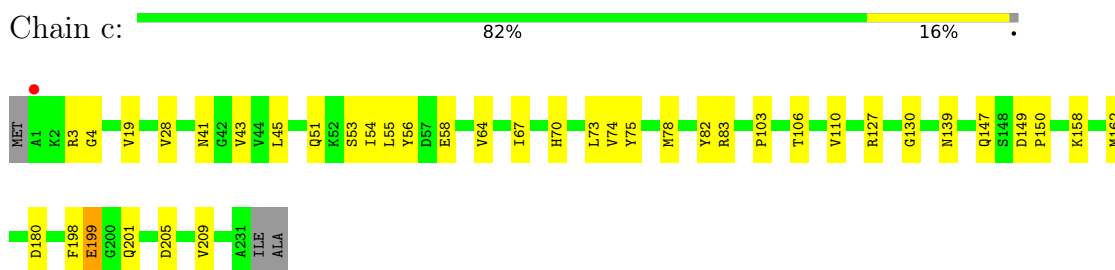
- Molecule 1: Proteasome subunit alpha type-2



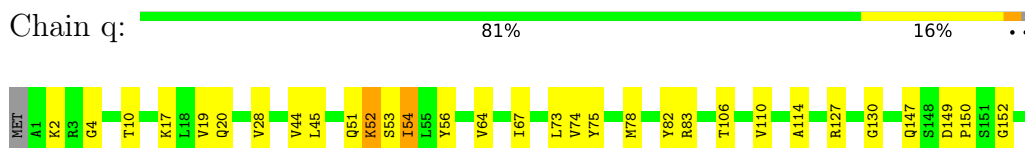
- Molecule 1: Proteasome subunit alpha type-2

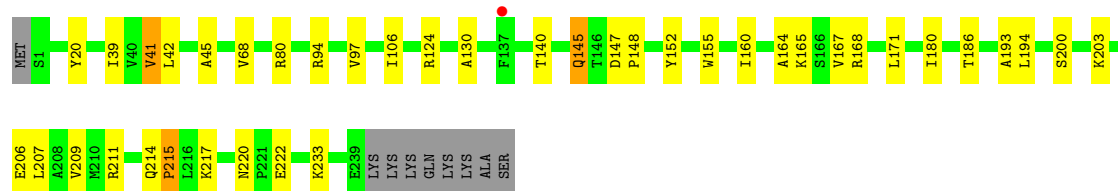


- Molecule 1: Proteasome subunit alpha type-2



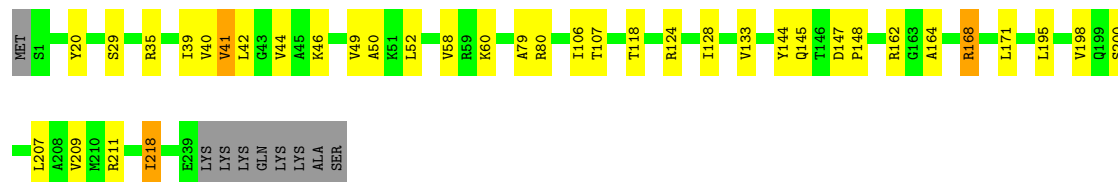
- Molecule 1: Proteasome subunit alpha type-2





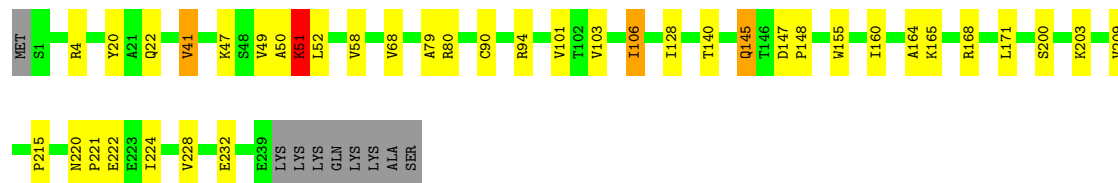
• Molecule 3: Proteasome subunit alpha type-7

Chain Q: 81% 14% . .



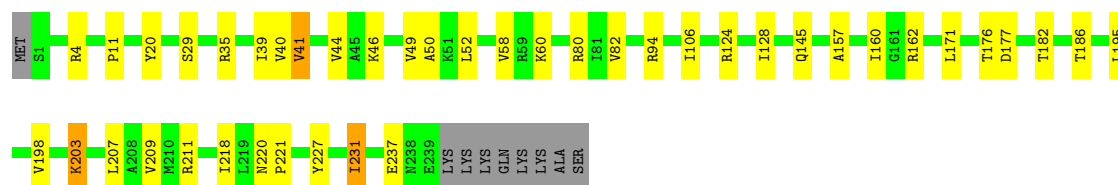
• Molecule 3: Proteasome subunit alpha type-7

Chain e: 81% 14% . .



• Molecule 3: Proteasome subunit alpha type-7

Chain s: 79% 16% . .



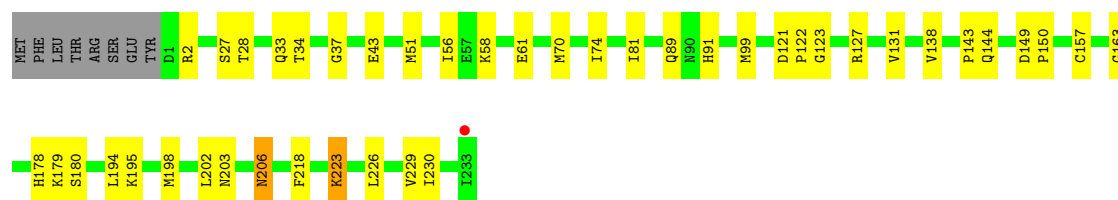
• Molecule 4: Proteasome subunit alpha type-5

Chain D: 83% 13% .



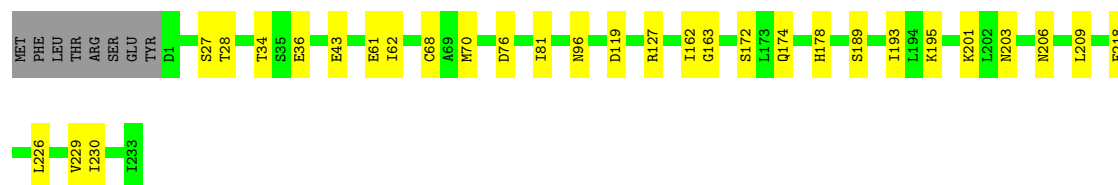
• Molecule 4: Proteasome subunit alpha type-5

Chain R:  79% 17% ..



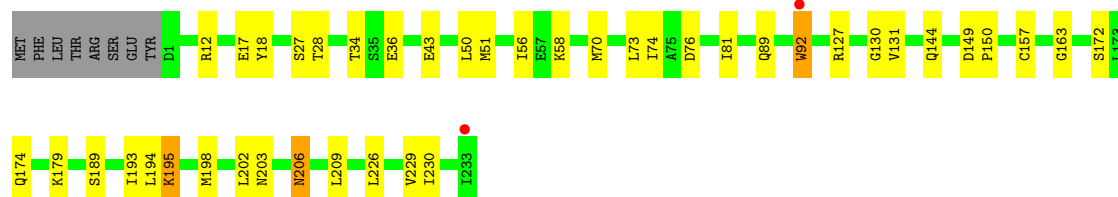
- Molecule 4: Proteasome subunit alpha type-5

Chain f:  84% 12% .



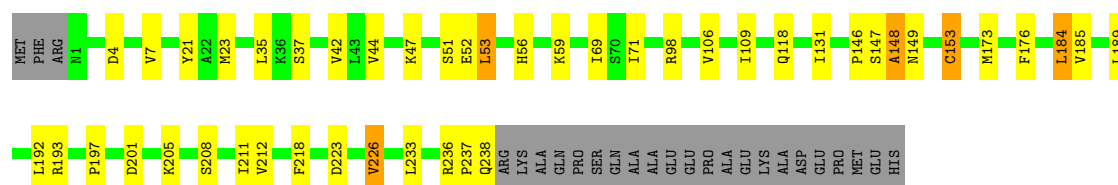
- Molecule 4: Proteasome subunit alpha type-5

Chain t:  79% 16% ..



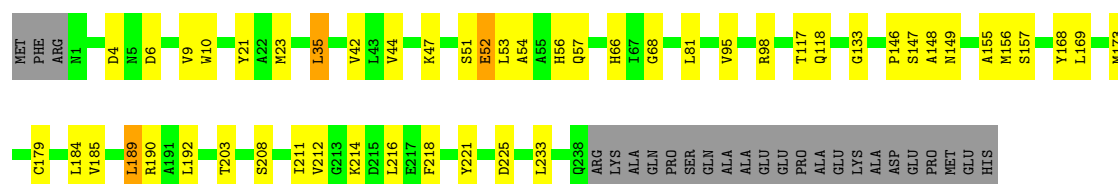
- Molecule 5: Proteasome subunit alpha type-1

Chain E:  73% 16% . 10%



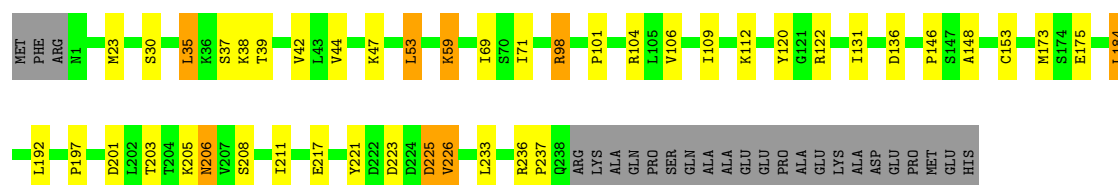
- Molecule 5: Proteasome subunit alpha type-1

Chain S:  71% 18% . 10%



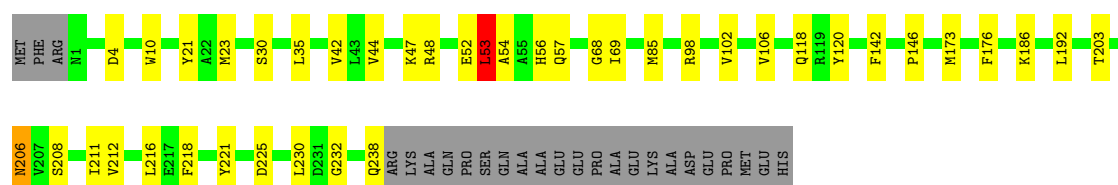
- Molecule 5: Proteasome subunit alpha type-1

Chain g:  73% 14% 10%



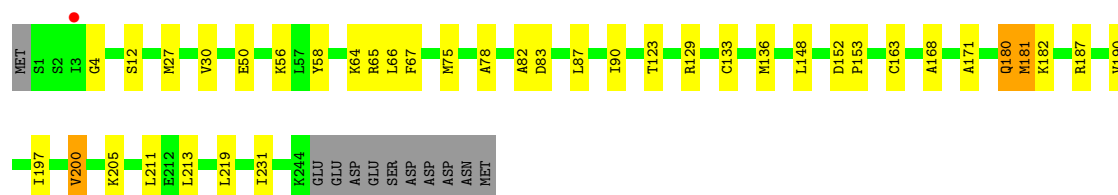
- Molecule 5: Proteasome subunit alpha type-1

Chain u:  75% 15% 10%



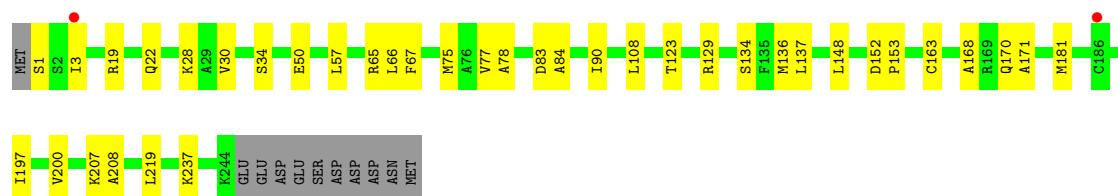
- Molecule 6: Proteasome subunit alpha type-3

Chain F:  80% 14% 10%



- Molecule 6: Proteasome subunit alpha type-3

Chain T:  81% 15% 10%



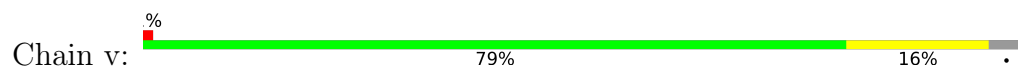
- Molecule 6: Proteasome subunit alpha type-3

Chain h:  79% 15% 10%

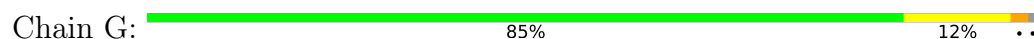




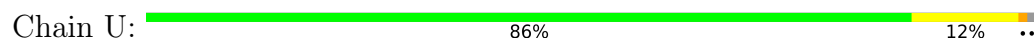
- Molecule 6: Proteasome subunit alpha type-3



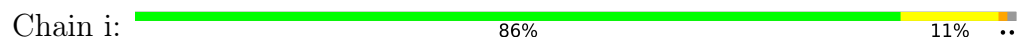
- Molecule 7: Proteasome subunit alpha type-6



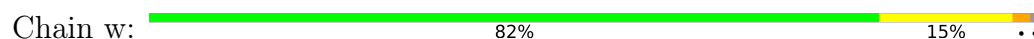
- Molecule 7: Proteasome subunit alpha type-6

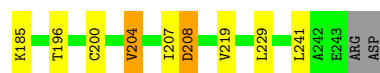


- Molecule 7: Proteasome subunit alpha type-6



- Molecule 7: Proteasome subunit alpha type-6





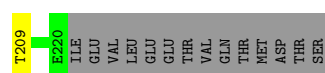
• Molecule 8: Proteasome subunit beta type-7

Chain H: 76% 16% 6%



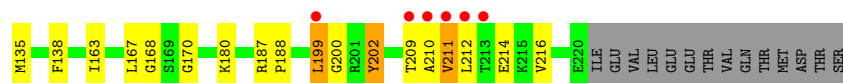
• Molecule 8: Proteasome subunit beta type-7

Chain V: 80% 13% 6%



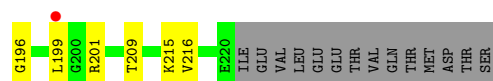
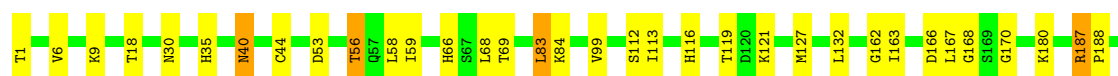
• Molecule 8: Proteasome subunit beta type-7

Chain j: 3% 73% 18% 6%



• Molecule 8: Proteasome subunit beta type-7

Chain x: 77% 15% 6%

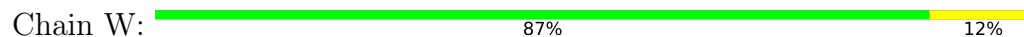


• Molecule 9: Proteasome subunit beta type-3

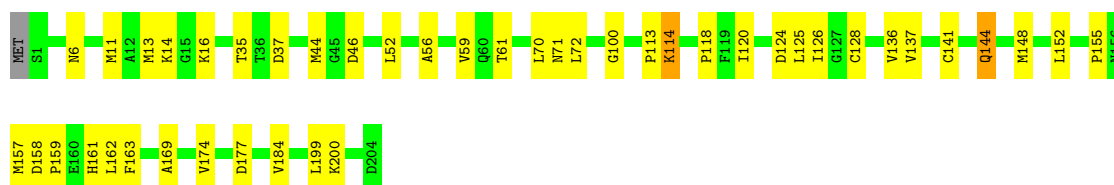
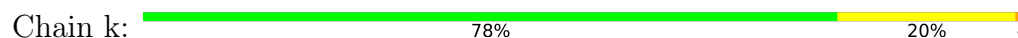
Chain I: 85% 14% 1%



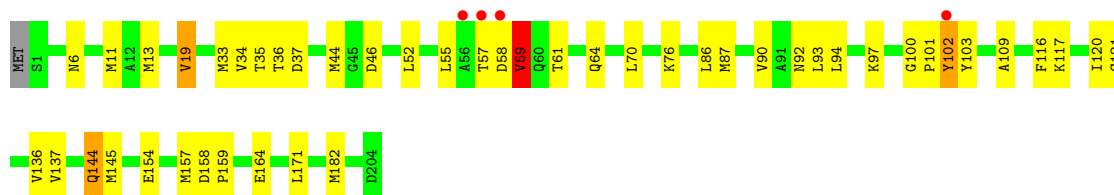
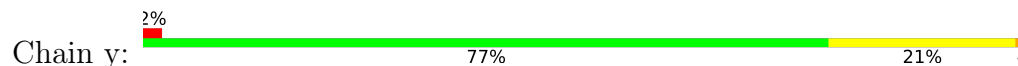
- Molecule 9: Proteasome subunit beta type-3



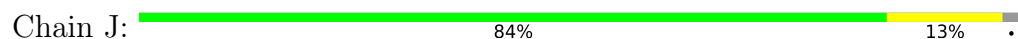
- Molecule 9: Proteasome subunit beta type-3



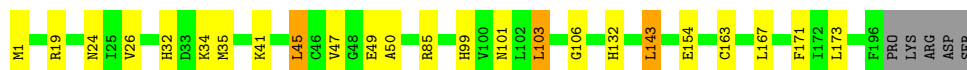
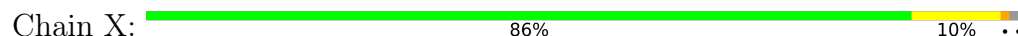
- Molecule 9: Proteasome subunit beta type-3



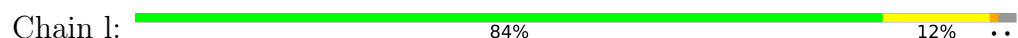
- Molecule 10: Proteasome subunit beta type-2



- Molecule 10: Proteasome subunit beta type-2

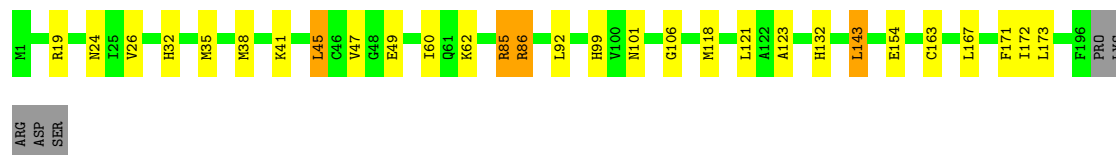
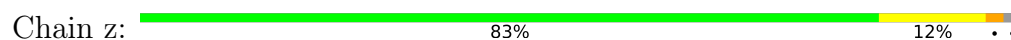


- Molecule 10: Proteasome subunit beta type-2

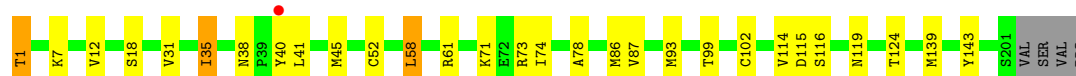
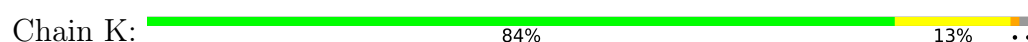




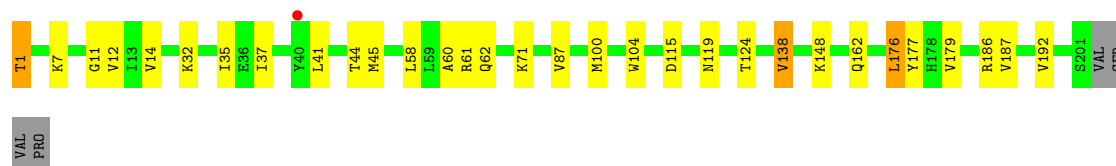
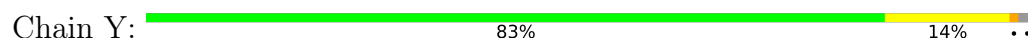
- Molecule 10: Proteasome subunit beta type-2



- Molecule 11: Proteasome subunit beta type-5



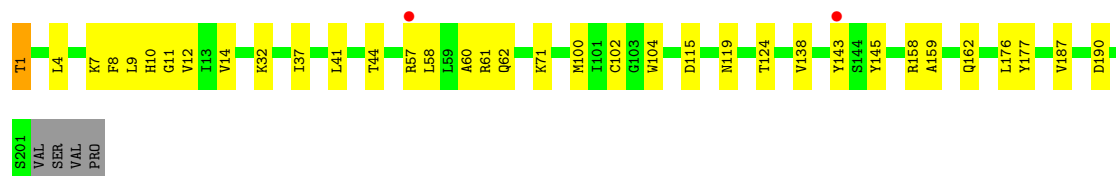
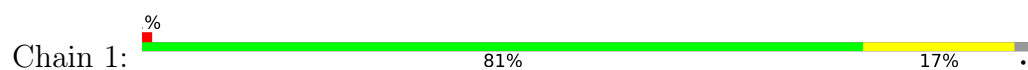
- Molecule 11: Proteasome subunit beta type-5



- Molecule 11: Proteasome subunit beta type-5



- Molecule 11: Proteasome subunit beta type-5



- Molecule 12: Proteasome subunit beta type-1

Chain L:  91% 8% .



- Molecule 12: Proteasome subunit beta type-1

Chain Z:  88% 11% .



- Molecule 12: Proteasome subunit beta type-1

Chain n:  88% 11% .



- Molecule 12: Proteasome subunit beta type-1

Chain 2:  86% 13% .



- Molecule 13: Proteasome subunit beta type-4

Chain M:  88% 10% ..



- Molecule 13: Proteasome subunit beta type-4

Chain a:  88% 10% ..



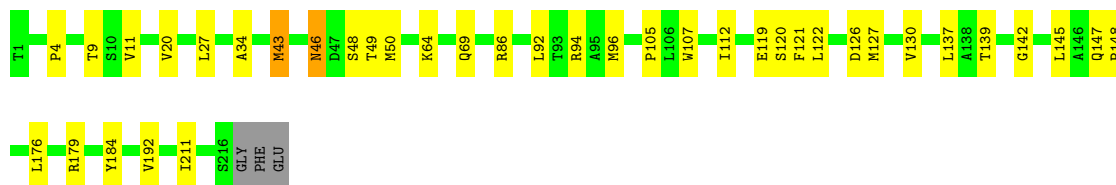
- Molecule 13: Proteasome subunit beta type-4

Chain o:  87% 11% ..



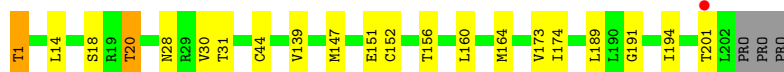
- Molecule 13: Proteasome subunit beta type-4

Chain 3:  81% 16% ..



• Molecule 14: Proteasome subunit beta type-6

Chain N:  88% 9% ..



• Molecule 14: Proteasome subunit beta type-6

Chain b:  89% 9% .



• Molecule 14: Proteasome subunit beta type-6

Chain p:  88% 8% ..



• Molecule 14: Proteasome subunit beta type-6

Chain 4:  91% 7% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	171.72Å 198.59Å 226.75Å 90.00° 106.59° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 15.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.0 (15.00-2.90) 95.3 (15.00-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.6.0119	Depositor
R, R_{free}	0.230 , 0.273 0.231 , 0.274	Depositor DCC
R_{free} test set	15447 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	56.0	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 63.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	99236	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 98.11 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.3244e-11. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 04C

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	0.52	0/1845	0.76	0/2498
1	O	0.51	0/1845	0.75	0/2498
1	c	0.51	0/1845	0.75	0/2498
1	q	0.51	0/1845	0.75	0/2498
2	B	0.49	0/1980	0.73	0/2667
2	P	0.48	0/1980	0.75	0/2667
2	d	0.48	0/1980	0.74	0/2667
2	r	0.48	0/1980	0.76	0/2667
3	C	0.47	0/1908	0.75	0/2576
3	Q	0.48	0/1908	0.77	0/2576
3	e	0.47	0/1908	0.75	0/2576
3	s	0.48	0/1908	0.75	0/2576
4	D	0.52	0/1805	0.78	0/2437
4	R	0.51	0/1805	0.75	0/2437
4	f	0.53	0/1805	0.77	0/2437
4	t	0.52	0/1805	0.75	0/2437
5	E	0.56	0/1907	0.77	0/2578
5	S	0.57	0/1907	0.78	0/2578
5	g	0.57	0/1907	0.76	0/2578
5	u	0.58	0/1907	0.79	1/2578 (0.0%)
6	F	0.52	0/1938	0.75	0/2608
6	T	0.51	0/1938	0.76	0/2608
6	h	0.52	0/1938	0.75	0/2608
6	v	0.51	0/1938	0.76	0/2608
7	G	0.49	0/1924	0.78	0/2600
7	U	0.49	0/1924	0.80	1/2600 (0.0%)
7	i	0.48	0/1924	0.77	0/2600
7	w	0.49	0/1924	0.78	1/2600 (0.0%)
8	H	0.55	1/1683 (0.1%)	0.84	2/2276 (0.1%)
8	V	0.58	1/1683 (0.1%)	0.80	2/2276 (0.1%)
8	j	0.52	1/1683 (0.1%)	0.81	3/2276 (0.1%)
8	x	0.58	1/1683 (0.1%)	0.83	2/2276 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	I	0.46	0/1621	0.74	0/2185
9	W	0.48	0/1621	0.77	0/2185
9	k	0.46	0/1621	0.73	0/2185
9	y	0.47	0/1621	0.77	1/2185 (0.0%)
10	J	0.52	0/1602	0.74	0/2167
10	X	0.52	0/1602	0.74	0/2167
10	l	0.51	0/1602	0.73	0/2167
10	z	0.52	0/1602	0.75	0/2167
11	1	0.56	1/1588 (0.1%)	0.74	0/2145
11	K	0.58	1/1588 (0.1%)	0.74	0/2145
11	Y	0.60	1/1588 (0.1%)	0.72	0/2145
11	m	0.59	1/1588 (0.1%)	0.74	0/2145
12	2	0.49	0/1685	0.73	0/2271
12	L	0.50	0/1685	0.75	0/2271
12	Z	0.49	0/1685	0.74	0/2271
12	n	0.49	0/1685	0.74	0/2271
13	3	0.50	0/1718	0.75	0/2325
13	M	0.51	0/1718	0.74	0/2325
13	a	0.51	0/1718	0.77	0/2325
13	o	0.50	0/1718	0.73	0/2325
14	4	0.55	1/1546 (0.1%)	0.74	0/2094
14	N	0.57	1/1546 (0.1%)	0.77	0/2094
14	b	0.57	1/1546 (0.1%)	0.75	0/2094
14	p	0.57	1/1546 (0.1%)	0.75	0/2094
All	All	0.52	12/99000 (0.0%)	0.76	13/133708 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
8	H	0	1
8	V	0	1
8	j	0	1
11	1	0	1
11	K	0	1
11	Y	0	1
11	m	0	1
14	4	0	1
14	N	0	1
14	b	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
14	p	0	1
All	All	0	11

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Y	1	THR	C-N	12.66	1.51	1.33
11	m	1	THR	C-N	12.04	1.50	1.33
8	V	1	THR	C-N	11.11	1.48	1.33
8	x	1	THR	C-N	11.05	1.47	1.33
11	K	1	THR	C-N	10.56	1.48	1.33
14	p	1	THR	C-N	9.49	1.46	1.33
14	b	1	THR	C-N	8.95	1.46	1.33
14	N	1	THR	C-N	8.84	1.45	1.33
11	1	1	THR	C-N	8.83	1.45	1.33
8	H	1	THR	C-N	8.72	1.44	1.33
14	4	1	THR	C-N	7.95	1.44	1.33
8	j	1	THR	C-N	5.91	1.41	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	1	THR	CA-C-N	10.35	137.36	122.77
8	H	1	THR	C-N-CA	10.35	137.36	122.77
5	u	53	LEU	N-CA-C	-8.51	104.92	114.62
8	x	1	THR	CA-C-N	8.31	134.48	122.77
8	x	1	THR	C-N-CA	8.31	134.48	122.77
8	V	1	THR	CA-C-N	7.86	133.85	122.77
8	V	1	THR	C-N-CA	7.86	133.85	122.77
8	j	1	THR	CA-C-N	6.67	132.40	123.00
8	j	1	THR	C-N-CA	6.67	132.40	123.00
9	y	59	VAL	N-CA-C	-5.83	104.83	110.42
7	w	229	LEU	N-CA-C	5.69	118.42	111.82
7	U	229	LEU	N-CA-C	5.63	118.35	111.82
8	j	212	LEU	N-CA-C	-5.34	106.78	113.72

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	1	1	THR	Peptide

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Mol	Chain	Res	Type	Group
14	4	1	THR	Peptide
8	H	1	THR	Peptide
11	K	1	THR	Peptide
14	N	1	THR	Peptide
8	V	1	THR	Mainchain
11	Y	1	THR	Peptide
14	b	1	THR	Peptide
8	j	1	THR	Mainchain
11	m	1	THR	Peptide
14	p	1	THR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1806	0	1805	22	0
1	O	1806	0	1805	25	0
1	c	1806	0	1805	25	0
1	q	1806	0	1805	25	0
2	B	1950	0	1973	13	0
2	P	1950	0	1973	15	0
2	d	1950	0	1973	18	0
2	r	1950	0	1973	18	0
3	C	1881	0	1907	19	0
3	Q	1881	0	1907	18	0
3	e	1881	0	1907	19	0
3	s	1881	0	1907	20	0
4	D	1778	0	1767	14	0
4	R	1778	0	1767	21	0
4	f	1778	0	1767	15	0
4	t	1778	0	1767	29	0
5	E	1872	0	1859	24	0
5	S	1872	0	1859	27	0
5	g	1872	0	1859	26	0
5	u	1872	0	1859	26	0
6	F	1903	0	1894	22	0
6	T	1903	0	1894	22	0
6	h	1903	0	1894	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	v	1903	0	1894	19	0
7	G	1890	0	1900	18	0
7	U	1890	0	1900	17	0
7	i	1890	0	1900	16	0
7	w	1890	0	1900	22	0
8	H	1656	0	1682	26	0
8	V	1656	0	1683	17	0
8	j	1656	0	1682	39	0
8	x	1656	0	1683	22	0
9	I	1592	0	1612	15	0
9	W	1592	0	1612	16	0
9	k	1592	0	1612	27	0
9	y	1592	0	1612	27	0
10	J	1570	0	1573	13	0
10	X	1570	0	1573	13	0
10	l	1570	0	1573	16	0
10	z	1570	0	1573	17	0
11	1	1557	0	1523	16	0
11	K	1557	0	1524	16	0
11	Y	1557	0	1523	13	0
11	m	1557	0	1524	15	0
12	2	1654	0	1652	20	0
12	L	1654	0	1652	10	0
12	Z	1654	0	1652	15	0
12	n	1654	0	1652	16	0
13	3	1685	0	1664	25	0
13	M	1685	0	1664	14	0
13	a	1685	0	1664	14	0
13	o	1685	0	1664	19	0
14	4	1519	0	1485	9	0
14	N	1519	0	1486	9	0
14	b	1519	0	1486	11	0
14	p	1519	0	1485	11	0
15	1	42	0	42	0	0
15	4	42	0	42	2	0
15	H	42	0	42	5	0
15	K	42	0	42	0	0
15	N	42	0	42	1	0
15	V	42	0	42	3	0
15	Y	42	0	42	0	0
15	b	42	0	42	2	0
15	j	42	0	42	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	m	42	0	42	5	0
15	p	42	0	42	3	0
15	x	42	0	42	2	0
16	1	27	0	0	1	0
16	2	33	0	0	0	0
16	3	37	0	0	5	0
16	4	30	0	0	0	0
16	A	19	0	0	1	0
16	B	24	0	0	0	0
16	C	13	0	0	0	0
16	D	16	0	0	0	0
16	E	21	0	0	1	0
16	F	20	0	0	0	0
16	G	22	0	0	0	0
16	H	31	0	0	0	0
16	I	32	0	0	0	0
16	J	25	0	0	0	0
16	K	28	0	0	1	0
16	L	23	0	0	0	0
16	M	27	0	0	0	0
16	N	33	0	0	0	0
16	O	33	0	0	1	0
16	P	38	0	0	0	0
16	Q	16	0	0	0	0
16	R	19	0	0	0	0
16	S	25	0	0	0	0
16	T	25	0	0	0	0
16	U	37	0	0	0	0
16	V	35	0	0	0	0
16	W	37	0	0	0	0
16	X	33	0	0	2	0
16	Y	16	0	0	0	0
16	Z	32	0	0	0	0
16	a	33	0	0	0	0
16	b	40	0	0	1	0
16	c	21	0	0	0	0
16	d	19	0	0	0	0
16	e	14	0	0	0	0
16	f	13	0	0	0	0
16	g	15	0	0	1	0
16	h	19	0	0	1	0
16	i	29	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	j	25	0	0	1	0
16	k	30	0	0	0	0
16	l	22	0	0	2	0
16	m	20	0	0	0	0
16	n	29	0	0	1	0
16	o	27	0	0	0	0
16	p	32	0	0	0	0
16	q	26	0	0	0	0
16	r	34	0	0	0	0
16	s	19	0	0	0	0
16	t	17	0	0	0	0
16	u	27	0	0	0	0
16	v	31	0	0	0	0
16	w	27	0	0	0	0
16	x	34	0	0	1	0
16	y	32	0	0	0	0
16	z	38	0	0	1	0
All	All	99236	0	97694	969	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 5.

All (969) 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)
10:J:60:ILE:HG21	10:J:84:THR:HG22	1.36	1.07
11:m:45:MET:HE2	15:m:301:04C:H44	1.43	1.01
10:l:60:ILE:HG21	10:l:84:THR:HG22	1.49	0.92
7:i:2:ARG:H	7:i:18:GLU:HG2	1.35	0.91
8:x:187:ARG:HB3	8:x:188:PRO:HD3	1.55	0.88
11:m:45:MET:HG2	11:m:52:CYS:HB3	1.55	0.88
13:M:212:ALA:HA	14:b:30:VAL:HG21	1.53	0.88
9:y:33:MET:HE3	9:y:36:THR:HG23	1.55	0.86
8:V:187:ARG:HB3	8:V:188:PRO:HD3	1.56	0.86
8:j:187:ARG:HB3	8:j:188:PRO:HD3	1.58	0.85
8:H:187:ARG:HB3	8:H:188:PRO:HD3	1.60	0.83
12:L:8:ASN:HD22	12:L:58:HIS:H	1.28	0.82
7:i:142:ILE:HG12	7:i:219:VAL:HG12	1.60	0.82
12:n:8:ASN:HD22	12:n:58:HIS:H	1.27	0.82
3:s:39:ILE:HG22	3:s:211:ARG:HG3	1.61	0.82
1:A:4:GLY:HA2	7:G:129:GLU:HG2	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:47:LYS:HE3	5:S:208:SER:HB2	1.63	0.81
13:o:96:MET:HE3	13:o:127:MET:HA	1.61	0.81
12:L:123:SER:HB3	12:L:136:LYS:HG2	1.63	0.78
1:c:4:GLY:HA2	7:i:129:GLU:HG2	1.65	0.78
5:u:203:THR:H	5:u:206:ASN:HD21	1.31	0.78
5:g:203:THR:H	5:g:206:ASN:HD21	1.31	0.78
9:y:64:GLN:HE22	10:z:85:ARG:HH12	1.33	0.77
8:j:132:LEU:HB3	16:3:333:HOH:O	1.83	0.76
6:T:136:MET:HE3	6:T:163:CYS:HB3	1.68	0.76
1:O:51:GLN:O	1:O:52:LYS:HB2	1.87	0.74
7:G:142:ILE:HD12	7:G:219:VAL:HG12	1.69	0.74
8:V:97:ALA:HB1	8:V:127:MET:HE3	1.68	0.74
12:Z:8:ASN:HD22	12:Z:58:HIS:H	1.35	0.74
6:F:65:ARG:HH12	6:F:78:ALA:HA	1.52	0.74
13:o:122:LEU:HG	13:o:137:LEU:HD12	1.70	0.73
4:D:34:THR:HG22	4:D:36:GLU:H	1.54	0.73
3:s:94:ARG:HB3	10:z:62:LYS:HE2	1.70	0.73
7:w:38:SER:HB3	7:w:51:THR:HG23	1.70	0.73
13:M:96:MET:HE3	13:M:127:MET:HA	1.71	0.72
4:f:34:THR:HG22	4:f:36:GLU:H	1.53	0.72
11:m:45:MET:CE	15:m:301:04C:H44	2.19	0.72
6:v:136:MET:HE3	6:v:163:CYS:HB3	1.72	0.72
15:x:301:04C:H24	15:x:301:04C:H8	1.73	0.71
5:u:47:LYS:HB3	5:u:56:HIS:HB3	1.72	0.71
13:M:46:ASN:HD22	13:M:48:SER:H	1.37	0.71
13:o:46:ASN:HD22	13:o:48:SER:H	1.36	0.71
13:o:212:ALA:HA	14:4:30:VAL:HG21	1.72	0.70
5:u:47:LYS:HE3	5:u:208:SER:HB2	1.73	0.70
4:D:203:ASN:HB3	4:D:206:ASN:HB2	1.72	0.70
5:S:47:LYS:HB3	5:S:56:HIS:HB3	1.72	0.70
1:q:149:ASP:HB2	1:q:150:PRO:HD2	1.74	0.70
4:t:34:THR:HG22	4:t:36:GLU:H	1.55	0.70
6:v:65:ARG:HH21	6:v:78:ALA:HA	1.54	0.70
12:2:13:LEU:HD11	12:2:149:LEU:HD11	1.74	0.70
2:d:160:ALA:HB1	2:d:174:LEU:HD23	1.74	0.70
14:b:49:ALA:HA	16:b:407:HOH:O	1.92	0.69
3:C:45:ALA:HB2	3:C:194:LEU:HD22	1.74	0.69
1:q:4:GLY:HA2	7:w:129:GLU:HG2	1.74	0.69
1:O:67:ILE:HD11	1:O:73:LEU:HD12	1.74	0.69
8:j:132:LEU:CB	16:3:333:HOH:O	2.37	0.69
7:U:122:GLN:O	7:U:125:THR:HG22	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:122:LEU:HG	13:M:137:LEU:HD12	1.75	0.68
6:h:136:MET:HE3	6:h:163:CYS:HB3	1.76	0.68
13:a:46:ASN:HD21	13:a:49:THR:HG22	1.59	0.67
6:v:123:THR:O	7:w:131:ARG:NH1	2.28	0.67
12:L:162:GLU:O	12:L:163:HIS:HB2	1.94	0.67
4:f:174:GLN:HG3	5:g:53:LEU:HD23	1.76	0.67
8:x:112:SER:HB2	8:x:127:MET:HE2	1.76	0.67
6:T:123:THR:O	7:U:131:ARG:NH1	2.28	0.67
1:A:149:ASP:HB2	1:A:150:PRO:HD2	1.77	0.67
13:3:50:MET:HE2	13:3:192:VAL:HG23	1.77	0.67
1:A:127:ARG:HH21	7:G:125:THR:HG22	1.59	0.66
1:c:67:ILE:HD11	1:c:73:LEU:HG	1.77	0.66
1:c:149:ASP:HB2	1:c:150:PRO:HD2	1.77	0.66
13:3:27:LEU:HD11	13:3:34:ALA:HB1	1.75	0.66
5:E:47:LYS:HE3	5:E:208:SER:HB2	1.76	0.66
13:a:96:MET:HE3	13:a:127:MET:HA	1.77	0.66
4:f:172:SER:HB3	4:f:193:ILE:HD12	1.78	0.66
7:U:142:ILE:HG12	7:U:219:VAL:HG12	1.77	0.66
7:w:49:ILE:HG21	7:w:78:VAL:HB	1.77	0.66
5:u:206:ASN:H	5:u:206:ASN:HD22	1.43	0.66
1:A:67:ILE:HD11	1:A:73:LEU:HG	1.78	0.66
1:O:178:ASN:HB2	1:O:181:LEU:HG	1.77	0.66
3:s:39:ILE:CG2	3:s:211:ARG:HG3	2.25	0.66
15:H:301:04C:H8	15:H:301:04C:H24	1.77	0.65
1:q:67:ILE:HD11	1:q:73:LEU:HD12	1.78	0.65
1:q:178:ASN:HB2	1:q:181:LEU:HG	1.77	0.65
1:c:75:TYR:HB3	1:c:82:TYR:CD1	2.32	0.65
12:n:123:SER:HB3	12:n:136:LYS:HG2	1.79	0.65
12:Z:13:LEU:HD11	12:Z:149:LEU:HD11	1.78	0.65
10:l:60:ILE:HG21	10:l:84:THR:CG2	2.26	0.65
7:G:2:ARG:H	7:G:18:GLU:HG2	1.61	0.65
1:c:127:ARG:HH21	7:i:125:THR:HG22	1.62	0.64
1:A:75:TYR:HB3	1:A:82:TYR:CD1	2.33	0.64
1:O:149:ASP:HB2	1:O:150:PRO:HD2	1.78	0.64
1:q:127:ARG:HH21	7:w:125:THR:HG22	1.62	0.64
6:T:65:ARG:HH21	6:T:78:ALA:HA	1.63	0.64
6:h:181:MET:HG2	16:h:307:HOH:O	1.99	0.63
4:t:189:SER:O	4:t:193:ILE:HG12	1.99	0.63
2:r:189:LEU:HD23	2:r:235:LEU:HD21	1.79	0.63
8:V:44:CYS:HB2	8:V:99:VAL:HB	1.79	0.63
4:t:172:SER:HB3	4:t:193:ILE:HD12	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:f:203:ASN:HB3	4:f:206:ASN:HB2	1.81	0.62
6:F:136:MET:HE3	6:F:163:CYS:HB3	1.82	0.62
1:A:67:ILE:HD13	1:A:71:ILE:HG22	1.82	0.62
4:R:27:SER:HB2	4:R:43:GLU:HG3	1.81	0.62
13:3:142:GLY:HA2	13:3:176:LEU:HD21	1.80	0.62
6:h:12:SER:HA	7:i:131:ARG:HG2	1.82	0.62
8:j:211:VAL:HG11	8:j:214:GLU:HB2	1.83	0.61
3:e:94:ARG:HB3	10:l:62:LYS:HE2	1.82	0.61
1:q:51:GLN:HG3	1:q:56:TYR:HB2	1.82	0.61
9:y:144:GLN:H	9:y:144:GLN:HE21	1.49	0.61
15:V:301:04C:H8	15:V:301:04C:H24	1.81	0.61
3:e:50:ALA:C	3:e:52:LEU:H	2.09	0.61
6:h:136:MET:HE2	6:h:148:LEU:HD11	1.83	0.60
5:E:44:VAL:HG12	5:E:192:LEU:HD22	1.83	0.60
13:3:96:MET:HE3	13:3:127:MET:HA	1.83	0.60
1:O:75:TYR:HB3	1:O:82:TYR:CD1	2.36	0.60
5:g:47:LYS:HE2	5:g:208:SER:HB2	1.82	0.60
3:Q:46:LYS:HE2	3:Q:162:ARG:HB3	1.83	0.60
7:U:77:CYS:HB3	7:U:139:LEU:HD23	1.83	0.60
1:q:51:GLN:O	1:q:52:LYS:HB3	2.00	0.60
5:g:101:PRO:HB2	5:g:104:ARG:HG3	1.84	0.60
12:n:153:VAL:HG13	12:n:166:LEU:HD11	1.82	0.60
4:D:226:LEU:O	4:D:230:ILE:HG12	2.01	0.60
4:f:189:SER:O	4:f:193:ILE:HG12	2.00	0.60
4:f:226:LEU:O	4:f:230:ILE:HG12	2.01	0.60
13:a:15:LYS:HB3	13:a:20:VAL:HG22	1.83	0.60
2:P:117:LYS:HZ1	2:P:149:SER:HB3	1.67	0.59
13:3:46:ASN:HD21	13:3:49:THR:HG22	1.66	0.59
6:T:136:MET:HE2	6:T:148:LEU:HD11	1.85	0.59
13:a:50:MET:HE2	13:a:192:VAL:HG23	1.83	0.59
1:c:45:LEU:HD13	1:c:74:VAL:HG23	1.83	0.59
9:y:35:THR:HG22	9:y:37:ASP:H	1.66	0.59
11:1:143:TYR:HD1	16:1:425:HOH:O	1.85	0.59
12:Z:8:ASN:ND2	12:Z:58:HIS:H	2.00	0.59
4:f:96:ASN:HD22	11:m:57:ARG:HH22	1.49	0.59
11:1:115:ASP:HB2	11:1:119:ASN:HB2	1.84	0.59
8:H:40:ASN:H	8:H:40:ASN:HD22	1.50	0.59
11:K:115:ASP:HB2	11:K:119:ASN:HB2	1.85	0.59
13:M:46:ASN:HD21	13:M:49:THR:HG23	1.66	0.59
7:U:49:ILE:HG21	7:U:78:VAL:HB	1.82	0.59
2:r:44:LEU:HD13	2:r:74:SER:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:s:44:VAL:HG21	3:s:60:LYS:HB2	1.83	0.59
2:d:20:VAL:HG11	2:d:152:SER:HB3	1.85	0.59
13:o:46:ASN:HB3	13:o:71:VAL:HG21	1.84	0.59
12:L:16:ALA:HB2	12:L:121:VAL:HG23	1.84	0.58
13:3:145:LEU:HG	16:3:333:HOH:O	2.03	0.58
4:t:27:SER:HB2	4:t:43:GLU:HG3	1.85	0.58
1:A:67:ILE:HG13	16:A:315:HOH:O	2.03	0.58
2:B:44:LEU:HD13	2:B:74:SER:HB2	1.85	0.58
9:I:124:ASP:HB2	9:I:128:CYS:H	1.68	0.58
2:P:117:LYS:NZ	2:P:149:SER:HB3	2.18	0.58
8:x:163:ILE:HG23	8:x:170:GLY:HA2	1.85	0.58
4:D:27:SER:HB2	4:D:43:GLU:HG3	1.86	0.58
11:K:87:VAL:HG11	11:K:116:SER:HA	1.84	0.58
3:Q:44:VAL:HG21	3:Q:60:LYS:HB2	1.85	0.58
3:C:152:TYR:HE2	4:D:78:LYS:HE2	1.69	0.57
1:O:51:GLN:O	1:O:52:LYS:CB	2.52	0.57
13:M:35:ARG:HD2	13:M:36:PHE:CE1	2.39	0.57
4:R:226:LEU:O	4:R:230:ILE:HG12	2.03	0.57
8:j:1:THR:HG23	8:j:33:LYS:HD3	1.86	0.57
13:a:46:ASN:ND2	13:a:49:THR:HG22	2.20	0.57
8:x:44:CYS:HB2	8:x:99:VAL:HB	1.86	0.57
9:W:144:GLN:H	9:W:144:GLN:HE21	1.51	0.57
9:y:44:MET:HE3	9:y:70:LEU:HD22	1.87	0.57
9:W:6:ASN:ND2	9:W:56:ALA:H	2.03	0.57
10:X:99:HIS:HB3	16:X:306:HOH:O	2.03	0.57
11:m:45:MET:HE2	15:m:301:04C:C2	2.27	0.57
2:P:44:LEU:HD13	2:P:74:SER:HB2	1.87	0.57
5:S:51:SER:O	5:S:53:LEU:N	2.38	0.57
5:S:118:GLN:HG3	6:T:129:ARG:HG3	1.87	0.57
11:Y:138:VAL:HG11	11:Y:162:GLN:HG3	1.86	0.57
14:b:48:SER:HB3	14:b:51:ASP:HB2	1.87	0.57
9:k:44:MET:HE3	9:k:70:LEU:HD22	1.87	0.57
13:3:46:ASN:HD22	13:3:48:SER:H	1.53	0.57
1:q:149:ASP:HB2	1:q:150:PRO:CD	2.34	0.57
4:t:92:TRP:HE3	4:t:92:TRP:C	2.13	0.57
9:W:167:SER:O	9:W:171:LEU:HB2	2.05	0.56
2:d:68:ASN:HD22	2:d:93:ALA:HB1	1.70	0.56
8:x:113:ILE:HG12	8:x:119:THR:HG22	1.87	0.56
7:U:142:ILE:HG12	7:U:219:VAL:CG1	2.35	0.56
2:r:135:TYR:HE1	2:r:149:SER:HB2	1.70	0.56
9:k:11:MET:HG3	9:k:137:VAL:HG12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:w:112:MET:HE1	8:x:69:THR:HG22	1.87	0.56
6:F:168:ALA:HB3	6:F:200:VAL:HG13	1.86	0.56
4:R:202:LEU:HD21	4:R:230:ILE:HD12	1.86	0.56
5:g:30:SER:HB2	5:g:59:LYS:HE3	1.88	0.56
5:g:206:ASN:H	5:g:206:ASN:HD22	1.53	0.56
8:j:40:ASN:H	8:j:40:ASN:HD22	1.53	0.56
6:h:168:ALA:HB3	6:h:200:VAL:HG13	1.87	0.56
1:q:51:GLN:O	1:q:52:LYS:CB	2.54	0.56
2:d:44:LEU:HD13	2:d:74:SER:HB2	1.88	0.56
3:e:164:ALA:O	3:e:168:ARG:HB2	2.06	0.56
5:u:203:THR:H	5:u:206:ASN:ND2	2.02	0.56
13:M:212:ALA:CA	14:b:30:VAL:HG21	2.32	0.56
7:w:136:CYS:SG	7:w:152:LYS:HE2	2.46	0.56
5:g:44:VAL:HG12	5:g:192:LEU:HD22	1.88	0.55
13:a:27:LEU:HD11	13:a:34:ALA:HB1	1.87	0.55
8:H:199:LEU:HB3	12:Z:173:ARG:HH11	1.71	0.55
3:C:214:GLN:HB3	3:C:215:PRO:HD2	1.89	0.55
5:E:23:MET:HA	5:E:146:PRO:HG2	1.88	0.55
3:Q:50:ALA:C	3:Q:52:LEU:H	2.14	0.55
4:f:27:SER:HB2	4:f:43:GLU:HG3	1.89	0.55
7:i:2:ARG:N	7:i:18:GLU:HG2	2.14	0.55
12:L:12:VAL:HG21	12:L:53:GLY:HA3	1.88	0.55
12:n:16:ALA:HB2	12:n:121:VAL:HG23	1.87	0.55
9:I:204:ASP:HB3	11:Y:192:VAL:HG11	1.88	0.55
10:z:35:MET:HG2	10:z:45:LEU:HD13	1.87	0.55
11:l:7:LYS:HE2	11:l:124:THR:HA	1.88	0.55
4:R:194:LEU:O	4:R:198:MET:HG3	2.07	0.55
2:P:36:ILE:HD11	2:P:188:ALA:CB	2.37	0.55
8:j:209:THR:CG2	9:k:163:PHE:HZ	2.20	0.55
13:M:27:LEU:HD11	13:M:34:ALA:HB1	1.89	0.55
8:j:135:MET:HE2	13:3:179:ARG:CZ	2.38	0.54
7:U:112:MET:HE1	8:V:69:THR:HG22	1.88	0.54
9:W:124:ASP:HB2	9:W:128:CYS:H	1.72	0.54
8:H:31:CYS:SG	15:H:301:04C:H42	2.48	0.54
9:I:157:MET:HE2	9:I:161:HIS:HB3	1.89	0.54
11:m:115:ASP:HB2	11:m:119:ASN:HB2	1.89	0.54
2:r:206:SER:HB3	2:r:209:LYS:HD3	1.89	0.54
5:E:47:LYS:CE	5:E:208:SER:HB2	2.38	0.54
1:O:78:MET:HE2	1:O:130:GLY:HA3	1.90	0.54
8:H:152:LYS:HE2	8:H:177:VAL:HG21	1.88	0.54
13:a:122:LEU:HG	13:a:137:LEU:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:199:ILE:HD12	14:b:199:ILE:H	1.72	0.54
9:y:52:LEU:HB2	9:y:59:VAL:HG13	1.89	0.54
12:2:145:LEU:HD22	12:2:178:VAL:HB	1.90	0.54
8:H:24:MET:HE3	12:Z:187:VAL:HG21	1.90	0.54
1:O:4:GLY:HA2	7:U:129:GLU:HG2	1.90	0.54
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.89	0.54
8:j:209:THR:HG22	9:k:199:LEU:HD23	1.90	0.53
4:t:92:TRP:C	4:t:92:TRP:CE3	2.86	0.53
2:B:196:LEU:O	2:B:200:MET:HB2	2.08	0.53
5:g:23:MET:HA	5:g:146:PRO:HG2	1.90	0.53
9:k:125:LEU:HD12	9:k:126:ILE:HG23	1.91	0.53
3:Q:118:THR:O	4:R:127:ARG:NH1	2.41	0.53
9:k:157:MET:HE2	9:k:161:HIS:HB3	1.90	0.53
7:G:181:LYS:HD3	7:G:196:THR:HG23	1.91	0.53
14:N:20:THR:HG22	14:N:31:THR:OG1	2.09	0.53
2:P:153:GLY:O	3:Q:80:ARG:NH2	2.42	0.53
13:o:46:ASN:HD21	13:o:49:THR:HG23	1.73	0.53
1:q:53:SER:O	1:q:54:ILE:HB	2.08	0.53
2:B:20:VAL:HG11	2:B:152:SER:HB3	1.89	0.53
11:K:139:MET:O	11:K:143:TYR:HB2	2.09	0.53
2:d:135:TYR:HE1	2:d:149:SER:HB2	1.72	0.53
10:X:35:MET:HG2	10:X:45:LEU:HD13	1.89	0.53
7:i:77:CYS:HB3	7:i:139:LEU:HD23	1.91	0.53
3:s:195:LEU:HA	3:s:198:VAL:HG12	1.90	0.53
12:n:8:ASN:ND2	12:n:58:HIS:H	2.03	0.53
11:K:7:LYS:HB3	11:K:12:VAL:HG22	1.91	0.53
8:V:209:THR:HG21	9:W:167:SER:HB3	1.91	0.53
7:G:140:ILE:HG22	7:G:150:VAL:HG22	1.91	0.53
3:e:41:VAL:HB	3:e:209:VAL:HG12	1.90	0.53
13:o:27:LEU:HD11	13:o:34:ALA:HB1	1.90	0.53
10:z:171:PHE:CE2	10:z:173:LEU:HB2	2.44	0.53
14:b:48:SER:HB2	15:b:301:04C:H25	1.91	0.53
5:g:47:LYS:CE	5:g:208:SER:HB2	2.39	0.52
7:w:77:CYS:HB3	7:w:139:LEU:HD23	1.91	0.52
3:C:68:VAL:HG11	3:C:106:ILE:HG21	1.91	0.52
6:F:67:PHE:HB2	6:F:75:MET:HB3	1.90	0.52
9:I:11:MET:HG3	9:I:137:VAL:HG12	1.91	0.52
4:t:89:GLN:HB3	11:l:61:ARG:HG3	1.89	0.52
7:G:2:ARG:H	7:G:18:GLU:CG	2.22	0.52
2:P:36:ILE:HD11	2:P:188:ALA:HB1	1.92	0.52
9:W:157:MET:HE2	9:W:161:HIS:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:136:LYS:HA	12:Z:146:GLN:NE2	2.25	0.52
1:c:106:THR:H	1:c:139:ASN:HD21	1.58	0.52
8:V:168:GLY:O	15:V:301:04C:H33	2.10	0.52
13:a:126:ASP:HB3	13:a:128:LEU:H	1.74	0.52
2:d:94:GLN:HE22	9:k:71:ASN:HD22	1.57	0.52
11:1:176:LEU:HB3	11:1:187:VAL:HB	1.90	0.52
2:r:153:GLY:O	3:s:80:ARG:NH2	2.38	0.52
12:2:8:ASN:HD22	12:2:58:HIS:H	1.55	0.52
6:F:12:SER:HA	7:G:131:ARG:HG2	1.92	0.52
7:G:77:CYS:HB3	7:G:139:LEU:HD23	1.92	0.52
13:a:46:ASN:C	13:a:46:ASN:HD22	2.17	0.52
7:U:136:CYS:SG	7:U:152:LYS:HE2	2.49	0.52
12:n:148:LEU:HB2	16:n:321:HOH:O	2.10	0.52
3:s:227:TYR:O	3:s:231:ILE:HD12	2.09	0.52
3:C:152:TYR:CE2	4:D:78:LYS:HE2	2.45	0.52
1:O:127:ARG:HH21	7:U:125:THR:HG23	1.73	0.52
12:L:8:ASN:ND2	12:L:58:HIS:H	2.04	0.52
14:N:20:THR:CG2	14:N:28:ASN:HB3	2.39	0.52
1:O:203:THR:H	1:O:206:ASN:HB2	1.75	0.52
1:c:3:ARG:HH22	4:f:119:ASP:H	1.57	0.52
3:Q:29:SER:HB2	3:Q:60:LYS:HE2	1.92	0.52
5:S:44:VAL:HG12	5:S:192:LEU:HD22	1.91	0.52
3:e:90:CYS:HA	3:e:101:VAL:HG21	1.91	0.52
3:s:220:ASN:HB2	3:s:221:PRO:HD2	1.92	0.52
5:S:10:TRP:H	6:T:22:GLN:HE22	1.58	0.51
8:j:22:GLU:HG2	8:j:27:ALA:HB2	1.91	0.51
4:t:149:ASP:HB2	4:t:150:PRO:HD2	1.92	0.51
13:3:46:ASN:ND2	13:3:49:THR:HG22	2.24	0.51
5:S:23:MET:HA	5:S:146:PRO:HG2	1.92	0.51
13:o:33:LEU:HD13	14:4:134:TYR:CE2	2.46	0.51
13:o:212:ALA:CA	14:4:30:VAL:HG21	2.40	0.51
10:z:99:HIS:HB3	16:z:302:HOH:O	2.09	0.51
12:2:8:ASN:ND2	12:2:58:HIS:H	2.09	0.51
8:H:22:GLU:HG2	8:H:27:ALA:HB2	1.92	0.51
12:L:137:ALA:H	12:L:146:GLN:HE21	1.57	0.51
14:b:18:SER:HB2	14:b:30:VAL:HA	1.92	0.51
5:u:23:MET:HA	5:u:146:PRO:HG2	1.93	0.51
6:T:34:SER:HB2	6:T:50:GLU:HG3	1.92	0.51
1:A:106:THR:H	1:A:139:ASN:HD21	1.58	0.51
6:F:64:LYS:H	6:F:64:LYS:HD2	1.76	0.51
8:V:106:THR:HB	8:V:109:HIS:HE2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:q:75:TYR:HB3	1:q:82:TYR:CD1	2.45	0.51
11:K:45:MET:HB2	11:K:52:CYS:HB3	1.92	0.51
11:K:99:THR:HG23	11:K:114:VAL:HB	1.93	0.51
6:T:83:ASP:OD2	6:T:129:ARG:NH2	2.44	0.51
1:c:45:LEU:HB3	1:c:74:VAL:HG21	1.92	0.51
1:c:78:MET:HE2	1:c:130:GLY:HA3	1.93	0.51
9:y:58:ASP:HB2	9:y:102:TYR:HE2	1.75	0.51
10:z:172:ILE:HG13	10:z:173:LEU:HD22	1.92	0.51
12:2:159:GLN:HG2	12:2:160:ASN:H	1.76	0.51
1:O:147:GLN:HG3	1:O:162:MET:HE1	1.92	0.51
6:h:87:LEU:HD12	6:h:133:CYS:SG	2.51	0.51
4:t:203:ASN:H	4:t:206:ASN:ND2	2.09	0.51
7:w:200:CYS:O	7:w:204:VAL:HB	2.11	0.51
8:x:187:ARG:HB3	8:x:188:PRO:CD	2.35	0.51
4:D:76:ASP:OD2	4:D:127:ARG:NH2	2.44	0.51
8:H:97:ALA:HB1	8:H:127:MET:HE3	1.91	0.51
9:I:35:THR:HG22	9:I:37:ASP:H	1.75	0.51
14:N:152:CYS:O	14:N:156:THR:HG22	2.11	0.51
4:R:70:MET:HE3	4:R:74:ILE:HG23	1.92	0.51
10:X:103:LEU:HD13	10:X:132:HIS:HD2	1.76	0.51
11:Y:176:LEU:HB3	11:Y:187:VAL:HB	1.92	0.51
2:d:174:LEU:HD12	2:d:195:VAL:HG21	1.93	0.51
9:k:144:GLN:H	9:k:144:GLN:HE21	1.57	0.51
12:n:173:ARG:CZ	8:x:199:LEU:HB2	2.41	0.51
14:p:20:THR:HG23	14:p:31:THR:OG1	2.11	0.51
14:p:160:LEU:O	14:p:164:MET:HG3	2.11	0.51
4:t:203:ASN:H	4:t:206:ASN:HD21	1.59	0.51
14:4:14:LEU:HD23	14:4:44:CYS:SG	2.50	0.51
14:4:48:SER:HB3	14:4:51:ASP:HB2	1.92	0.51
8:j:100:LEU:HB3	8:j:111:TYR:HB2	1.93	0.51
8:V:187:ARG:HB3	8:V:188:PRO:CD	2.36	0.50
9:k:61:THR:HG23	10:l:86:ARG:HH22	1.76	0.50
4:t:195:LYS:HB3	4:t:202:LEU:HD13	1.93	0.50
1:A:45:LEU:HB3	1:A:74:VAL:HG21	1.93	0.50
12:L:123:SER:CB	12:L:136:LYS:HG2	2.36	0.50
4:f:76:ASP:OD2	4:f:127:ARG:NH2	2.43	0.50
6:h:180:GLN:O	6:h:182:LYS:N	2.44	0.50
8:j:167:LEU:HB3	12:2:187:VAL:CG1	2.41	0.50
6:v:30:VAL:HG21	6:v:134:SER:HB2	1.93	0.50
5:g:106:VAL:HA	5:g:109:ILE:HD12	1.94	0.50
8:j:202:TYR:HB2	16:j:401:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:87:LEU:HD12	6:F:133:CYS:SG	2.52	0.50
7:G:112:MET:HE1	8:H:69:THR:HG22	1.92	0.50
6:T:30:VAL:HG21	6:T:134:SER:HB2	1.94	0.50
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.94	0.50
5:u:44:VAL:HG12	5:u:192:LEU:HD22	1.92	0.50
6:v:136:MET:HE2	6:v:148:LEU:HD11	1.92	0.50
9:y:55:LEU:O	9:y:57:THR:N	2.39	0.50
2:B:135:TYR:HE1	2:B:149:SER:HB2	1.76	0.50
3:Q:164:ALA:O	3:Q:168:ARG:HB2	2.12	0.50
8:V:18:THR:HB	8:V:30:ASN:HA	1.93	0.50
5:g:233:LEU:HD23	5:g:233:LEU:H	1.77	0.50
3:s:58:VAL:O	3:s:58:VAL:HG12	2.11	0.50
5:u:30:SER:HB3	5:u:48:ARG:HG3	1.93	0.50
2:P:75:VAL:HG11	2:P:82:ALA:CB	2.42	0.50
1:q:78:MET:HE2	1:q:130:GLY:HA3	1.94	0.50
9:y:137:VAL:HG11	9:y:145:MET:HB3	1.93	0.50
8:j:132:LEU:HB2	16:3:333:HOH:O	2.08	0.50
10:l:143:LEU:HD13	10:l:163:CYS:SG	2.52	0.50
1:q:147:GLN:HG3	1:q:162:MET:HE1	1.94	0.50
1:A:53:SER:C	1:A:55:LEU:H	2.20	0.49
10:J:23:SER:HB2	10:J:28:MET:HE2	1.94	0.49
3:Q:107:THR:HG21	3:Q:144:TYR:HB3	1.94	0.49
4:R:203:ASN:H	4:R:206:ASN:ND2	2.10	0.49
8:j:59:ILE:HD12	8:j:82:MET:HB3	1.94	0.49
12:n:123:SER:CB	12:n:136:LYS:HG2	2.41	0.49
4:t:194:LEU:HG	4:t:198:MET:CE	2.42	0.49
9:W:11:MET:HG3	9:W:137:VAL:HG12	1.93	0.49
11:Y:115:ASP:HB2	11:Y:119:ASN:HB2	1.93	0.49
6:h:129:ARG:CG	6:h:129:ARG:HH11	2.25	0.49
8:j:187:ARG:HB3	8:j:188:PRO:CD	2.38	0.49
2:d:13:PRO:HA	3:e:20:TYR:CE2	2.48	0.49
7:w:24:VAL:HG21	7:w:125:THR:HG23	1.95	0.49
7:G:49:ILE:HG21	7:G:78:VAL:HB	1.93	0.49
9:I:47:ARG:HG2	9:I:111:LEU:HB2	1.95	0.49
11:Y:14:VAL:HB	11:Y:177:TYR:HB2	1.95	0.49
8:j:97:ALA:HB1	8:j:127:MET:HE3	1.93	0.49
13:o:50:MET:HE2	13:o:192:VAL:HG23	1.94	0.49
12:2:12:VAL:HG21	12:2:53:GLY:HA3	1.94	0.49
6:F:83:ASP:OD2	6:F:129:ARG:NH2	2.45	0.49
1:O:53:SER:O	1:O:54:ILE:HB	2.12	0.49
14:b:127:ILE:HD12	14:b:132:SER:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:l:1:MET:HE1	10:l:134:TYR:H	1.76	0.49
1:O:64:VAL:HG22	1:O:74:VAL:HG22	1.95	0.49
12:Z:12:VAL:HG23	12:Z:109:ILE:HD12	1.93	0.49
8:j:44:CYS:HB2	8:j:99:VAL:HB	1.95	0.49
15:j:301:04C:H8	15:j:301:04C:H24	1.95	0.49
2:P:89:LEU:HG	2:P:113:LEU:HD13	1.95	0.49
3:Q:195:LEU:HA	3:Q:198:VAL:HG12	1.94	0.49
14:N:30:VAL:HG13	14:N:30:VAL:O	2.12	0.49
6:h:213:LEU:HD12	6:h:232:ARG:HG3	1.93	0.49
1:q:74:VAL:HG12	1:q:75:TYR:N	2.28	0.49
8:x:35:HIS:CG	8:x:56:THR:HG21	2.48	0.49
8:x:59:ILE:HG12	8:x:83:LEU:HD13	1.95	0.49
13:3:46:ASN:ND2	13:3:48:SER:H	2.10	0.49
2:B:13:PRO:HA	3:C:20:TYR:CE2	2.48	0.49
5:E:69:ILE:HG22	5:E:131:ILE:HG12	1.95	0.49
6:F:136:MET:HE2	6:F:148:LEU:HD11	1.94	0.49
12:n:137:ALA:H	12:n:146:GLN:HE21	1.60	0.49
2:r:87:ASN:HD21	9:y:76:LYS:HE2	1.78	0.49
1:O:51:GLN:HG3	1:O:56:TYR:HB2	1.94	0.49
5:S:35:LEU:HD13	5:S:184:LEU:HD22	1.94	0.49
11:m:7:LYS:HB3	11:m:12:VAL:HG22	1.95	0.49
15:m:301:04C:H24	15:m:301:04C:H6	1.95	0.49
3:Q:35:ARG:HA	3:Q:40:VAL:HG13	1.95	0.48
8:x:119:THR:H	14:4:53:GLN:HE22	1.61	0.48
8:j:200:GLY:N	12:2:173:ARG:HH11	2.11	0.48
5:u:69:ILE:HG21	5:u:85:MET:HE1	1.94	0.48
5:E:42:VAL:HG22	5:E:211:ILE:HG12	1.96	0.48
10:J:60:ILE:HG21	10:J:84:THR:CG2	2.24	0.48
10:J:101:ASN:HB3	10:J:132:HIS:CE1	2.48	0.48
1:O:188:HIS:HD2	16:O:325:HOH:O	1.96	0.48
5:S:4:ASP:HB2	5:S:21:TYR:HE1	1.77	0.48
13:3:92:LEU:HD23	13:3:112:ILE:HD11	1.96	0.48
1:A:149:ASP:HB2	1:A:150:PRO:CD	2.43	0.48
8:j:202:TYR:HE1	12:2:170:ARG:HE	1.61	0.48
1:q:114:ALA:HB1	1:q:152:GLY:O	2.14	0.48
12:2:123:SER:HB3	12:2:136:LYS:HG2	1.96	0.48
11:K:102:CYS:HB2	16:K:427:HOH:O	2.13	0.48
7:i:140:ILE:HG22	7:i:150:VAL:HG22	1.94	0.48
7:i:142:ILE:HG12	7:i:219:VAL:CG1	2.38	0.48
3:s:82:VAL:HG11	3:s:128:ILE:HD11	1.96	0.48
14:4:48:SER:HB2	15:4:301:04C:H25	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:233:LEU:H	5:S:233:LEU:HD23	1.79	0.48
9:y:61:THR:HG23	10:z:86:ARG:HH22	1.78	0.48
3:C:145:GLN:HG2	3:C:155:TRP:NE1	2.29	0.48
5:S:4:ASP:HB2	5:S:21:TYR:CE1	2.49	0.48
6:h:189:VAL:O	6:h:193:VAL:HG23	2.14	0.48
7:i:181:LYS:HD3	7:i:196:THR:HG23	1.95	0.48
13:o:150:LEU:HD23	13:o:168:LEU:HD22	1.95	0.48
3:C:164:ALA:O	3:C:168:ARG:HB2	2.14	0.48
1:c:51:GLN:HG3	1:c:56:TYR:HB2	1.96	0.48
4:t:70:MET:HE3	4:t:74:ILE:HG23	1.95	0.48
1:A:106:THR:O	1:A:110:VAL:HG23	2.13	0.47
5:E:148:ALA:HB3	6:F:82:ALA:HB1	1.96	0.47
6:h:240:LYS:HA	6:h:243:LEU:HD13	1.95	0.47
9:y:92:ASN:O	9:y:94:LEU:N	2.45	0.47
11:l:14:VAL:HB	11:l:177:TYR:HB2	1.96	0.47
5:E:37:SER:HB3	5:E:184:LEU:HG	1.96	0.47
6:T:152:ASP:HB2	6:T:153:PRO:HD2	1.97	0.47
2:d:178:TYR:HA	2:d:183:MET:HE3	1.95	0.47
6:h:67:PHE:HB2	6:h:75:MET:HB3	1.96	0.47
14:p:19:ARG:O	15:p:301:04C:H34	2.15	0.47
8:x:209:THR:HG22	9:y:164:GLU:OE1	2.14	0.47
9:y:144:GLN:HE21	9:y:144:GLN:N	2.10	0.47
10:l:16:ALA:HA	10:l:179:SER:O	2.14	0.47
10:z:101:ASN:HB3	10:z:132:HIS:CE1	2.48	0.47
5:S:185:VAL:O	5:S:189:LEU:HG	2.15	0.47
10:X:41:LYS:O	10:X:106:GLY:HA2	2.15	0.47
14:b:14:LEU:HD23	14:b:44:CYS:SG	2.54	0.47
7:i:112:MET:HE1	8:j:69:THR:HG22	1.95	0.47
15:4:301:04C:H8	15:4:301:04C:H22	1.97	0.47
11:K:18:SER:O	11:K:31:VAL:HG22	2.14	0.47
6:T:67:PHE:HB2	6:T:75:MET:HB3	1.95	0.47
9:k:148:MET:HG2	9:k:169:ALA:HA	1.96	0.47
6:T:1:SER:HB3	6:T:19:ARG:HH22	1.80	0.47
6:T:207:LYS:HG2	6:T:208:ALA:H	1.79	0.47
5:g:98:ARG:HH21	5:g:101:PRO:HD3	1.79	0.47
14:p:152:CYS:O	14:p:156:THR:HG22	2.15	0.47
7:w:71:ILE:HG21	7:w:113:LEU:HD11	1.96	0.47
9:y:64:GLN:NE2	10:z:85:ARG:HH12	2.07	0.47
11:l:138:VAL:CG2	11:l:159:ALA:HA	2.44	0.47
3:C:94:ARG:HB3	10:J:62:LYS:HE2	1.96	0.47
4:D:192:ILE:O	4:D:195:LYS:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:223:ASP:O	5:E:226:VAL:HG12	2.14	0.47
1:O:198:PHE:O	1:O:199:GLU:HG2	2.14	0.47
2:P:75:VAL:HG11	2:P:82:ALA:HB2	1.96	0.47
8:V:35:HIS:CG	8:V:56:THR:HG21	2.49	0.47
12:Z:14:ALA:HA	12:Z:22:ILE:O	2.14	0.47
6:h:99:ARG:HH11	13:o:69:GLN:HE22	1.61	0.47
8:j:167:LEU:HB3	12:2:187:VAL:HG13	1.97	0.47
1:q:106:THR:O	1:q:110:VAL:HG23	2.14	0.47
2:r:86:THR:HA	2:r:89:LEU:HD12	1.97	0.47
7:w:111:ASP:HB3	7:w:151:TYR:CZ	2.49	0.47
12:2:159:GLN:H	12:2:159:GLN:NE2	2.12	0.47
13:3:27:LEU:HD22	13:3:184:TYR:HB2	1.95	0.47
1:A:51:GLN:O	1:A:52:LYS:HG2	2.15	0.47
8:H:44:CYS:HB2	8:H:99:VAL:HB	1.96	0.47
8:H:59:ILE:HD12	8:H:82:MET:HB3	1.97	0.47
9:I:144:GLN:H	9:I:144:GLN:HE21	1.61	0.47
2:P:115:ASP:OD1	3:Q:80:ARG:NH1	2.47	0.47
11:Y:44:THR:HG21	11:Y:100:MET:HE3	1.97	0.47
1:c:64:VAL:HG22	1:c:74:VAL:HG22	1.97	0.47
1:c:158:LYS:HG3	2:d:56:ASP:HA	1.96	0.47
1:q:10:THR:HG23	1:q:20:GLN:HB2	1.96	0.47
6:v:27:MET:O	6:v:30:VAL:HG12	2.15	0.47
11:1:44:THR:HG21	11:1:100:MET:HE3	1.97	0.47
12:2:1:ARG:HD3	12:2:2:PHE:H	1.79	0.47
8:H:219:LEU:HD13	9:I:47:ARG:HD3	1.97	0.47
12:L:72:LEU:HG	12:L:83:MET:HE2	1.95	0.47
4:R:28:THR:HA	4:R:163:GLY:HA3	1.96	0.47
9:W:158:ASP:HB2	9:W:159:PRO:HD2	1.97	0.47
5:g:173:MET:C	5:g:175:GLU:H	2.23	0.47
8:j:81:ARG:HD3	8:j:84:LYS:HE2	1.95	0.47
10:l:38:MET:HE1	10:l:60:ILE:HG22	1.97	0.47
1:A:83:ARG:NH2	7:G:157:GLY:O	2.47	0.47
5:E:197:PRO:HG2	16:E:302:HOH:O	2.15	0.47
10:J:16:ALA:HA	10:J:179:SER:O	2.15	0.47
7:U:12:ILE:HG13	7:U:14:ILE:HG12	1.97	0.47
3:e:47:LYS:HB3	3:e:49:VAL:HG23	1.96	0.47
5:g:37:SER:HB3	5:g:184:LEU:HG	1.97	0.47
12:2:16:ALA:HB2	12:2:121:VAL:HG23	1.96	0.47
13:3:20:VAL:HG23	13:3:120:SER:HB2	1.96	0.47
5:E:212:VAL:HB	5:E:218:PHE:HD1	1.80	0.46
15:p:301:04C:H8	15:p:301:04C:H22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:t:194:LEU:O	4:t:198:MET:HB2	2.15	0.46
11:K:35:ILE:HD13	11:K:45:MET:HE3	1.97	0.46
4:R:157:CYS:HA	5:S:54:ALA:HA	1.97	0.46
9:W:44:MET:HE3	9:W:70:LEU:HD22	1.96	0.46
13:a:15:LYS:HE3	13:a:135:PRO:HA	1.96	0.46
15:b:301:04C:H8	15:b:301:04C:H22	1.97	0.46
1:q:64:VAL:HG22	1:q:74:VAL:HG22	1.97	0.46
2:r:193:VAL:HG21	2:r:235:LEU:HB3	1.98	0.46
4:t:92:TRP:HE3	4:t:92:TRP:O	1.98	0.46
5:u:212:VAL:HB	5:u:218:PHE:HD1	1.80	0.46
9:y:11:MET:HG3	9:y:137:VAL:HG12	1.97	0.46
5:E:118:GLN:HG3	6:F:129:ARG:HG3	1.97	0.46
8:H:106:THR:HB	8:H:109:HIS:HE2	1.81	0.46
9:I:44:MET:HE3	9:I:70:LEU:HD13	1.96	0.46
2:P:107:GLU:HG3	2:P:147:TYR:OH	2.15	0.46
3:Q:58:VAL:O	3:Q:58:VAL:HG12	2.16	0.46
13:a:46:ASN:ND2	13:a:48:SER:H	2.12	0.46
6:h:129:ARG:HH11	6:h:129:ARG:HG2	1.79	0.46
10:l:1:MET:HB2	16:l:306:HOH:O	2.15	0.46
14:p:173:VAL:HG21	14:p:190:LEU:HD23	1.97	0.46
1:q:203:THR:H	1:q:206:ASN:HB2	1.80	0.46
3:C:41:VAL:HB	3:C:209:VAL:HG12	1.98	0.46
5:E:185:VAL:O	5:E:189:LEU:HD12	2.16	0.46
4:R:178:HIS:CE1	4:R:180:SER:HB3	2.51	0.46
12:Z:16:ALA:HB2	12:Z:121:VAL:HG23	1.97	0.46
12:Z:72:LEU:HD23	12:Z:83:MET:HE3	1.97	0.46
6:F:190:VAL:HG13	6:F:213:LEU:HD22	1.97	0.46
4:t:226:LEU:O	4:t:230:ILE:HG12	2.15	0.46
10:z:92:LEU:HD11	10:z:121:LEU:HD23	1.98	0.46
5:E:106:VAL:HA	5:E:109:ILE:HD12	1.98	0.46
6:F:27:MET:O	6:F:30:VAL:HG12	2.16	0.46
8:H:40:ASN:H	8:H:40:ASN:ND2	2.13	0.46
9:I:6:ASN:ND2	9:I:56:ALA:H	2.14	0.46
14:N:14:LEU:HD23	14:N:44:CYS:SG	2.55	0.46
10:X:171:PHE:CE2	10:X:173:LEU:HB2	2.51	0.46
1:c:74:VAL:HG12	1:c:75:TYR:N	2.31	0.46
3:e:145:GLN:HG2	3:e:155:TRP:NE1	2.31	0.46
9:k:124:ASP:HB2	9:k:128:CYS:H	1.81	0.46
2:r:170:ALA:HB2	2:r:199:THR:HG21	1.98	0.46
8:H:40:ASN:HD21	8:H:74:PRO:HG2	1.81	0.46
11:K:40:TYR:OH	11:K:74:ILE:O	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:k:35:THR:HG22	9:k:37:ASP:H	1.81	0.46
12:n:162:GLU:O	12:n:163:HIS:HB2	2.16	0.46
13:3:46:ASN:HD22	13:3:46:ASN:C	2.23	0.46
5:g:206:ASN:HD22	5:g:206:ASN:N	2.14	0.46
8:j:199:LEU:HB3	12:2:173:ARG:CZ	2.46	0.46
13:o:20:VAL:HG11	13:o:122:LEU:HD13	1.97	0.46
3:s:41:VAL:HB	3:s:209:VAL:HG12	1.97	0.46
13:3:126:ASP:HB2	13:3:130:VAL:HB	1.98	0.46
13:3:211:ILE:HD12	13:3:211:ILE:H	1.80	0.46
2:P:178:TYR:HA	2:P:183:MET:HE3	1.98	0.46
3:Q:147:ASP:HB2	3:Q:148:PRO:HD2	1.98	0.46
5:g:148:ALA:HB3	6:h:82:ALA:HB1	1.98	0.46
8:j:163:ILE:HG23	8:j:170:GLY:HA2	1.96	0.46
5:u:118:GLN:HG3	6:v:129:ARG:HG3	1.98	0.46
13:3:92:LEU:CD2	13:3:112:ILE:HD11	2.46	0.46
1:c:147:GLN:HG3	1:c:162:MET:HE1	1.97	0.46
9:k:144:GLN:HE21	9:k:144:GLN:N	2.14	0.46
12:n:187:VAL:CG1	8:x:167:LEU:HB3	2.46	0.46
7:U:71:ILE:HG21	7:U:113:LEU:HD11	1.97	0.45
6:F:180:GLN:O	6:F:182:LYS:N	2.42	0.45
5:g:223:ASP:O	5:g:226:VAL:HG12	2.17	0.45
2:r:75:VAL:HG11	2:r:82:ALA:CB	2.46	0.45
2:r:178:TYR:HA	2:r:183:MET:HE3	1.97	0.45
2:d:1:SER:HB3	5:g:120:TYR:CZ	2.52	0.45
6:h:50:GLU:HB3	6:h:197:ILE:HG23	1.98	0.45
14:p:174:ILE:HB	14:p:189:LEU:HB2	1.97	0.45
6:v:108:LEU:HD11	6:v:137:LEU:HB3	1.97	0.45
11:1:11:GLY:HA2	11:1:104:TRP:HZ3	1.80	0.45
2:B:170:ALA:HB2	2:B:199:THR:HG21	1.98	0.45
5:S:95:VAL:HA	13:a:94:ARG:HG2	1.98	0.45
5:S:117:THR:O	6:T:129:ARG:NH1	2.48	0.45
5:S:212:VAL:HB	5:S:218:PHE:HD1	1.80	0.45
6:h:99:ARG:HD2	13:o:69:GLN:NE2	2.31	0.45
9:k:52:LEU:HB2	9:k:59:VAL:HG13	1.98	0.45
4:t:43:GLU:HB3	4:t:198:MET:HE2	1.98	0.45
7:w:12:ILE:HG13	7:w:14:ILE:HG12	1.99	0.45
9:y:36:THR:HG22	9:y:182:MET:HB3	1.97	0.45
4:D:28:THR:HA	4:D:163:GLY:HA3	1.99	0.45
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.97	0.45
7:i:72:THR:HG22	7:i:73:GLU:H	1.82	0.45
5:u:4:ASP:HB2	5:u:21:TYR:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:u:4:ASP:HB2	5:u:21:TYR:HE1	1.81	0.45
4:R:223:LYS:H	4:R:223:LYS:HD2	1.81	0.45
5:S:147:SER:C	5:S:149:ASN:H	2.25	0.45
13:o:46:ASN:ND2	13:o:49:THR:HG23	2.32	0.45
8:H:35:HIS:CG	8:H:56:THR:HG21	2.52	0.45
9:W:163:PHE:CE1	9:W:197:ARG:HD3	2.52	0.45
1:c:198:PHE:O	1:c:199:GLU:HG2	2.16	0.45
5:g:197:PRO:HG2	16:g:302:HOH:O	2.16	0.45
6:h:64:LYS:HD3	6:h:64:LYS:H	1.81	0.45
6:h:197:ILE:HG21	6:h:211:LEU:HD13	1.98	0.45
10:z:38:MET:HE1	10:z:60:ILE:HG22	1.98	0.45
12:2:72:LEU:HD23	12:2:83:MET:HE3	1.99	0.45
8:j:35:HIS:CG	8:j:56:THR:HG21	2.51	0.45
8:j:168:GLY:O	15:j:301:04C:H33	2.17	0.45
3:C:97:VAL:HG13	11:K:78:ALA:HB1	1.99	0.45
7:G:72:THR:HG22	7:G:73:GLU:H	1.82	0.45
3:s:29:SER:HB2	3:s:60:LYS:HE2	1.98	0.45
4:t:51:MET:SD	4:t:56:ILE:HD11	2.57	0.45
10:z:143:LEU:HD13	10:z:163:CYS:SG	2.57	0.45
5:E:51:SER:C	5:E:53:LEU:H	2.25	0.45
1:O:106:THR:O	1:O:110:VAL:HG23	2.17	0.45
10:X:1:MET:HB2	16:X:308:HOH:O	2.17	0.45
12:Z:149:LEU:HD23	12:Z:174:LEU:HD22	1.99	0.45
5:g:69:ILE:HG22	5:g:131:ILE:HG12	1.98	0.45
14:p:20:THR:HG22	15:p:301:04C:C5	2.47	0.45
3:s:46:LYS:HE2	3:s:162:ARG:HB3	1.97	0.45
5:u:10:TRP:H	6:v:22:GLN:HE22	1.65	0.45
7:w:78:VAL:HG12	7:w:138:ILE:HB	1.98	0.45
9:W:137:VAL:HG11	9:W:145:MET:HB3	2.00	0.44
10:X:101:ASN:HB3	10:X:132:HIS:CE1	2.51	0.44
12:Z:137:ALA:H	12:Z:146:GLN:HE21	1.65	0.44
9:k:13:MET:HB3	9:k:162:LEU:HD11	1.98	0.44
5:S:68:GLY:HA3	5:S:218:PHE:CZ	2.52	0.44
1:c:149:ASP:HB2	1:c:150:PRO:CD	2.46	0.44
15:j:301:04C:H41	15:j:301:04C:H29	1.86	0.44
11:m:139:MET:O	11:m:143:TYR:HB2	2.17	0.44
13:3:50:MET:CE	13:3:192:VAL:HG23	2.43	0.44
4:D:62:ILE:HD11	4:D:68:CYS:HB2	1.99	0.44
4:R:203:ASN:H	4:R:206:ASN:HD21	1.66	0.44
11:Y:35:ILE:HB	11:Y:45:MET:HE3	1.99	0.44
1:A:147:GLN:HG3	1:A:162:MET:HE1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:89:LEU:HG	2:B:113:LEU:HD13	1.99	0.44
2:B:153:GLY:O	3:C:80:ARG:NH2	2.50	0.44
3:C:167:VAL:HG13	3:C:193:ALA:HB1	1.99	0.44
4:D:44:LYS:HE3	4:D:208:GLU:HG3	1.99	0.44
8:H:18:THR:HB	8:H:31:CYS:H	1.81	0.44
4:R:149:ASP:HB2	4:R:150:PRO:HD2	2.00	0.44
5:S:47:LYS:CB	5:S:56:HIS:HB3	2.43	0.44
9:W:35:THR:HG22	9:W:37:ASP:H	1.83	0.44
11:m:18:SER:O	11:m:31:VAL:HG22	2.16	0.44
1:q:198:PHE:O	1:q:199:GLU:HG2	2.17	0.44
9:y:86:LEU:O	9:y:90:VAL:HG23	2.17	0.44
4:f:61:GLU:HB3	4:f:218:PHE:CD2	2.53	0.44
8:j:40:ASN:HD21	8:j:74:PRO:HG2	1.81	0.44
4:t:12:ARG:HD2	4:t:17:GLU:CD	2.43	0.44
4:t:28:THR:HA	4:t:163:GLY:HA3	1.98	0.44
7:w:181:LYS:NZ	7:w:196:THR:HG22	2.33	0.44
12:2:43:CYS:CB	12:2:196:CYS:SG	3.05	0.44
5:E:173:MET:HA	5:E:176:PHE:CD1	2.53	0.44
13:a:46:ASN:HD22	13:a:48:SER:H	1.66	0.44
5:u:221:TYR:HD2	5:u:225:ASP:HB3	1.82	0.44
10:z:118:MET:HA	10:z:123:ALA:O	2.17	0.44
9:I:141:CYS:HB2	9:I:144:GLN:HB2	2.00	0.44
10:J:35:MET:HG2	10:J:45:LEU:HD22	1.99	0.44
12:L:136:LYS:HA	12:L:146:GLN:NE2	2.33	0.44
13:M:59:ASP:HB3	13:M:108:ASN:HD21	1.82	0.44
5:S:42:VAL:HG22	5:S:211:ILE:HG12	2.00	0.44
6:T:34:SER:OG	6:T:65:ARG:NH1	2.51	0.44
9:W:64:GLN:HE22	10:X:85:ARG:NH1	2.16	0.44
11:Y:37:ILE:HG23	11:Y:60:ALA:HA	2.00	0.44
3:e:147:ASP:HB2	3:e:148:PRO:HD2	2.00	0.44
8:x:187:ARG:CB	8:x:188:PRO:HD3	2.37	0.44
9:I:52:LEU:HB2	9:I:59:VAL:HG13	1.99	0.44
8:V:75:ARG:HA	8:V:104:ASP:OD1	2.17	0.44
12:Z:153:VAL:HG13	12:Z:166:LEU:HD11	1.99	0.44
9:k:158:ASP:HB2	9:k:159:PRO:HD2	2.00	0.44
11:m:58:LEU:HD12	11:m:86:MET:SD	2.58	0.44
6:v:152:ASP:HB2	6:v:153:PRO:HD2	2.00	0.44
2:B:86:THR:HA	2:B:89:LEU:HD12	1.99	0.44
2:B:174:LEU:HD23	2:B:191:LEU:HD22	1.99	0.44
13:M:27:LEU:HD22	13:M:184:TYR:HB2	1.99	0.44
2:P:71:MET:HE3	2:P:71:MET:HB2	1.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:j:210:ALA:HB3	9:k:200:LYS:HB2	1.99	0.44
10:l:1:MET:HE2	10:l:1:MET:HB3	1.82	0.44
6:v:49:VAL:HG11	6:v:65:ARG:HB2	2.00	0.44
9:y:55:LEU:HB2	9:y:103:TYR:HB2	1.99	0.44
6:T:50:GLU:HB3	6:T:197:ILE:HG23	2.00	0.43
3:e:220:ASN:HD22	3:e:222:GLU:H	1.66	0.43
5:u:102:VAL:O	5:u:106:VAL:HG23	2.18	0.43
11:1:9:LEU:HB2	11:1:145:TYR:CE2	2.53	0.43
12:2:43:CYS:HB3	12:2:196:CYS:SG	2.58	0.43
8:H:31:CYS:SG	15:H:301:04C:C4	3.06	0.43
4:R:89:GLN:HB3	11:Y:61:ARG:HG3	1.99	0.43
6:F:197:ILE:HG21	6:F:211:LEU:HD13	1.98	0.43
13:M:46:ASN:ND2	13:M:49:THR:HG23	2.33	0.43
1:O:114:ALA:HB1	1:O:152:GLY:O	2.18	0.43
5:S:6:ASP:HB2	5:S:9:VAL:HG23	2.00	0.43
5:S:155:ALA:HB3	6:T:57:LEU:HD22	2.01	0.43
3:e:68:VAL:HG11	3:e:106:ILE:HG21	2.01	0.43
5:g:42:VAL:HG22	5:g:211:ILE:HG12	2.00	0.43
8:j:40:ASN:H	8:j:40:ASN:ND2	2.16	0.43
3:s:35:ARG:HA	3:s:40:VAL:HG13	1.99	0.43
3:s:182:THR:O	3:s:186:THR:HG22	2.18	0.43
6:v:66:LEU:HD22	6:v:212:GLU:HB3	2.00	0.43
1:A:51:GLN:HG3	1:A:56:TYR:HB2	2.00	0.43
6:F:152:ASP:HB2	6:F:153:PRO:HD2	2.00	0.43
8:H:168:GLY:O	15:H:301:04C:H33	2.18	0.43
9:I:105:GLU:HB2	9:I:138:SER:OG	2.18	0.43
11:Y:12:VAL:HB	11:Y:179:VAL:HB	1.99	0.43
6:h:27:MET:O	6:h:30:VAL:HG12	2.19	0.43
9:k:184:VAL:HB	9:k:199:LEU:HD12	1.99	0.43
3:s:50:ALA:C	3:s:52:LEU:H	2.26	0.43
7:w:49:ILE:CG2	7:w:78:VAL:HB	2.47	0.43
11:K:87:VAL:CG1	11:K:116:SER:HA	2.49	0.43
8:V:53:ASP:O	8:V:56:THR:HG22	2.19	0.43
9:W:106:PRO:HD2	9:W:123:LEU:HB2	2.00	0.43
1:c:58:GLU:HG2	1:c:205:ASP:HB3	1.99	0.43
9:k:141:CYS:HB3	9:k:177:ASP:HB2	1.99	0.43
10:z:41:LYS:O	10:z:106:GLY:HA2	2.18	0.43
1:A:45:LEU:HB3	1:A:74:VAL:CG2	2.48	0.43
1:A:158:LYS:HG3	2:B:56:ASP:HA	2.00	0.43
4:D:89:GLN:HB3	11:K:61:ARG:HG3	2.01	0.43
7:i:49:ILE:HG21	7:i:78:VAL:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:v:83:ASP:OD2	6:v:129:ARG:NH2	2.51	0.43
14:4:127:ILE:HD11	14:4:136:TYR:CE2	2.54	0.43
3:C:147:ASP:HB2	3:C:148:PRO:HD2	2.00	0.43
11:Y:11:GLY:HA2	11:Y:104:TRP:HZ3	1.83	0.43
12:Z:123:SER:HB3	12:Z:136:LYS:HG2	2.00	0.43
1:c:83:ARG:NH2	7:i:157:GLY:O	2.51	0.43
2:d:173:MET:HE1	2:d:198:LYS:HD2	2.00	0.43
4:f:96:ASN:ND2	11:m:57:ARG:HH22	2.16	0.43
6:h:108:LEU:HD11	6:h:137:LEU:HB3	1.99	0.43
9:k:35:THR:HG21	16:l:301:HOH:O	2.18	0.43
14:p:30:VAL:O	14:p:30:VAL:CG1	2.66	0.43
3:C:220:ASN:ND2	3:C:222:GLU:HB2	2.34	0.43
5:E:4:ASP:HB2	5:E:21:TYR:HE1	1.84	0.43
3:s:203:LYS:HE3	3:s:203:LYS:O	2.18	0.43
5:u:47:LYS:CB	5:u:56:HIS:HB3	2.46	0.43
4:D:42:VAL:HG11	4:D:58:LYS:HB2	2.01	0.43
10:J:146:TYR:HB2	10:J:159:LEU:HD13	2.00	0.43
8:V:20:ALA:HB2	15:V:301:04C:H42	2.00	0.43
12:Z:155:PHE:HA	12:Z:158:MET:HE2	2.01	0.43
1:c:67:ILE:HD11	1:c:73:LEU:CG	2.47	0.43
1:c:106:THR:O	1:c:110:VAL:HG23	2.18	0.43
4:f:119:ASP:HB2	5:g:122:ARG:HD3	2.01	0.43
5:g:221:TYR:HD2	5:g:225:ASP:HB2	1.83	0.43
6:h:99:ARG:HH11	13:o:69:GLN:NE2	2.17	0.43
12:2:12:VAL:HG13	12:2:109:ILE:HD12	2.00	0.43
6:T:50:GLU:HG3	6:T:50:GLU:O	2.19	0.43
5:g:35:LEU:HD13	5:g:184:LEU:HD13	2.01	0.43
5:g:201:ASP:HB3	5:g:236:ARG:HH11	1.83	0.43
11:m:20:ALA:HB2	15:m:301:04C:H42	2.01	0.43
12:n:83:MET:HG2	12:n:88:ILE:HG13	2.00	0.43
1:q:44:VAL:HG21	1:q:187:ILE:HA	2.01	0.43
4:t:202:LEU:HD21	4:t:230:ILE:HD12	2.00	0.43
13:3:147:GLN:HB3	13:3:148:PRO:HD3	2.01	0.43
8:H:6:VAL:HG23	8:H:124:TYR:HB3	2.01	0.42
11:K:7:LYS:HE2	11:K:124:THR:HA	2.00	0.42
1:O:149:ASP:HB2	1:O:150:PRO:CD	2.48	0.42
1:O:178:ASN:C	1:O:180:ASP:H	2.27	0.42
3:Q:218:ILE:H	3:Q:218:ILE:HG13	1.57	0.42
4:R:34:THR:HG22	4:R:37:GLY:O	2.19	0.42
4:R:58:LYS:HA	4:R:70:MET:HE2	2.01	0.42
11:Y:7:LYS:HE2	11:Y:124:THR:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:i:71:ILE:HD11	7:i:77:CYS:SG	2.59	0.42
10:l:23:SER:HB2	10:l:28:MET:HE2	2.01	0.42
10:l:54:VAL:O	10:l:58:GLU:HB2	2.19	0.42
6:v:51:LYS:HE2	6:v:210:GLU:HB2	2.01	0.42
6:F:123:THR:O	7:G:131:ARG:NH1	2.52	0.42
2:d:94:GLN:HG2	9:k:72:LEU:HD13	2.02	0.42
8:j:127:MET:C	8:j:131:SER:HB3	2.43	0.42
11:m:38:ASN:C	11:m:40:TYR:H	2.27	0.42
9:y:87:MET:HG3	9:y:121:CYS:SG	2.59	0.42
7:U:40:ALA:HB2	7:U:49:ILE:HD13	2.00	0.42
12:n:180:ILE:HD12	8:x:196:GLY:HA3	2.01	0.42
14:p:14:LEU:HD23	14:p:44:CYS:SG	2.59	0.42
6:v:111:LEU:O	6:v:115:VAL:HG23	2.19	0.42
5:E:233:LEU:HD23	5:E:233:LEU:H	1.83	0.42
4:R:138:VAL:HG22	4:R:143:PRO:HB3	2.02	0.42
10:X:143:LEU:HD13	10:X:163:CYS:SG	2.59	0.42
1:c:106:THR:H	1:c:139:ASN:ND2	2.18	0.42
2:d:86:THR:HA	2:d:89:LEU:HD12	1.99	0.42
3:e:220:ASN:HB2	3:e:221:PRO:HD2	2.01	0.42
10:l:35:MET:HG2	10:l:45:LEU:HD22	2.01	0.42
4:t:58:LYS:HA	4:t:70:MET:HE2	2.01	0.42
13:3:86:ARG:HG3	13:3:121:PHE:CE1	2.55	0.42
1:O:74:VAL:HG12	1:O:75:TYR:N	2.34	0.42
7:U:78:VAL:HG12	7:U:138:ILE:HB	2.01	0.42
5:u:68:GLY:HA3	5:u:218:PHE:CZ	2.54	0.42
5:u:173:MET:HA	5:u:176:PHE:CD1	2.54	0.42
9:y:92:ASN:O	9:y:93:LEU:HB3	2.20	0.42
13:3:122:LEU:HG	13:3:137:LEU:HD12	2.00	0.42
3:C:180:ILE:HA	3:C:186:THR:HG22	2.02	0.42
6:F:168:ALA:HB1	6:F:171:ALA:HB3	2.01	0.42
8:V:11:GLY:HA2	8:V:108:PRO:HB3	2.02	0.42
13:a:3:ASN:HA	13:a:4:PRO:HD2	1.93	0.42
1:c:53:SER:HB3	1:c:56:TYR:CD1	2.54	0.42
7:i:49:ILE:CG2	7:i:78:VAL:HB	2.49	0.42
13:o:126:ASP:HB3	13:o:128:LEU:H	1.84	0.42
2:r:171:VAL:HA	2:r:174:LEU:HD12	2.00	0.42
7:w:140:ILE:HD12	7:w:219:VAL:HG12	2.01	0.42
9:y:158:ASP:HB2	9:y:159:PRO:HD2	2.01	0.42
13:M:20:VAL:HG11	13:M:122:LEU:HD13	2.00	0.42
3:Q:41:VAL:HB	3:Q:209:VAL:HG12	2.01	0.42
7:U:49:ILE:CG2	7:U:78:VAL:HB	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:q:45:LEU:HD13	1:q:74:VAL:HG23	2.02	0.42
5:u:42:VAL:HG22	5:u:211:ILE:HG12	2.01	0.42
5:u:106:VAL:HG21	5:u:142:PHE:CG	2.55	0.42
9:y:33:MET:HE2	9:y:34:VAL:C	2.45	0.42
1:A:147:GLN:O	1:A:154:TYR:HA	2.20	0.42
10:J:9:GLY:HA3	10:J:12:TYR:CE2	2.55	0.42
6:T:168:ALA:HB1	6:T:171:ALA:HB3	2.00	0.42
3:e:50:ALA:O	3:e:52:LEU:N	2.47	0.42
5:g:38:LYS:HG3	5:g:39:THR:HG23	2.01	0.42
12:n:14:ALA:HA	12:n:22:ILE:O	2.19	0.42
2:r:13:PRO:HA	3:s:20:TYR:CE2	2.54	0.42
2:r:43:LEU:HG	2:r:189:LEU:HD12	2.00	0.42
6:v:34:SER:OG	6:v:65:ARG:NH1	2.52	0.42
8:x:162:GLY:O	8:x:166:ASP:HB3	2.19	0.42
5:E:51:SER:O	5:E:53:LEU:N	2.52	0.42
8:H:100:LEU:HB3	8:H:111:TYR:HB2	2.01	0.42
8:j:209:THR:HG22	9:k:199:LEU:CD2	2.50	0.42
4:t:73:LEU:HD12	4:t:130:GLY:HA3	2.01	0.42
5:u:186:LYS:NZ	5:u:232:GLY:HA3	2.34	0.42
3:C:130:ALA:O	3:C:145:GLN:HA	2.20	0.42
13:M:126:ASP:HB3	13:M:128:LEU:H	1.84	0.42
3:Q:39:ILE:HG22	3:Q:211:ARG:HG2	2.02	0.42
10:X:49:GLU:HB2	10:X:99:HIS:HB2	2.02	0.42
1:c:53:SER:C	1:c:55:LEU:H	2.28	0.42
3:e:50:ALA:C	3:e:52:LEU:N	2.76	0.42
10:l:1:MET:HE1	10:l:134:TYR:N	2.35	0.42
12:n:136:LYS:HA	12:n:146:GLN:NE2	2.35	0.42
1:q:83:ARG:NH1	7:w:119:ASP:OD1	2.53	0.42
1:q:147:GLN:HG3	1:q:162:MET:CE	2.50	0.42
8:x:116:HIS:HD2	16:x:402:HOH:O	2.03	0.42
5:E:47:LYS:CB	5:E:56:HIS:HB3	2.50	0.41
6:F:50:GLU:HB3	6:F:197:ILE:HG23	2.02	0.41
8:H:8:TYR:CE1	8:H:10:ASP:HB2	2.55	0.41
4:R:91:HIS:CG	4:R:99:MET:HG3	2.55	0.41
5:S:168:TYR:OH	5:S:190:ARG:HD2	2.20	0.41
4:f:28:THR:HA	4:f:163:GLY:HA3	2.02	0.41
6:h:111:LEU:O	6:h:115:VAL:HG23	2.20	0.41
8:j:6:VAL:HG23	8:j:124:TYR:HB3	2.01	0.41
9:k:113:PRO:O	9:k:114:LYS:HB2	2.20	0.41
14:p:164:MET:HB3	14:p:171:GLY:HA2	2.03	0.41
14:p:199:ILE:HD12	14:p:199:ILE:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:y:19:VAL:CG1	9:y:109:ALA:HB1	2.49	0.41
9:y:97:LYS:O	9:y:101:PRO:HA	2.20	0.41
9:y:154:GLU:HB2	9:y:157:MET:HE3	2.02	0.41
11:1:37:ILE:HG23	11:1:60:ALA:HA	2.02	0.41
12:2:14:ALA:HA	12:2:22:ILE:O	2.19	0.41
5:E:153:CYS:HB3	6:F:58:TYR:HD2	1.85	0.41
15:H:301:04C:H41	15:H:301:04C:H29	1.84	0.41
14:N:147:MET:HE2	14:N:151:GLU:HB3	2.02	0.41
4:R:61:GLU:HB3	4:R:218:PHE:CD2	2.55	0.41
5:S:221:TYR:HD2	5:S:225:ASP:HB3	1.86	0.41
14:b:148:THR:HG22	14:b:151:GLU:OE2	2.20	0.41
2:r:1:SER:HB3	5:u:120:TYR:CE2	2.56	0.41
6:v:168:ALA:HB1	6:v:171:ALA:HB3	2.01	0.41
11:1:138:VAL:HG21	11:1:159:ALA:HA	2.02	0.41
13:3:4:PRO:HG3	13:3:107:TRP:CE2	2.55	0.41
2:B:52:HIS:H	2:B:55:LEU:HD12	1.84	0.41
7:G:48:VAL:HG11	7:G:194:VAL:HA	2.01	0.41
8:H:11:GLY:HA2	8:H:108:PRO:HB3	2.01	0.41
10:J:38:MET:HE1	10:J:60:ILE:HG22	2.02	0.41
13:M:50:MET:HE2	13:M:192:VAL:HG23	2.02	0.41
8:V:50:ALA:HB2	9:W:128:CYS:HB2	2.02	0.41
6:h:37:ILE:HG22	6:h:197:ILE:HD11	2.00	0.41
6:h:152:ASP:HB2	6:h:153:PRO:HD2	2.01	0.41
6:h:207:LYS:HG2	6:h:208:ALA:H	1.85	0.41
9:k:14:LYS:HG3	9:k:120:ILE:HG12	2.02	0.41
9:k:148:MET:CG	9:k:169:ALA:HA	2.50	0.41
2:r:89:LEU:HG	2:r:113:LEU:HD13	2.02	0.41
10:J:138:LEU:HD21	10:X:26:VAL:HG12	2.01	0.41
14:N:18:SER:HB2	14:N:30:VAL:HA	2.01	0.41
14:N:174:ILE:HB	14:N:189:LEU:HB2	2.02	0.41
1:O:53:SER:C	1:O:55:LEU:H	2.28	0.41
7:U:140:ILE:HG22	7:U:150:VAL:HG22	2.01	0.41
3:e:50:ALA:O	3:e:51:LYS:HG3	2.20	0.41
6:h:39:ILE:HD11	6:h:181:MET:HB3	2.02	0.41
8:j:8:TYR:CE1	8:j:10:ASP:HB2	2.55	0.41
9:k:6:ASN:ND2	9:k:56:ALA:H	2.18	0.41
4:t:92:TRP:CE3	4:t:92:TRP:O	2.73	0.41
2:B:115:ASP:OD1	3:C:80:ARG:NH1	2.54	0.41
7:G:45:ASP:O	7:G:221:VAL:HG23	2.20	0.41
9:I:122:SER:HB3	9:I:136:VAL:HB	2.03	0.41
1:O:147:GLN:HG3	1:O:162:MET:CE	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:136:MET:CE	6:T:163:CYS:HB3	2.46	0.41
10:X:19:ARG:HA	10:X:32:HIS:O	2.21	0.41
2:d:36:ILE:HD11	2:d:192:ALA:HB2	2.03	0.41
4:f:62:ILE:HD11	4:f:68:CYS:HB2	2.03	0.41
11:m:11:GLY:HA2	11:m:104:TRP:HZ3	1.85	0.41
6:F:187:ARG:NH2	6:F:231:ILE:HG23	2.36	0.41
15:N:301:04C:H22	15:N:301:04C:H8	2.03	0.41
7:U:24:VAL:HG21	7:U:125:THR:OG1	2.21	0.41
11:Y:7:LYS:HB3	11:Y:12:VAL:HG22	2.01	0.41
2:d:115:ASP:OD1	3:e:80:ARG:NH1	2.53	0.41
8:j:31:CYS:SG	15:j:301:04C:H42	2.60	0.41
2:r:247:GLU:HB3	2:r:248:ARG:H	1.69	0.41
8:x:40:ASN:H	8:x:40:ASN:HD22	1.67	0.41
8:x:53:ASP:O	8:x:56:THR:HG22	2.20	0.41
11:l:8:PHE:CE1	11:l:10:HIS:HB2	2.55	0.41
1:A:212:CYS:HB2	1:A:217:PHE:HD1	1.86	0.41
3:C:39:ILE:HG22	3:C:211:ARG:HG2	2.01	0.41
2:P:13:PRO:HA	3:Q:20:TYR:CE2	2.55	0.41
13:o:37:ARG:HG2	13:o:184:TYR:CZ	2.56	0.41
8:x:18:THR:HB	8:x:30:ASN:HA	2.03	0.41
1:A:53:SER:HB3	1:A:56:TYR:CD1	2.56	0.41
14:N:160:LEU:O	14:N:164:MET:HG3	2.21	0.41
6:T:108:LEU:HD11	6:T:137:LEU:HB3	2.02	0.41
3:e:101:VAL:HG11	3:e:106:ILE:HG12	2.03	0.41
8:j:124:TYR:CD1	8:j:138:PHE:HB3	2.56	0.41
11:m:138:VAL:CG2	11:m:159:ALA:HA	2.51	0.41
7:G:174:SER:O	7:G:178:LEU:HD22	2.21	0.41
2:P:114:CYS:HB3	2:P:153:GLY:O	2.21	0.41
3:Q:79:ALA:HA	3:Q:128:ILE:HD13	2.02	0.41
5:S:156:MET:HE3	5:S:157:SER:H	1.86	0.41
3:e:228:VAL:O	3:e:232:GLU:HB2	2.21	0.41
8:j:187:ARG:CB	8:j:188:PRO:HD3	2.40	0.41
9:k:14:LYS:HG2	9:k:118:PRO:HB2	2.02	0.41
10:l:101:ASN:HB3	10:l:132:HIS:CE1	2.56	0.41
12:n:28:ARG:HG3	12:n:191:ASP:OD2	2.20	0.41
4:t:76:ASP:OD2	4:t:127:ARG:NH2	2.54	0.41
5:u:230:LEU:C	5:u:232:GLY:H	2.28	0.41
7:w:207:ILE:O	7:w:208:ASP:HB2	2.21	0.41
8:x:168:GLY:O	15:x:301:04C:H33	2.21	0.41
9:y:6:ASN:ND2	9:y:55:LEU:O	2.54	0.41
13:3:43:MET:SD	13:3:64:LYS:HG3	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ILE:HD11	1:A:73:LEU:CG	2.48	0.41
5:E:201:ASP:HB3	5:E:236:ARG:HH11	1.84	0.41
6:F:65:ARG:NH1	6:F:78:ALA:HA	2.27	0.41
5:S:66:HIS:O	5:S:133:GLY:HA2	2.21	0.41
5:S:169:LEU:O	5:S:173:MET:HB3	2.21	0.41
1:c:70:HIS:CE1	1:c:103:PRO:HB3	2.55	0.41
3:e:79:ALA:HB2	3:e:128:ILE:HG21	2.01	0.41
2:r:118:GLN:HE22	2:r:122:GLN:NE2	2.20	0.41
3:s:11:PRO:HA	4:t:18:TYR:CD2	2.56	0.41
11:1:4:LEU:HD21	11:1:159:ALA:HB3	2.03	0.41
13:3:11:VAL:H	13:3:139:THR:HG1	1.67	0.41
14:4:127:ILE:HD12	14:4:132:SER:HB2	2.02	0.41
5:E:147:SER:C	5:E:149:ASN:H	2.29	0.40
5:E:193:ARG:HD3	5:E:236:ARG:HD3	2.03	0.40
8:H:187:ARG:CB	8:H:188:PRO:HD3	2.40	0.40
10:J:102:LEU:HD11	10:J:118:MET:HE2	2.03	0.40
1:O:45:LEU:HD13	1:O:74:VAL:HG23	2.03	0.40
6:T:77:VAL:HG11	6:T:84:ALA:HB1	2.03	0.40
7:w:9:ASP:HA	7:w:14:ILE:HG13	2.02	0.40
10:z:49:GLU:HB2	10:z:99:HIS:HB2	2.03	0.40
13:3:105:PRO:HB2	16:3:334:HOH:O	2.20	0.40
8:H:53:ASP:O	8:H:56:THR:HG22	2.21	0.40
10:J:15:VAL:HB	10:J:45:LEU:HD11	2.03	0.40
11:K:58:LEU:HD12	11:K:86:MET:SD	2.61	0.40
9:W:144:GLN:HE21	9:W:144:GLN:N	2.18	0.40
10:X:32:HIS:ND1	10:X:34:LYS:HE3	2.36	0.40
14:b:127:ILE:HD11	14:b:136:TYR:CE2	2.56	0.40
10:l:138:LEU:HD21	10:z:26:VAL:HG12	2.02	0.40
7:G:49:ILE:CG2	7:G:78:VAL:HB	2.52	0.40
4:R:51:MET:SD	4:R:56:ILE:HD11	2.61	0.40
4:R:121:ASP:HB3	4:R:122:PRO:HD2	2.03	0.40
1:q:187:ILE:O	1:q:191:ILE:HD12	2.22	0.40
4:t:157:CYS:HA	5:u:54:ALA:HA	2.02	0.40
11:1:7:LYS:HB3	11:1:12:VAL:HG22	2.02	0.40
11:K:38:ASN:C	11:K:40:TYR:H	2.30	0.40
1:O:73:LEU:HD21	1:O:133:LEU:HB3	2.03	0.40
8:j:18:THR:HB	8:j:31:CYS:H	1.86	0.40
13:o:46:ASN:ND2	13:o:48:SER:H	2.11	0.40
3:s:157:ALA:HB3	4:t:50:LEU:HD22	2.02	0.40
4:t:174:GLN:HG2	5:u:53:LEU:HD23	2.02	0.40
6:v:67:PHE:HB2	6:v:75:MET:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:v:77:VAL:HG11	6:v:84:ALA:HB1	2.04	0.40
7:w:106:TYR:OH	8:x:66:HIS:HE1	2.05	0.40
10:z:19:ARG:HA	10:z:32:HIS:O	2.21	0.40
4:D:61:GLU:HB3	4:D:218:PHE:CD2	2.57	0.40
9:I:144:GLN:HE21	9:I:144:GLN:N	2.19	0.40
2:d:71:MET:HE3	2:d:71:MET:HB2	1.87	0.40
2:d:200:MET:HE1	2:d:209:LYS:HB3	2.04	0.40
8:j:53:ASP:O	8:j:56:THR:HG22	2.22	0.40
7:w:40:ALA:HB2	7:w:49:ILE:HD13	2.02	0.40
11:l:158:ARG:HE	11:l:162:GLN:HE21	1.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	229/234 (98%)	214 (93%)	9 (4%)	6 (3%)	4	17
1	O	229/234 (98%)	215 (94%)	9 (4%)	5 (2%)	5	20
1	c	229/234 (98%)	217 (95%)	7 (3%)	5 (2%)	5	20
1	q	229/234 (98%)	216 (94%)	9 (4%)	4 (2%)	7	26
2	B	246/261 (94%)	239 (97%)	7 (3%)	0	100	100
2	P	246/261 (94%)	238 (97%)	8 (3%)	0	100	100
2	d	246/261 (94%)	237 (96%)	9 (4%)	0	100	100
2	r	246/261 (94%)	239 (97%)	6 (2%)	1 (0%)	30	59
3	C	237/248 (96%)	220 (93%)	15 (6%)	2 (1%)	16	44
3	Q	237/248 (96%)	227 (96%)	8 (3%)	2 (1%)	16	44
3	e	237/248 (96%)	224 (94%)	10 (4%)	3 (1%)	9	32
3	s	237/248 (96%)	225 (95%)	11 (5%)	1 (0%)	30	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	231/241 (96%)	222 (96%)	9 (4%)	0	100	100
4	R	231/241 (96%)	220 (95%)	10 (4%)	1 (0%)	30	59
4	f	231/241 (96%)	217 (94%)	14 (6%)	0	100	100
4	t	231/241 (96%)	219 (95%)	12 (5%)	0	100	100
5	E	236/263 (90%)	223 (94%)	10 (4%)	3 (1%)	9	32
5	S	236/263 (90%)	219 (93%)	15 (6%)	2 (1%)	16	44
5	g	236/263 (90%)	220 (93%)	15 (6%)	1 (0%)	30	59
5	u	236/263 (90%)	221 (94%)	14 (6%)	1 (0%)	30	59
6	F	242/255 (95%)	232 (96%)	8 (3%)	2 (1%)	16	44
6	T	242/255 (95%)	234 (97%)	8 (3%)	0	100	100
6	h	242/255 (95%)	235 (97%)	5 (2%)	2 (1%)	16	44
6	v	242/255 (95%)	233 (96%)	7 (3%)	2 (1%)	16	44
7	G	241/246 (98%)	235 (98%)	3 (1%)	3 (1%)	10	34
7	U	241/246 (98%)	235 (98%)	6 (2%)	0	100	100
7	i	241/246 (98%)	234 (97%)	5 (2%)	2 (1%)	16	44
7	w	241/246 (98%)	234 (97%)	6 (2%)	1 (0%)	30	59
8	H	218/234 (93%)	213 (98%)	5 (2%)	0	100	100
8	V	218/234 (93%)	210 (96%)	8 (4%)	0	100	100
8	j	218/234 (93%)	212 (97%)	6 (3%)	0	100	100
8	x	218/234 (93%)	210 (96%)	7 (3%)	1 (0%)	24	54
9	I	202/205 (98%)	188 (93%)	9 (4%)	5 (2%)	4	17
9	W	202/205 (98%)	189 (94%)	12 (6%)	1 (0%)	24	54
9	k	202/205 (98%)	187 (93%)	12 (6%)	3 (2%)	8	28
9	y	202/205 (98%)	183 (91%)	16 (8%)	3 (2%)	8	28
10	J	194/201 (96%)	187 (96%)	6 (3%)	1 (0%)	24	54
10	X	194/201 (96%)	188 (97%)	4 (2%)	2 (1%)	12	39
10	l	194/201 (96%)	186 (96%)	7 (4%)	1 (0%)	24	54
10	z	194/201 (96%)	186 (96%)	7 (4%)	1 (0%)	24	54
11	1	199/205 (97%)	192 (96%)	7 (4%)	0	100	100
11	K	199/205 (97%)	193 (97%)	6 (3%)	0	100	100
11	Y	199/205 (97%)	196 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	m	199/205 (97%)	192 (96%)	7 (4%)	0	100	100
12	2	211/213 (99%)	204 (97%)	5 (2%)	2 (1%)	14	41
12	L	211/213 (99%)	204 (97%)	6 (3%)	1 (0%)	24	54
12	Z	211/213 (99%)	200 (95%)	11 (5%)	0	100	100
12	n	211/213 (99%)	205 (97%)	6 (3%)	0	100	100
13	3	214/219 (98%)	200 (94%)	13 (6%)	1 (0%)	24	54
13	M	214/219 (98%)	203 (95%)	10 (5%)	1 (0%)	24	54
13	a	214/219 (98%)	202 (94%)	11 (5%)	1 (0%)	24	54
13	o	214/219 (98%)	206 (96%)	7 (3%)	1 (0%)	24	54
14	4	200/205 (98%)	193 (96%)	7 (4%)	0	100	100
14	N	200/205 (98%)	191 (96%)	8 (4%)	1 (0%)	24	54
14	b	200/205 (98%)	189 (94%)	10 (5%)	1 (0%)	24	54
14	p	200/205 (98%)	188 (94%)	11 (6%)	1 (0%)	24	54
All	All	12400/12920 (96%)	11841 (96%)	482 (4%)	77 (1%)	21	51

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	181	MET
14	N	191	GLY
1	O	54	ILE
5	S	52	GLU
10	X	24	ASN
6	h	181	MET
10	l	24	ASN
1	q	52	LYS
5	u	52	GLU
10	z	24	ASN
12	2	163	HIS
1	A	41	ASN
3	C	200	SER
10	J	24	ASN
12	L	163	HIS
1	O	52	LYS
1	O	199	GLU
3	Q	49	VAL
5	S	148	ALA

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Mol	Chain	Res	Type
14	b	191	GLY
1	c	41	ASN
1	c	180	ASP
3	e	51	LYS
9	k	46	ASP
14	p	191	GLY
1	q	54	ILE
9	y	100	GLY
1	A	54	ILE
1	A	180	ASP
1	A	199	GLU
5	E	52	GLU
7	G	2	ARG
9	I	100	GLY
9	W	46	ASP
1	c	199	GLU
3	e	200	SER
1	q	199	GLU
3	s	49	VAL
9	y	46	ASP
9	y	116	PHE
13	3	9	THR
1	A	201	GLN
3	C	215	PRO
9	I	155	PRO
13	M	9	THR
1	O	41	ASN
3	Q	200	SER
10	X	50	ALA
1	c	201	GLN
5	g	237	PRO
6	h	207	LYS
7	i	2	ARG
9	k	155	PRO
13	o	9	THR
6	v	207	LYS
5	E	148	ALA
5	E	237	PRO
7	G	208	ASP
7	G	242	ALA
9	I	16	LYS
13	a	9	THR

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Mol	Chain	Res	Type
7	i	208	ASP
1	q	201	GLN
2	r	205	LEU
12	2	191	ASP
6	F	4	GLY
9	I	45	GLY
9	I	116	PHE
1	O	201	GLN
9	k	100	GLY
6	v	3	ILE
7	w	208	ASP
1	c	54	ILE
4	R	123	GLY
3	e	215	PRO
8	x	187	ARG
1	A	200	GLY

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	189/191 (99%)	183 (97%)	6 (3%)	34	68
1	O	189/191 (99%)	185 (98%)	4 (2%)	47	77
1	c	189/191 (99%)	185 (98%)	4 (2%)	47	77
1	q	189/191 (99%)	183 (97%)	6 (3%)	34	68
2	B	208/221 (94%)	195 (94%)	13 (6%)	16	45
2	P	208/221 (94%)	194 (93%)	14 (7%)	15	43
2	d	208/221 (94%)	195 (94%)	13 (6%)	16	45
2	r	208/221 (94%)	196 (94%)	12 (6%)	18	49
3	C	202/210 (96%)	189 (94%)	13 (6%)	16	44
3	Q	202/210 (96%)	192 (95%)	10 (5%)	22	53
3	e	202/210 (96%)	188 (93%)	14 (7%)	14	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	s	202/210 (96%)	188 (93%)	14 (7%)	14	41
4	D	195/203 (96%)	186 (95%)	9 (5%)	24	57
4	R	195/203 (96%)	185 (95%)	10 (5%)	21	53
4	f	195/203 (96%)	187 (96%)	8 (4%)	27	61
4	t	195/203 (96%)	186 (95%)	9 (5%)	24	57
5	E	204/224 (91%)	193 (95%)	11 (5%)	20	51
5	S	204/224 (91%)	194 (95%)	10 (5%)	22	54
5	g	204/224 (91%)	190 (93%)	14 (7%)	14	41
5	u	204/224 (91%)	197 (97%)	7 (3%)	32	66
6	F	200/211 (95%)	192 (96%)	8 (4%)	28	62
6	T	200/211 (95%)	191 (96%)	9 (4%)	24	58
6	h	200/211 (95%)	190 (95%)	10 (5%)	22	53
6	v	200/211 (95%)	189 (94%)	11 (6%)	19	50
7	G	207/210 (99%)	197 (95%)	10 (5%)	23	55
7	U	207/210 (99%)	196 (95%)	11 (5%)	20	52
7	i	207/210 (99%)	195 (94%)	12 (6%)	18	49
7	w	207/210 (99%)	196 (95%)	11 (5%)	20	52
8	H	181/195 (93%)	173 (96%)	8 (4%)	25	59
8	V	181/195 (93%)	175 (97%)	6 (3%)	33	67
8	j	181/195 (93%)	169 (93%)	12 (7%)	15	43
8	x	181/195 (93%)	167 (92%)	14 (8%)	12	35
9	I	174/175 (99%)	170 (98%)	4 (2%)	44	76
9	W	174/175 (99%)	171 (98%)	3 (2%)	53	82
9	k	174/175 (99%)	168 (97%)	6 (3%)	32	66
9	y	174/175 (99%)	165 (95%)	9 (5%)	21	52
10	J	166/171 (97%)	160 (96%)	6 (4%)	31	65
10	X	166/171 (97%)	160 (96%)	6 (4%)	31	65
10	l	166/171 (97%)	158 (95%)	8 (5%)	23	55
10	z	166/171 (97%)	159 (96%)	7 (4%)	26	60
11	1	157/161 (98%)	149 (95%)	8 (5%)	21	53
11	K	157/161 (98%)	151 (96%)	6 (4%)	29	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	Y	157/161 (98%)	147 (94%)	10 (6%)	16	44
11	m	157/161 (98%)	152 (97%)	5 (3%)	34	68
12	2	178/178 (100%)	173 (97%)	5 (3%)	38	72
12	L	178/178 (100%)	171 (96%)	7 (4%)	28	63
12	Z	178/178 (100%)	173 (97%)	5 (3%)	38	72
12	n	178/178 (100%)	172 (97%)	6 (3%)	32	66
13	3	178/180 (99%)	173 (97%)	5 (3%)	38	72
13	M	178/180 (99%)	172 (97%)	6 (3%)	32	66
13	a	178/180 (99%)	173 (97%)	5 (3%)	38	72
13	o	178/180 (99%)	172 (97%)	6 (3%)	32	66
14	4	159/162 (98%)	154 (97%)	5 (3%)	35	69
14	N	159/162 (98%)	154 (97%)	5 (3%)	35	69
14	b	159/162 (98%)	154 (97%)	5 (3%)	35	69
14	p	159/162 (98%)	153 (96%)	6 (4%)	29	64
All	All	10392/10768 (96%)	9925 (96%)	467 (4%)	24	58

All (467) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	19	VAL
1	A	28	VAL
1	A	43	VAL
1	A	74	VAL
1	A	229	LEU
2	B	24	MET
2	B	27	ILE
2	B	43	LEU
2	B	49	ARG
2	B	51	ILE
2	B	79	THR
2	B	97	LEU
2	B	186	LYS
2	B	191	LEU
2	B	200	MET
2	B	204	LYS
2	B	217	ARG

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Mol	Chain	Res	Type
2	B	221	LYS
3	C	41	VAL
3	C	42	LEU
3	C	124	ARG
3	C	140	THR
3	C	145	GLN
3	C	160	ILE
3	C	165	LYS
3	C	171	LEU
3	C	203	LYS
3	C	206	GLU
3	C	207	LEU
3	C	217	LYS
3	C	233	LYS
4	D	12	ARG
4	D	70	MET
4	D	81	ILE
4	D	131	VAL
4	D	162	ILE
4	D	195	LYS
4	D	209	LEU
4	D	216	GLN
4	D	229	VAL
5	E	7	VAL
5	E	35	LEU
5	E	53	LEU
5	E	59	LYS
5	E	71	ILE
5	E	98	ARG
5	E	153	CYS
5	E	184	LEU
5	E	205	LYS
5	E	226	VAL
5	E	238	GLN
6	F	56	LYS
6	F	66	LEU
6	F	90	ILE
6	F	180	GLN
6	F	181	MET
6	F	200	VAL
6	F	205	LYS
6	F	219	LEU

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Mol	Chain	Res	Type
7	G	51	THR
7	G	59	LEU
7	G	113	LEU
7	G	131	ARG
7	G	142	ILE
7	G	165	THR
7	G	178	LEU
7	G	185	LYS
7	G	204	VAL
7	G	220	THR
8	H	6	VAL
8	H	12	ILE
8	H	40	ASN
8	H	56	THR
8	H	68	LEU
8	H	121	LYS
8	H	180	LYS
8	H	198	ARG
9	I	19	VAL
9	I	70	LEU
9	I	144	GLN
9	I	174	VAL
10	J	47	VAL
10	J	68	LYS
10	J	85	ARG
10	J	143	LEU
10	J	154	GLU
10	J	167	LEU
11	K	35	ILE
11	K	41	LEU
11	K	58	LEU
11	K	71	LYS
11	K	73	ARG
11	K	93	MET
12	L	43	CYS
12	L	72	LEU
12	L	148	LEU
12	L	160	ASN
12	L	174	LEU
12	L	208	VAL
12	L	212	LYS
13	M	46	ASN

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Mol	Chain	Res	Type
13	M	49	THR
13	M	94	ARG
13	M	152	GLU
13	M	192	VAL
13	M	195	LYS
14	N	20	THR
14	N	139	VAL
14	N	173	VAL
14	N	194	ILE
14	N	201	THR
1	O	2	LYS
1	O	19	VAL
1	O	28	VAL
1	O	54	ILE
2	P	24	MET
2	P	27	ILE
2	P	36	ILE
2	P	43	LEU
2	P	51	ILE
2	P	55	LEU
2	P	63	LYS
2	P	97	LEU
2	P	149	SER
2	P	216	THR
2	P	217	ARG
2	P	221	LYS
2	P	240	GLU
2	P	247	GLU
3	Q	41	VAL
3	Q	42	LEU
3	Q	106	ILE
3	Q	124	ARG
3	Q	133	VAL
3	Q	145	GLN
3	Q	168	ARG
3	Q	171	LEU
3	Q	207	LEU
3	Q	218	ILE
4	R	2	ARG
4	R	33	GLN
4	R	81	ILE
4	R	131	VAL

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Mol	Chain	Res	Type
4	R	144	GLN
4	R	179	LYS
4	R	195	LYS
4	R	206	ASN
4	R	223	LYS
4	R	229	VAL
5	S	35	LEU
5	S	52	GLU
5	S	57	GLN
5	S	81	LEU
5	S	98	ARG
5	S	179	CYS
5	S	189	LEU
5	S	203	THR
5	S	214	LYS
5	S	216	LEU
6	T	3	ILE
6	T	28	LYS
6	T	66	LEU
6	T	90	ILE
6	T	170	GLN
6	T	181	MET
6	T	200	VAL
6	T	219	LEU
6	T	237	LYS
7	U	51	THR
7	U	58	LYS
7	U	72	THR
7	U	80	THR
7	U	113	LEU
7	U	125	THR
7	U	165	THR
7	U	178	LEU
7	U	185	LYS
7	U	204	VAL
7	U	220	THR
8	V	6	VAL
8	V	12	ILE
8	V	40	ASN
8	V	56	THR
8	V	68	LEU
8	V	204	CYS

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Mol	Chain	Res	Type
9	W	117	LYS
9	W	144	GLN
9	W	174	VAL
10	X	45	LEU
10	X	47	VAL
10	X	103	LEU
10	X	143	LEU
10	X	154	GLU
10	X	167	LEU
11	Y	32	LYS
11	Y	41	LEU
11	Y	58	LEU
11	Y	62	GLN
11	Y	71	LYS
11	Y	87	VAL
11	Y	138	VAL
11	Y	148	LYS
11	Y	176	LEU
11	Y	186	ARG
12	Z	106	VAL
12	Z	148	LEU
12	Z	158	MET
12	Z	174	LEU
12	Z	201	GLU
13	a	14	VAL
13	a	37	ARG
13	a	46	ASN
13	a	94	ARG
13	a	119	GLU
14	b	68	ILE
14	b	72	GLU
14	b	139	VAL
14	b	194	ILE
14	b	201	THR
1	c	19	VAL
1	c	28	VAL
1	c	43	VAL
1	c	209	VAL
2	d	24	MET
2	d	27	ILE
2	d	36	ILE
2	d	43	LEU

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Mol	Chain	Res	Type
2	d	51	ILE
2	d	63	LYS
2	d	97	LEU
2	d	186	LYS
2	d	209	LYS
2	d	217	ARG
2	d	240	GLU
2	d	242	GLU
2	d	248	ARG
3	e	4	ARG
3	e	22	GLN
3	e	41	VAL
3	e	51	LYS
3	e	58	VAL
3	e	103	VAL
3	e	106	ILE
3	e	140	THR
3	e	145	GLN
3	e	160	ILE
3	e	165	LYS
3	e	171	LEU
3	e	203	LYS
3	e	224	ILE
4	f	70	MET
4	f	81	ILE
4	f	162	ILE
4	f	178	HIS
4	f	195	LYS
4	f	201	LYS
4	f	209	LEU
4	f	229	VAL
5	g	35	LEU
5	g	53	LEU
5	g	59	LYS
5	g	71	ILE
5	g	98	ARG
5	g	112	LYS
5	g	136	ASP
5	g	153	CYS
5	g	184	LEU
5	g	205	LYS
5	g	206	ASN

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Mol	Chain	Res	Type
5	g	217	GLU
5	g	225	ASP
5	g	226	VAL
6	h	39	ILE
6	h	66	LEU
6	h	90	ILE
6	h	124	LEU
6	h	129	ARG
6	h	165	ILE
6	h	181	MET
6	h	200	VAL
6	h	219	LEU
6	h	240	LYS
7	i	18	GLU
7	i	51	THR
7	i	58	LYS
7	i	83	THR
7	i	113	LEU
7	i	131	ARG
7	i	165	THR
7	i	178	LEU
7	i	185	LYS
7	i	204	VAL
7	i	220	THR
7	i	241	LEU
8	j	6	VAL
8	j	12	ILE
8	j	40	ASN
8	j	56	THR
8	j	68	LEU
8	j	89	ARG
8	j	121	LYS
8	j	180	LYS
8	j	199	LEU
8	j	202	TYR
8	j	211	VAL
8	j	216	VAL
9	k	16	LYS
9	k	114	LYS
9	k	136	VAL
9	k	144	GLN
9	k	152	LEU

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Mol	Chain	Res	Type
9	k	174	VAL
10	l	1	MET
10	l	47	VAL
10	l	68	LYS
10	l	85	ARG
10	l	95	ARG
10	l	143	LEU
10	l	154	GLU
10	l	167	LEU
11	m	35	ILE
11	m	41	LEU
11	m	58	LEU
11	m	87	VAL
11	m	97	MET
12	n	43	CYS
12	n	72	LEU
12	n	148	LEU
12	n	160	ASN
12	n	173	ARG
12	n	174	LEU
13	o	46	ASN
13	o	49	THR
13	o	94	ARG
13	o	152	GLU
13	o	192	VAL
13	o	195	LYS
14	p	6	VAL
14	p	30	VAL
14	p	31	THR
14	p	139	VAL
14	p	190	LEU
14	p	196	LYS
1	q	2	LYS
1	q	17	LYS
1	q	19	VAL
1	q	28	VAL
1	q	176	ARG
1	q	191	ILE
2	r	24	MET
2	r	27	ILE
2	r	43	LEU
2	r	51	ILE

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Mol	Chain	Res	Type
2	r	99	GLN
2	r	198	LYS
2	r	217	ARG
2	r	228	LYS
2	r	230	LYS
2	r	238	LYS
2	r	240	GLU
2	r	247	GLU
3	s	4	ARG
3	s	41	VAL
3	s	106	ILE
3	s	124	ARG
3	s	145	GLN
3	s	160	ILE
3	s	171	LEU
3	s	176	THR
3	s	177	ASP
3	s	203	LYS
3	s	207	LEU
3	s	218	ILE
3	s	231	ILE
3	s	237	GLU
4	t	81	ILE
4	t	92	TRP
4	t	131	VAL
4	t	144	GLN
4	t	179	LYS
4	t	195	LYS
4	t	206	ASN
4	t	209	LEU
4	t	229	VAL
5	u	35	LEU
5	u	53	LEU
5	u	57	GLN
5	u	98	ARG
5	u	206	ASN
5	u	216	LEU
5	u	238	GLN
6	v	28	LYS
6	v	53	VAL
6	v	56	LYS
6	v	64	LYS

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Mol	Chain	Res	Type
6	v	66	LEU
6	v	90	ILE
6	v	170	GLN
6	v	181	MET
6	v	200	VAL
6	v	229	LYS
6	v	244	LYS
7	w	51	THR
7	w	54	LYS
7	w	55	VAL
7	w	113	LEU
7	w	142	ILE
7	w	146	GLN
7	w	165	THR
7	w	178	LEU
7	w	185	LYS
7	w	204	VAL
7	w	241	LEU
8	x	6	VAL
8	x	9	LYS
8	x	40	ASN
8	x	56	THR
8	x	58	LEU
8	x	68	LEU
8	x	83	LEU
8	x	84	LYS
8	x	121	LYS
8	x	132	LEU
8	x	180	LYS
8	x	201	ARG
8	x	215	LYS
8	x	216	VAL
9	y	13	MET
9	y	19	VAL
9	y	59	VAL
9	y	102	TYR
9	y	117	LYS
9	y	120	ILE
9	y	136	VAL
9	y	144	GLN
9	y	171	LEU
10	z	45	LEU

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Mol	Chain	Res	Type
10	z	47	VAL
10	z	85	ARG
10	z	86	ARG
10	z	143	LEU
10	z	154	GLU
10	z	167	LEU
11	1	32	LYS
11	1	41	LEU
11	1	57	ARG
11	1	58	LEU
11	1	62	GLN
11	1	71	LYS
11	1	102	CYS
11	1	190	ASP
12	2	1	ARG
12	2	106	VAL
12	2	159	GLN
12	2	166	LEU
12	2	173	ARG
13	3	43	MET
13	3	46	ASN
13	3	69	GLN
13	3	94	ARG
13	3	119	GLU
14	4	70	LEU
14	4	72	GLU
14	4	139	VAL
14	4	190	LEU
14	4	194	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (244) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	108	GLN
1	A	111	GLN
1	A	139	ASN
1	A	206	ASN
2	B	94	GLN
2	B	108	GLN
2	B	122	GLN
2	B	154	ASN

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Mol	Chain	Res	Type
3	C	22	GLN
3	C	121	ASN
4	D	33	GLN
4	D	156	GLN
4	D	196	GLN
4	D	216	GLN
5	E	2	GLN
5	E	28	GLN
5	E	238	GLN
6	F	110	HIS
6	F	147	GLN
6	F	170	GLN
6	F	180	GLN
6	F	201	HIS
7	G	32	ASN
7	G	52	GLN
7	G	67	HIS
8	H	40	ASN
8	H	62	ASN
8	H	66	HIS
9	I	6	ASN
9	I	32	GLN
9	I	39	GLN
9	I	64	GLN
9	I	144	GLN
9	I	168	GLN
9	I	172	ASN
10	J	27	GLN
10	J	55	GLN
10	J	71	ASN
10	J	82	ASN
10	J	101	ASN
10	J	132	HIS
11	K	29	GLN
11	K	196	HIS
12	L	8	ASN
12	L	79	ASN
12	L	146	GLN
12	L	151	ASN
12	L	159	GLN
12	L	160	ASN
13	M	3	ASN

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Mol	Chain	Res	Type
13	M	38	ASN
13	M	46	ASN
13	M	104	ASN
13	M	108	ASN
13	M	157	GLN
14	N	66	HIS
14	N	187	GLN
14	N	193	GLN
1	O	41	ASN
1	O	62	HIS
1	O	111	GLN
1	O	122	GLN
1	O	139	ASN
1	O	178	ASN
1	O	188	HIS
2	P	29	HIS
2	P	94	GLN
2	P	99	GLN
2	P	101	GLN
2	P	122	GLN
2	P	145	GLN
2	P	148	GLN
2	P	197	ASN
3	Q	22	GLN
3	Q	121	ASN
3	Q	204	ASN
4	R	89	GLN
4	R	91	HIS
4	R	147	HIS
4	R	178	HIS
4	R	196	GLN
4	R	206	ASN
5	S	180	ASN
6	T	22	GLN
6	T	63	ASN
7	U	89	GLN
7	U	91	GLN
7	U	99	ASN
7	U	126	GLN
7	U	146	GLN
8	V	40	ASN
8	V	66	HIS

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Mol	Chain	Res	Type
8	V	116	HIS
9	W	6	ASN
9	W	32	GLN
9	W	39	GLN
9	W	71	ASN
9	W	144	GLN
10	X	55	GLN
10	X	71	ASN
10	X	82	ASN
10	X	132	HIS
11	Y	29	GLN
11	Y	162	GLN
12	Z	8	ASN
12	Z	79	ASN
12	Z	146	GLN
12	Z	152	GLN
12	Z	157	ASN
12	Z	159	GLN
13	a	2	GLN
13	a	46	ASN
13	a	65	GLN
13	a	81	HIS
13	a	157	GLN
13	a	208	ASN
14	b	53	GLN
14	b	106	GLN
14	b	193	GLN
1	c	51	GLN
1	c	62	HIS
1	c	101	GLN
1	c	111	GLN
1	c	139	ASN
1	c	206	ASN
2	d	94	GLN
2	d	99	GLN
2	d	197	ASN
2	d	234	GLN
3	e	121	ASN
3	e	220	ASN
4	f	91	HIS
4	f	96	ASN
4	f	144	GLN

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Mol	Chain	Res	Type
5	g	28	GLN
5	g	62	HIS
5	g	143	GLN
5	g	187	HIS
5	g	206	ASN
5	g	238	GLN
6	h	110	HIS
6	h	147	GLN
6	h	170	GLN
6	h	180	GLN
6	h	201	HIS
7	i	33	GLN
7	i	52	GLN
7	i	67	HIS
7	i	91	GLN
7	i	171	GLN
7	i	192	GLN
8	j	30	ASN
8	j	40	ASN
8	j	66	HIS
9	k	6	ASN
9	k	32	GLN
9	k	39	GLN
9	k	64	GLN
9	k	144	GLN
9	k	172	ASN
10	l	27	GLN
10	l	55	GLN
10	l	63	ASN
10	l	71	ASN
10	l	82	ASN
10	l	101	ASN
10	l	132	HIS
11	m	178	HIS
11	m	196	HIS
12	n	8	ASN
12	n	79	ASN
12	n	146	GLN
12	n	151	ASN
12	n	159	GLN
12	n	163	HIS
13	o	3	ASN

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Mol	Chain	Res	Type
13	o	46	ASN
13	o	69	GLN
13	o	81	HIS
13	o	104	ASN
13	o	147	GLN
13	o	157	GLN
14	p	53	GLN
14	p	66	HIS
14	p	106	GLN
14	p	187	GLN
1	q	41	ASN
1	q	139	ASN
1	q	178	ASN
1	q	188	HIS
2	r	29	HIS
2	r	87	ASN
2	r	99	GLN
2	r	101	GLN
2	r	122	GLN
2	r	197	ASN
3	s	22	GLN
3	s	145	GLN
3	s	238	ASN
4	t	89	GLN
4	t	91	HIS
4	t	144	GLN
4	t	196	GLN
4	t	206	ASN
5	u	40	HIS
5	u	62	HIS
5	u	206	ASN
6	v	110	HIS
6	v	201	HIS
7	w	67	HIS
7	w	99	ASN
7	w	126	GLN
7	w	223	ASN
8	x	40	ASN
8	x	66	HIS
8	x	116	HIS
9	y	6	ASN
9	y	39	GLN

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Mol	Chain	Res	Type
9	y	64	GLN
9	y	80	GLN
9	y	144	GLN
10	z	27	GLN
10	z	55	GLN
10	z	71	ASN
10	z	82	ASN
10	z	132	HIS
11	1	29	GLN
11	1	162	GLN
12	2	8	ASN
12	2	36	HIS
12	2	79	ASN
12	2	146	GLN
12	2	151	ASN
12	2	159	GLN
13	3	46	ASN
13	3	65	GLN
13	3	104	ASN
13	3	157	GLN
14	4	62	GLN
14	4	110	GLN
14	4	123	GLN
14	4	158	ASN
14	4	193	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

12 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	04C	V	301	8	44,44,44	1.35	7 (15%)	54,58,58	0.90	2 (3%)
15	04C	j	301	8	44,44,44	1.36	5 (11%)	54,58,58	0.85	0
15	04C	x	301	8	44,44,44	1.32	4 (9%)	54,58,58	0.93	2 (3%)
15	04C	m	301	11	44,44,44	1.32	5 (11%)	54,58,58	1.12	2 (3%)
15	04C	b	301	14	44,44,44	1.26	2 (4%)	54,58,58	1.02	3 (5%)
15	04C	N	301	14	44,44,44	1.31	4 (9%)	54,58,58	1.08	2 (3%)
15	04C	Y	301	11	44,44,44	1.45	6 (13%)	54,58,58	1.07	2 (3%)
15	04C	1	301	11	44,44,44	1.97	8 (18%)	54,58,58	0.97	3 (5%)
15	04C	K	301	11	44,44,44	1.34	4 (9%)	54,58,58	1.23	2 (3%)
15	04C	H	301	8	44,44,44	1.42	6 (13%)	54,58,58	0.89	1 (1%)
15	04C	p	301	14	44,44,44	1.35	5 (11%)	54,58,58	1.12	4 (7%)
15	04C	4	301	14	44,44,44	1.32	3 (6%)	54,58,58	1.02	3 (5%)

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	04C	V	301	8	-	11/44/52/52	0/3/3/3
15	04C	j	301	8	-	15/44/52/52	0/3/3/3
15	04C	x	301	8	-	10/44/52/52	0/3/3/3
15	04C	m	301	11	-	14/44/52/52	0/3/3/3
15	04C	b	301	14	-	15/44/52/52	0/3/3/3
15	04C	N	301	14	-	13/44/52/52	0/3/3/3
15	04C	Y	301	11	-	14/44/52/52	0/3/3/3
15	04C	1	301	11	-	14/44/52/52	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	04C	K	301	11	-	11/44/52/52	0/3/3/3
15	04C	H	301	8	-	14/44/52/52	0/3/3/3
15	04C	p	301	14	-	14/44/52/52	0/3/3/3
15	04C	4	301	14	-	15/44/52/52	0/3/3/3

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	1	301	04C	O45-C44	-9.21	1.19	1.37
15	H	301	04C	C12-C10	3.66	1.56	1.52
15	j	301	04C	C12-C10	3.54	1.56	1.52
15	H	301	04C	C10-C9	3.53	1.59	1.53
15	K	301	04C	C10-C9	3.51	1.59	1.53
15	V	301	04C	C12-C10	3.50	1.56	1.52
15	x	301	04C	C12-C10	3.49	1.56	1.52
15	p	301	04C	C10-C9	3.49	1.59	1.53
15	j	301	04C	C5-C6	3.47	1.45	1.38
15	1	301	04C	C47-C44	3.46	1.45	1.38
15	1	301	04C	C10-C9	3.45	1.59	1.53
15	4	301	04C	C12-C10	3.43	1.56	1.52
15	4	301	04C	C10-C9	3.37	1.59	1.53
15	V	301	04C	C10-C9	3.35	1.59	1.53
15	Y	301	04C	C10-C9	3.34	1.59	1.53
15	m	301	04C	C10-C9	3.31	1.59	1.53
15	N	301	04C	C10-C9	3.30	1.59	1.53
15	b	301	04C	C10-C9	3.28	1.59	1.53
15	m	301	04C	C12-C10	3.27	1.56	1.52
15	Y	301	04C	O45-C44	3.20	1.43	1.37
15	K	301	04C	C12-C10	3.20	1.56	1.52
15	p	301	04C	C12-C10	3.17	1.56	1.52
15	x	301	04C	C10-C9	3.10	1.58	1.53
15	b	301	04C	C12-C10	3.09	1.56	1.52
15	j	301	04C	C10-C9	3.09	1.58	1.53
15	Y	301	04C	C12-C10	3.05	1.56	1.52
15	p	301	04C	C7-C6	3.01	1.58	1.51
15	N	301	04C	C12-C10	2.97	1.56	1.52
15	1	301	04C	C12-C10	2.94	1.56	1.52
15	Y	301	04C	C5-C6	2.86	1.44	1.38
15	H	301	04C	O45-C44	-2.70	1.32	1.37
15	H	301	04C	C47-C44	2.67	1.43	1.38
15	m	301	04C	C5-C6	2.62	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	j	301	04C	C2-C3	2.62	1.44	1.38
15	N	301	04C	C7-C6	2.50	1.57	1.51
15	V	301	04C	C5-C6	2.49	1.43	1.38
15	K	301	04C	C5-C6	2.47	1.43	1.38
15	H	301	04C	C9-C8	2.39	1.57	1.53
15	V	301	04C	C47-C44	2.39	1.43	1.38
15	Y	301	04C	C9-C8	2.34	1.57	1.53
15	x	301	04C	C5-C6	2.34	1.43	1.38
15	H	301	04C	C5-C6	2.33	1.43	1.38
15	l	301	04C	C9-C8	2.32	1.57	1.53
15	l	301	04C	C48-C41	2.31	1.43	1.38
15	K	301	04C	C9-C8	2.29	1.57	1.53
15	l	301	04C	C5-C6	2.28	1.43	1.38
15	l	301	04C	C40-C41	2.22	1.56	1.51
15	p	301	04C	C9-C8	2.19	1.57	1.53
15	Y	301	04C	C2-C3	2.15	1.43	1.38
15	V	301	04C	C42-C43	2.12	1.42	1.38
15	V	301	04C	C2-C3	2.10	1.42	1.38
15	m	301	04C	C2-C3	2.09	1.42	1.38
15	j	301	04C	C47-C44	2.09	1.42	1.38
15	N	301	04C	C2-C1	2.05	1.42	1.38
15	V	301	04C	C9-C8	2.04	1.57	1.53
15	x	301	04C	C42-C43	2.04	1.42	1.38
15	4	301	04C	C9-C8	2.02	1.57	1.53
15	m	301	04C	C9-C8	2.01	1.57	1.53
15	p	301	04C	C2-C1	2.00	1.42	1.38

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	K	301	04C	C11-C10-C12	-5.50	102.76	109.76
15	p	301	04C	C11-C10-C12	-4.97	103.44	109.76
15	m	301	04C	C11-C10-C12	-4.82	103.62	109.76
15	N	301	04C	C11-C10-C12	-4.82	103.63	109.76
15	Y	301	04C	C6-C7-C8	4.62	121.23	113.40
15	b	301	04C	C11-C10-C12	-4.42	104.13	109.76
15	K	301	04C	C30-N31-C36	4.19	117.66	111.14
15	4	301	04C	C11-C10-C12	-3.96	104.72	109.76
15	m	301	04C	C30-N31-C36	3.91	117.23	111.14
15	V	301	04C	C11-C10-C12	-3.56	105.22	109.76
15	l	301	04C	C6-C7-C8	3.49	119.31	113.40
15	x	301	04C	C11-C10-C12	-3.16	105.73	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	p	301	04C	C6-C7-C8	2.65	117.90	113.40
15	Y	301	04C	C41-C40-C24	-2.64	106.34	113.36
15	N	301	04C	C7-C8-N22	-2.58	106.42	110.08
15	1	301	04C	C11-C10-C12	-2.53	106.54	109.76
15	x	301	04C	C32-N31-C36	2.35	113.90	108.84
15	b	301	04C	C32-N31-C36	2.16	113.50	108.84
15	p	301	04C	C7-C8-N22	-2.15	107.02	110.08
15	1	301	04C	C32-N31-C36	2.10	113.36	108.84
15	H	301	04C	C11-C10-C12	-2.10	107.09	109.76
15	V	301	04C	C32-N31-C36	2.10	113.36	108.84
15	b	301	04C	C7-C8-N22	-2.08	107.12	110.08
15	p	301	04C	C30-N31-C32	2.05	114.33	111.14
15	4	301	04C	C30-N31-C32	2.05	114.33	111.14
15	4	301	04C	O37-C29-C30	-2.02	117.48	121.02

There are no chirality outliers.

All (160) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	H	301	04C	C6-C7-C8-N22
15	H	301	04C	C6-C7-C8-C9
15	K	301	04C	C29-C30-N31-C36
15	N	301	04C	C6-C7-C8-N22
15	N	301	04C	C6-C7-C8-C9
15	V	301	04C	C6-C7-C8-N22
15	V	301	04C	C6-C7-C8-C9
15	Y	301	04C	C11-C10-C9-C8
15	Y	301	04C	C12-C10-C9-C8
15	b	301	04C	C6-C7-C8-N22
15	b	301	04C	C6-C7-C8-C9
15	j	301	04C	C6-C7-C8-N22
15	j	301	04C	C6-C7-C8-C9
15	j	301	04C	C11-C10-C12-O13
15	m	301	04C	C29-C30-N31-C36
15	p	301	04C	C6-C7-C8-N22
15	p	301	04C	C6-C7-C8-C9
15	x	301	04C	C6-C7-C8-N22
15	x	301	04C	C6-C7-C8-C9
15	1	301	04C	C11-C10-C9-C8
15	1	301	04C	C12-C10-C9-C8
15	4	301	04C	C6-C7-C8-N22
15	4	301	04C	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
15	b	301	04C	C43-C44-O45-C46
15	b	301	04C	C47-C44-O45-C46
15	m	301	04C	C47-C44-O45-C46
15	m	301	04C	C43-C44-O45-C46
15	l	301	04C	C43-C44-O45-C46
15	4	301	04C	C47-C44-O45-C46
15	4	301	04C	C43-C44-O45-C46
15	K	301	04C	C47-C44-O45-C46
15	K	301	04C	C43-C44-O45-C46
15	l	301	04C	C47-C44-O45-C46
15	H	301	04C	C47-C44-O45-C46
15	H	301	04C	C43-C44-O45-C46
15	N	301	04C	C47-C44-O45-C46
15	N	301	04C	C43-C44-O45-C46
15	Y	301	04C	C47-C44-O45-C46
15	Y	301	04C	C43-C44-O45-C46
15	j	301	04C	C43-C44-O45-C46
15	p	301	04C	C47-C44-O45-C46
15	p	301	04C	C43-C44-O45-C46
15	x	301	04C	C47-C44-O45-C46
15	V	301	04C	C43-C44-O45-C46
15	x	301	04C	C43-C44-O45-C46
15	j	301	04C	C47-C44-O45-C46
15	V	301	04C	C47-C44-O45-C46
15	H	301	04C	C1-C6-C7-C8
15	x	301	04C	C1-C6-C7-C8
15	l	301	04C	C5-C6-C7-C8
15	H	301	04C	C5-C6-C7-C8
15	Y	301	04C	C1-C6-C7-C8
15	Y	301	04C	C5-C6-C7-C8
15	x	301	04C	C5-C6-C7-C8
15	Y	301	04C	C11-C10-C9-O21
15	Y	301	04C	C12-C10-C9-O21
15	l	301	04C	C12-C10-C9-O21
15	l	301	04C	C1-C6-C7-C8
15	j	301	04C	C1-C6-C7-C8
15	V	301	04C	C1-C6-C7-C8
15	V	301	04C	C5-C6-C7-C8
15	j	301	04C	C5-C6-C7-C8
15	H	301	04C	C11-C10-C9-C8
15	N	301	04C	C11-C10-C9-C8
15	V	301	04C	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
15	b	301	04C	C11-C10-C9-C8
15	j	301	04C	C11-C10-C9-C8
15	p	301	04C	C11-C10-C9-C8
15	4	301	04C	C11-C10-C9-C8
15	H	301	04C	C11-C10-C12-O13
15	m	301	04C	C5-C6-C7-C8
15	K	301	04C	C5-C6-C7-C8
15	m	301	04C	C1-C6-C7-C8
15	b	301	04C	C11-C10-C9-O21
15	j	301	04C	C11-C10-C9-O21
15	p	301	04C	C11-C10-C9-O21
15	x	301	04C	C11-C10-C9-O21
15	l	301	04C	C11-C10-C9-O21
15	4	301	04C	C11-C10-C9-O21
15	K	301	04C	C1-C6-C7-C8
15	H	301	04C	N28-C29-C30-N31
15	K	301	04C	N28-C29-C30-N31
15	j	301	04C	N28-C29-C30-N31
15	m	301	04C	N28-C29-C30-N31
15	l	301	04C	N25-C24-C40-C41
15	H	301	04C	O37-C29-C30-N31
15	j	301	04C	O37-C29-C30-N31
15	m	301	04C	N25-C24-C40-C41
15	K	301	04C	O37-C29-C30-N31
15	m	301	04C	O37-C29-C30-N31
15	b	301	04C	N25-C24-C40-C41
15	4	301	04C	N25-C24-C40-C41
15	N	301	04C	C1-C6-C7-C8
15	m	301	04C	C11-C10-C9-C8
15	x	301	04C	C11-C10-C9-C8
15	x	301	04C	N28-C29-C30-N31
15	4	301	04C	N28-C29-C30-N31
15	4	301	04C	C1-C6-C7-C8
15	N	301	04C	C5-C6-C7-C8
15	H	301	04C	C11-C10-C9-O21
15	N	301	04C	C11-C10-C9-O21
15	V	301	04C	C11-C10-C9-O21
15	x	301	04C	O37-C29-C30-N31
15	4	301	04C	C5-C6-C7-C8
15	b	301	04C	C1-C6-C7-C8
15	Y	301	04C	C6-C7-C8-N22
15	m	301	04C	C6-C7-C8-N22

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Mol	Chain	Res	Type	Atoms
15	l	301	04C	C6-C7-C8-N22
15	b	301	04C	C5-C6-C7-C8
15	j	301	04C	C9-C10-C12-O13
15	j	301	04C	C12-C10-C9-C8
15	p	301	04C	N25-C24-C40-C41
15	N	301	04C	N25-C24-C40-C41
15	m	301	04C	C23-C24-C40-C41
15	p	301	04C	C1-C6-C7-C8
15	K	301	04C	C29-C30-N31-C32
15	N	301	04C	C29-C30-N31-C32
15	p	301	04C	C29-C30-N31-C32
15	K	301	04C	N25-C24-C40-C41
15	N	301	04C	C29-C30-N31-C36
15	p	301	04C	C29-C30-N31-C36
15	p	301	04C	C5-C6-C7-C8
15	4	301	04C	O49-C23-C24-N25
15	V	301	04C	N28-C29-C30-N31
15	b	301	04C	C29-C30-N31-C36
15	l	301	04C	O49-C23-C24-N25
15	Y	301	04C	N25-C24-C40-C41
15	p	301	04C	O49-C23-C24-N25
15	b	301	04C	N28-C29-C30-N31
15	b	301	04C	C23-C24-C40-C41
15	4	301	04C	O37-C29-C30-N31
15	H	301	04C	N25-C24-C40-C41
15	l	301	04C	N22-C23-C24-N25
15	b	301	04C	O49-C23-C24-N25
15	K	301	04C	C23-C24-C40-C41
15	4	301	04C	C23-C24-C40-C41
15	p	301	04C	C23-C24-C40-C41
15	m	301	04C	C11-C10-C9-O21
15	Y	301	04C	O49-C23-C24-N25
15	4	301	04C	N22-C23-C24-N25
15	b	301	04C	N22-C23-C24-N25
15	H	301	04C	C12-C10-C9-C8
15	p	301	04C	N22-C23-C24-N25
15	Y	301	04C	C23-C24-C40-C41
15	j	301	04C	N25-C24-C40-C41
15	Y	301	04C	C6-C7-C8-C9
15	m	301	04C	C6-C7-C8-C9
15	l	301	04C	C6-C7-C8-C9
15	H	301	04C	C12-C10-C9-O21

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Mol	Chain	Res	Type	Atoms
15	j	301	04C	C12-C10-C9-O21
15	N	301	04C	C23-C24-C40-C41
15	N	301	04C	O49-C23-C24-N25
15	V	301	04C	O49-C23-C24-N25
15	V	301	04C	O37-C29-C30-N31
15	Y	301	04C	N28-C29-C30-N31
15	1	301	04C	C23-C24-C40-C41
15	4	301	04C	N25-C26-C27-N28
15	m	301	04C	O49-C23-C24-N25
15	b	301	04C	O37-C29-C30-N31
15	K	301	04C	C11-C10-C9-O21

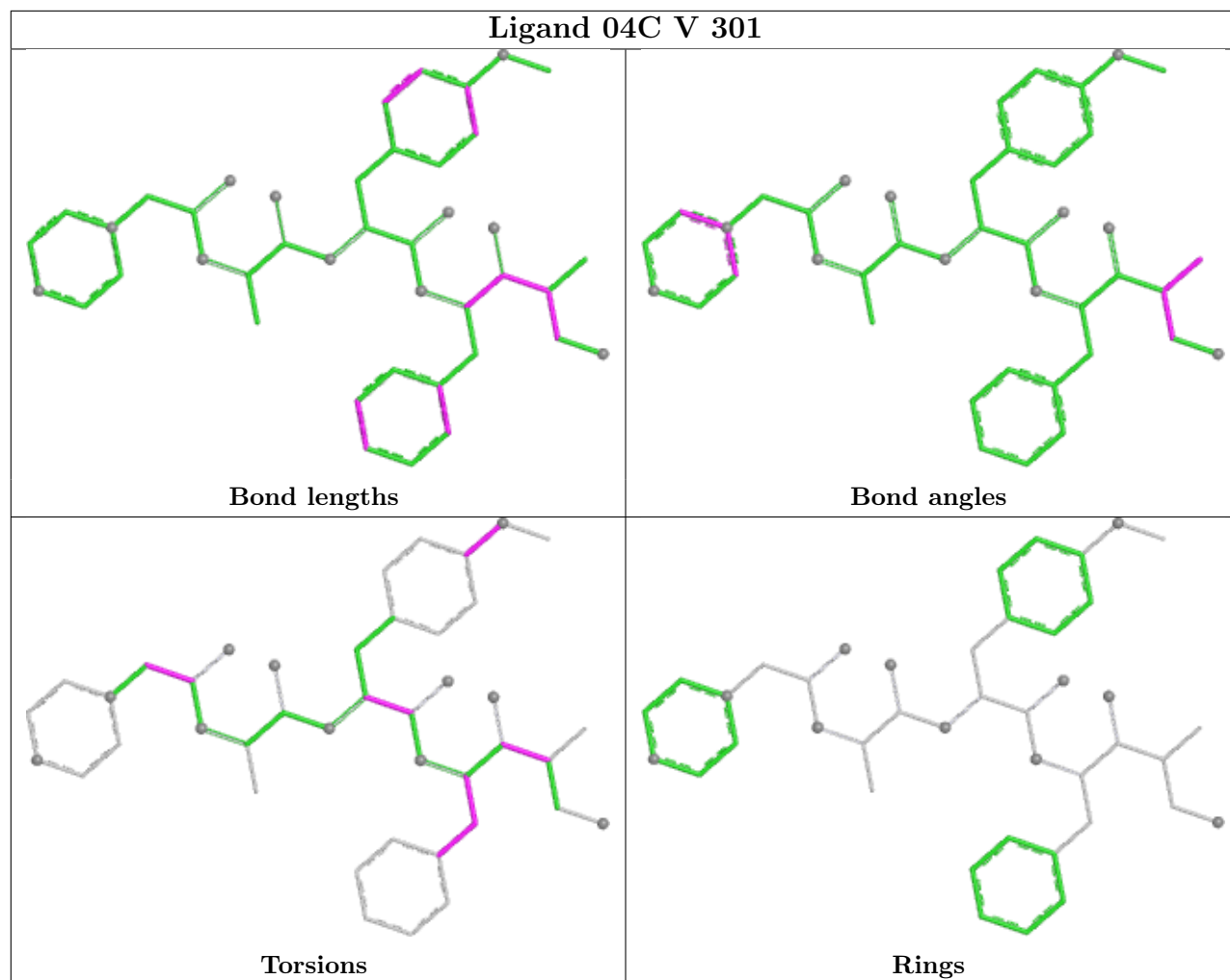
There are no ring outliers.

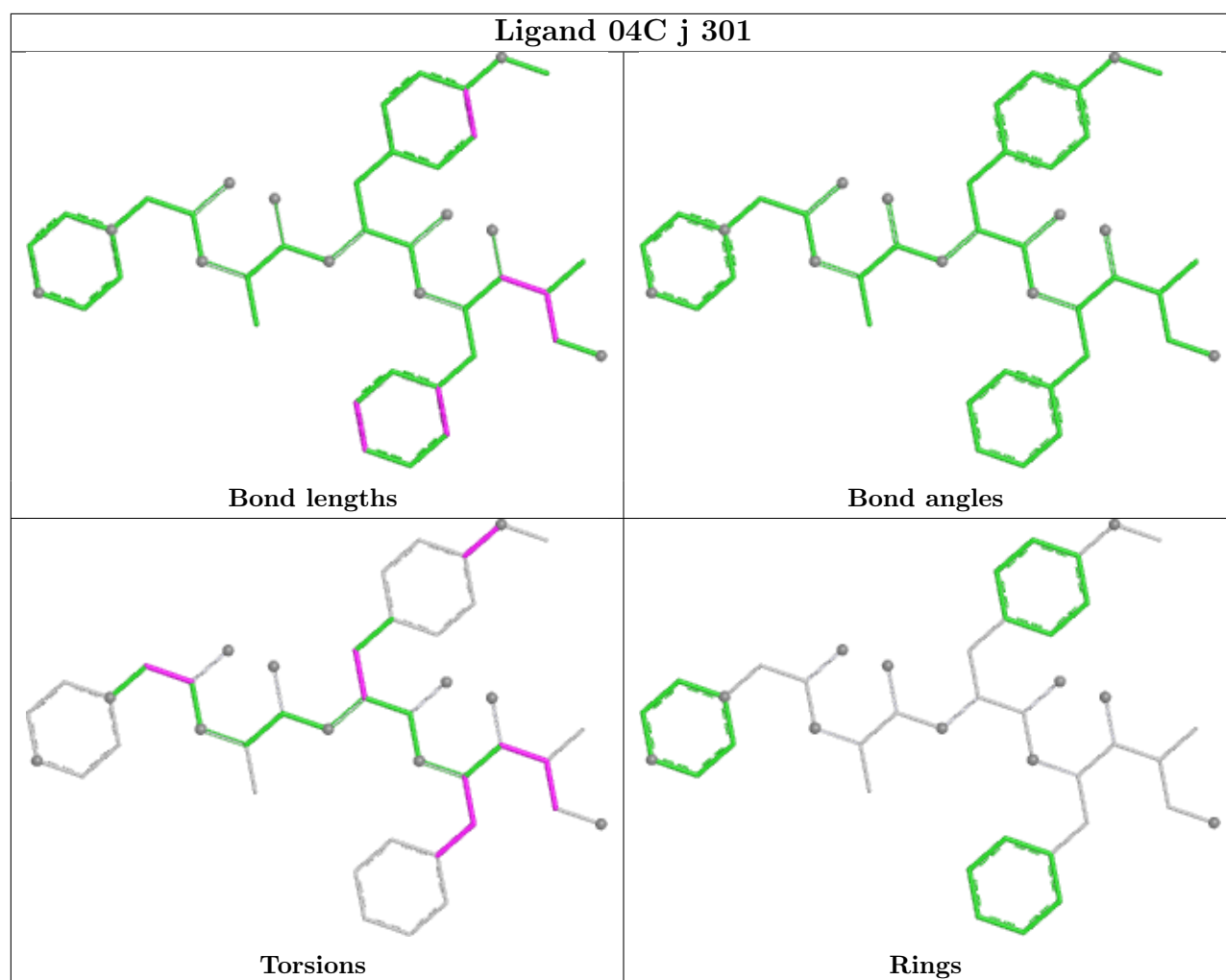
9 monomers are involved in 27 short contacts:

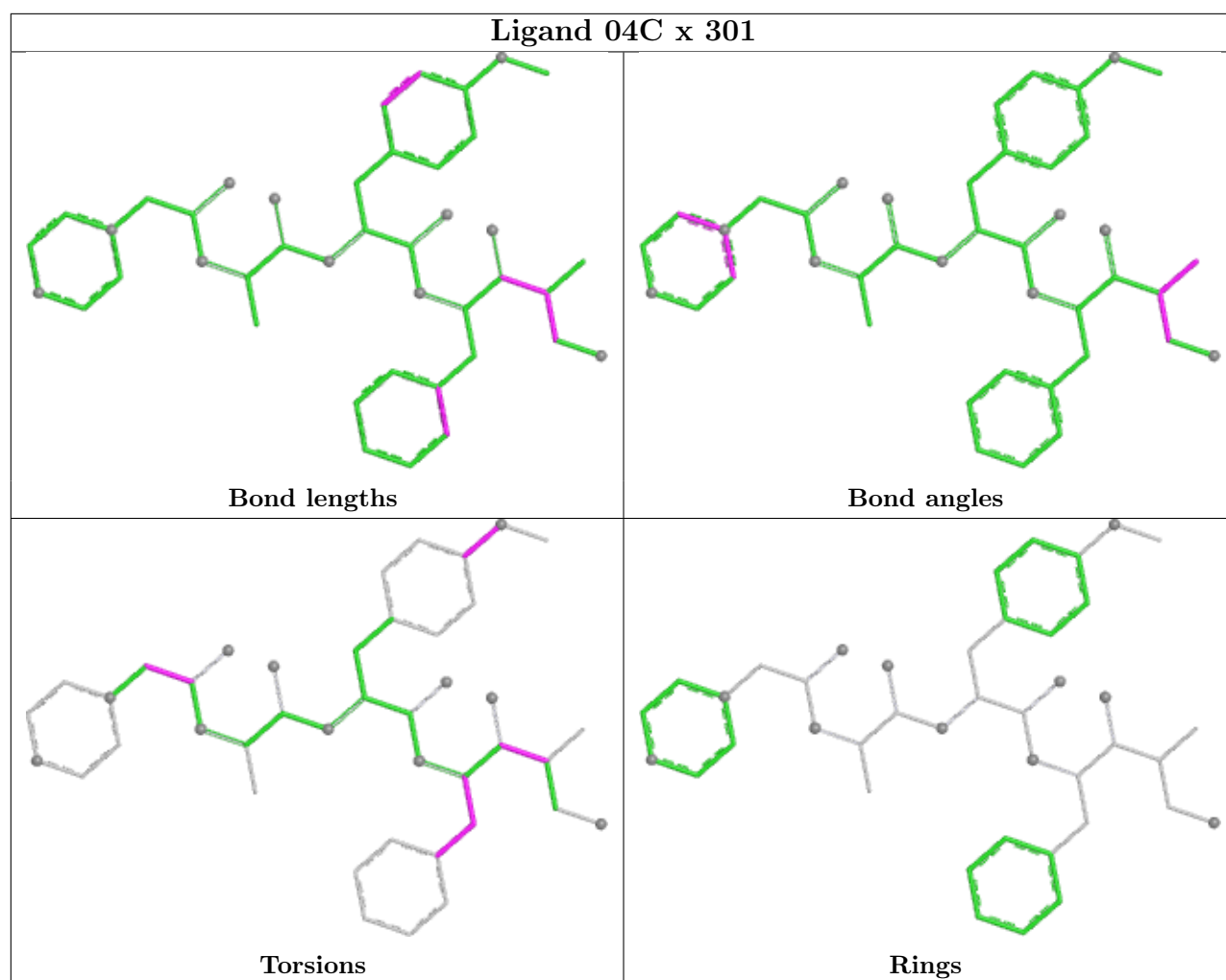
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	V	301	04C	3	0
15	j	301	04C	4	0
15	x	301	04C	2	0
15	m	301	04C	5	0
15	b	301	04C	2	0
15	N	301	04C	1	0
15	H	301	04C	5	0
15	p	301	04C	3	0
15	4	301	04C	2	0

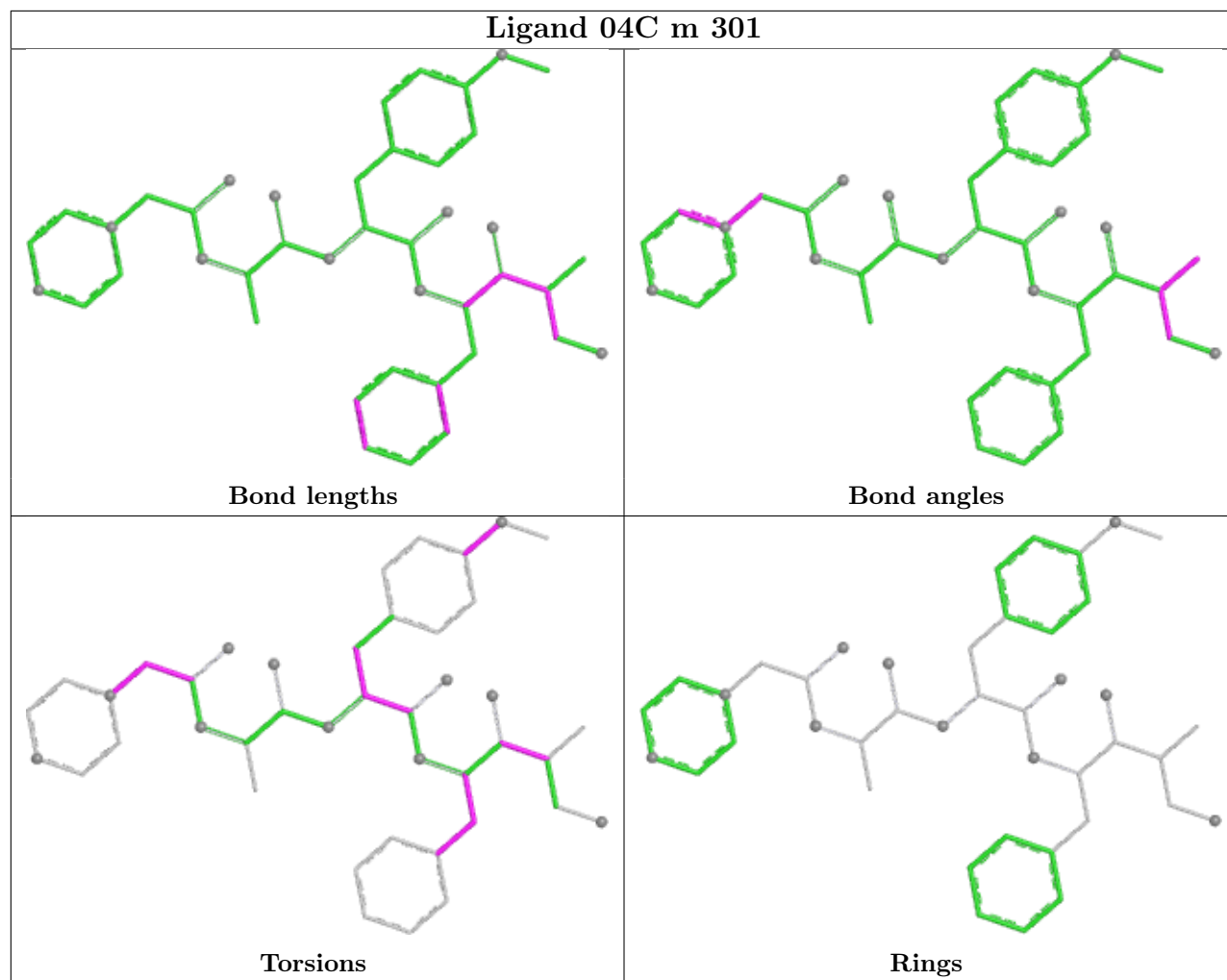
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

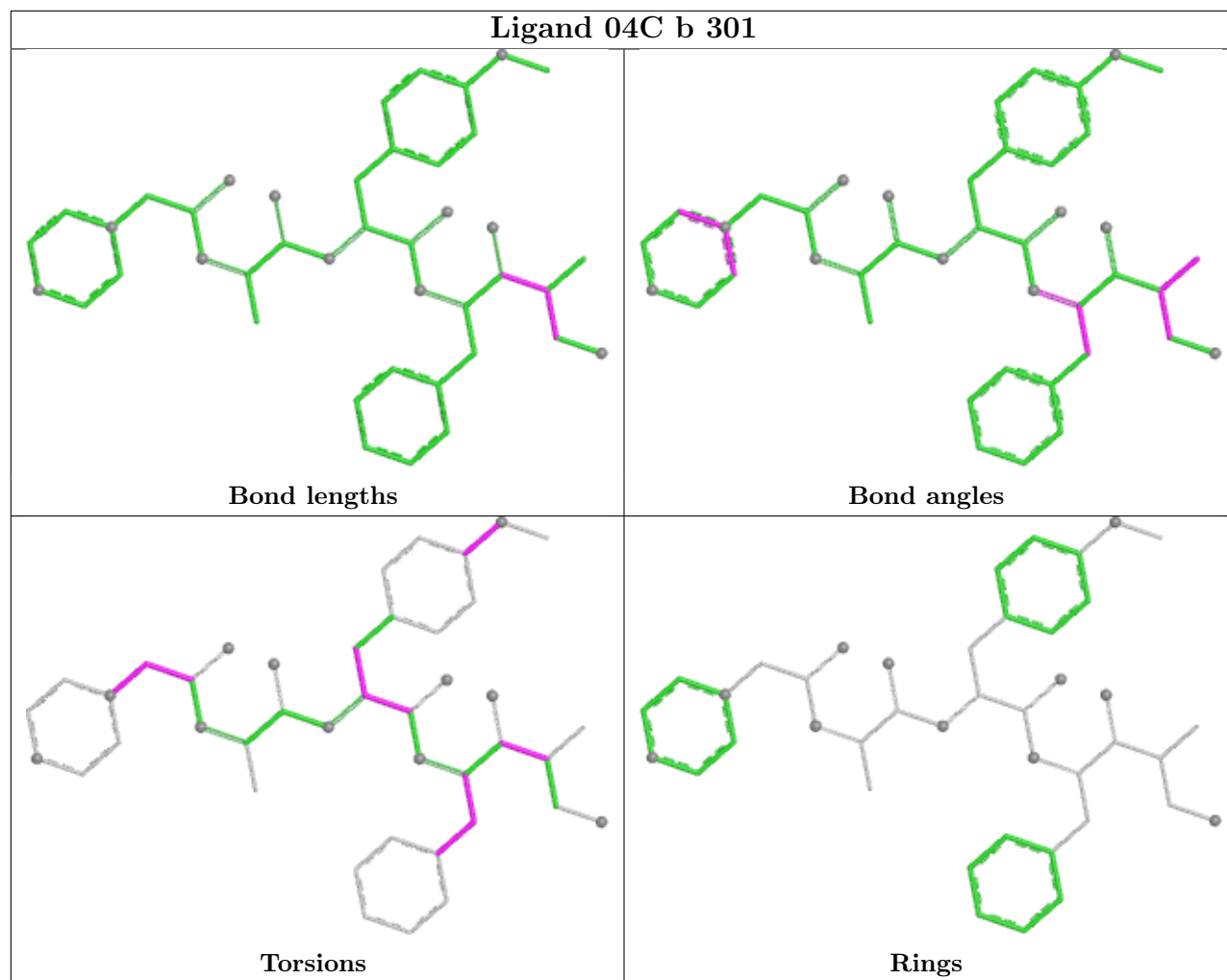
Ligand 04C V 301

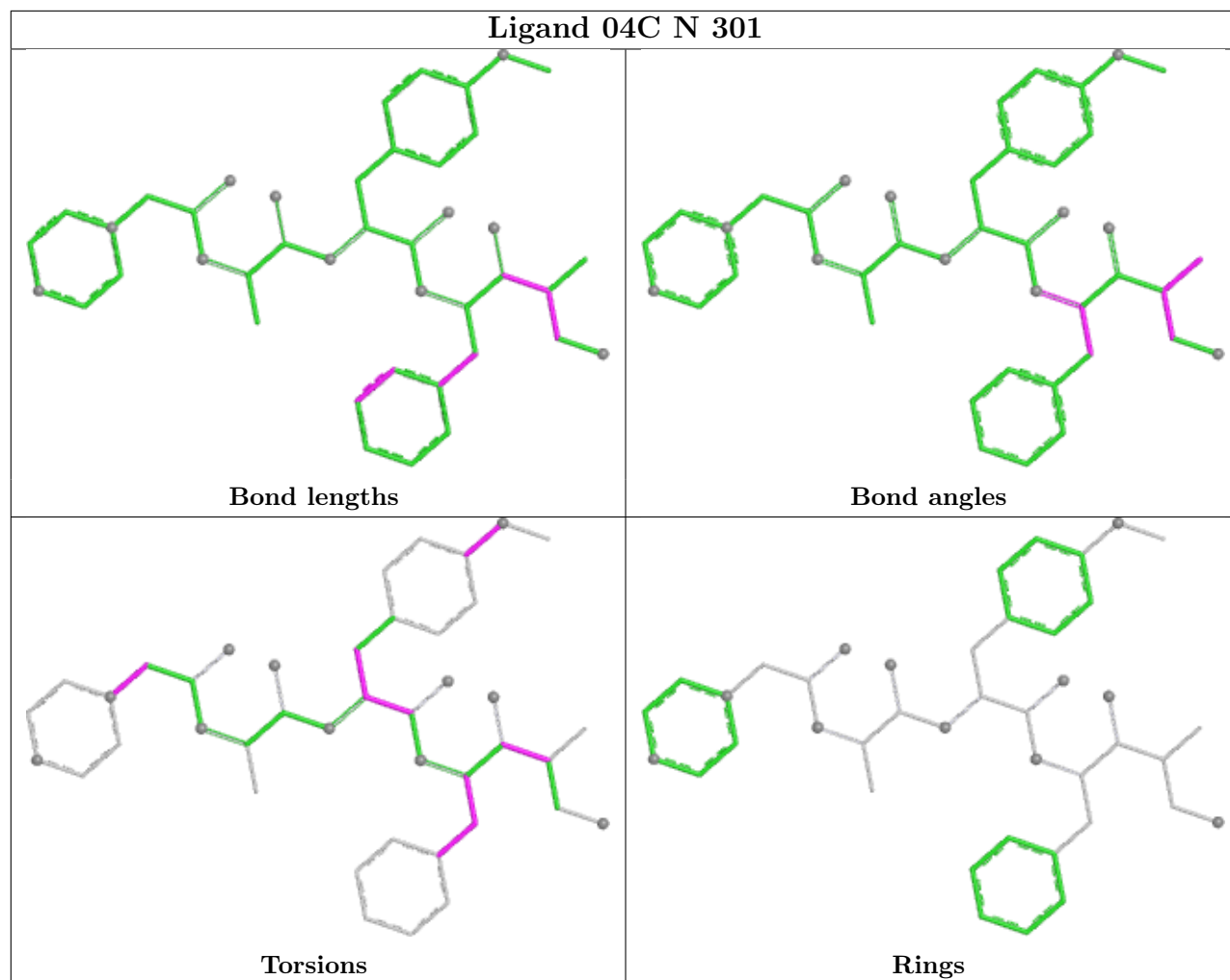




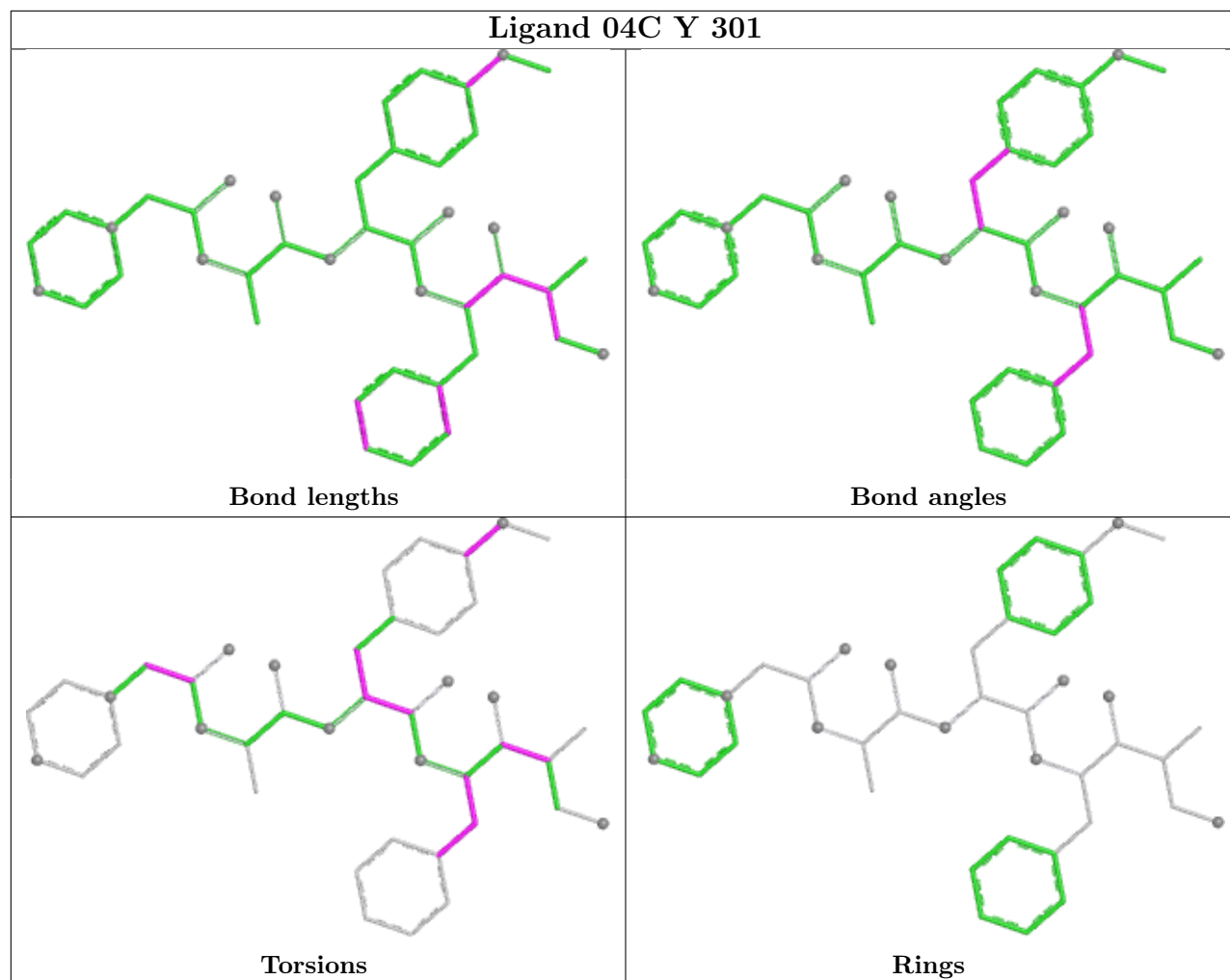




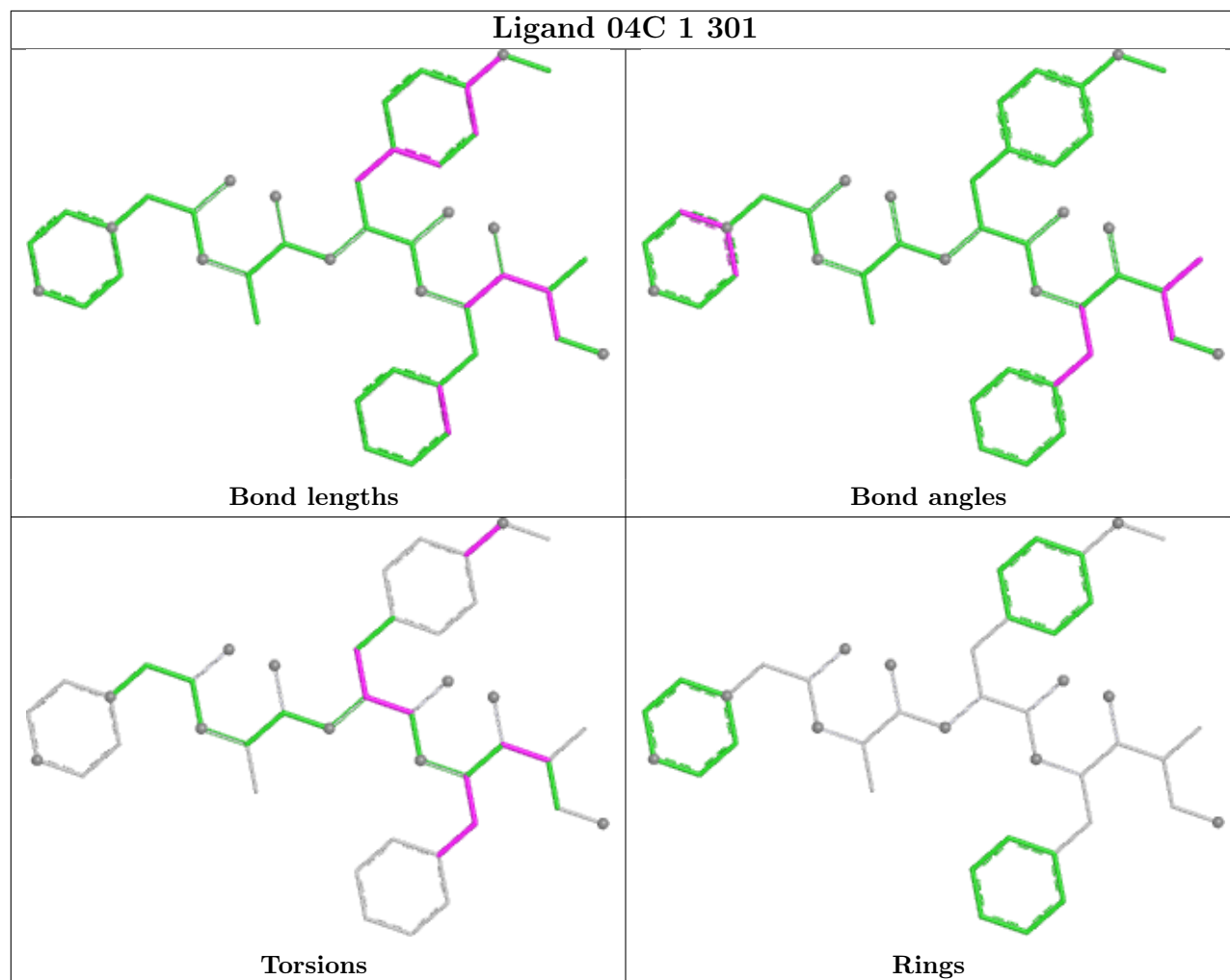




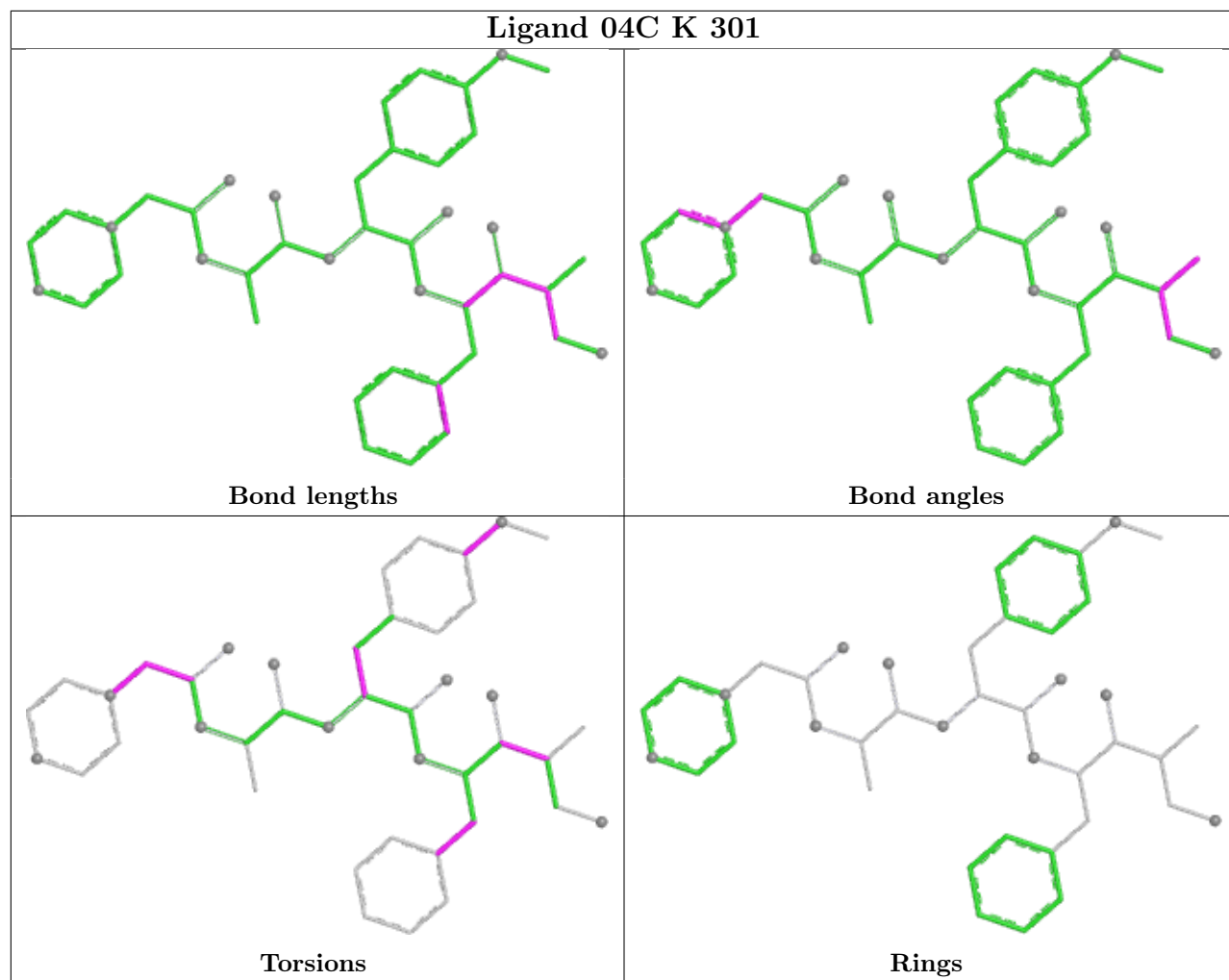
Ligand 04C Y 301



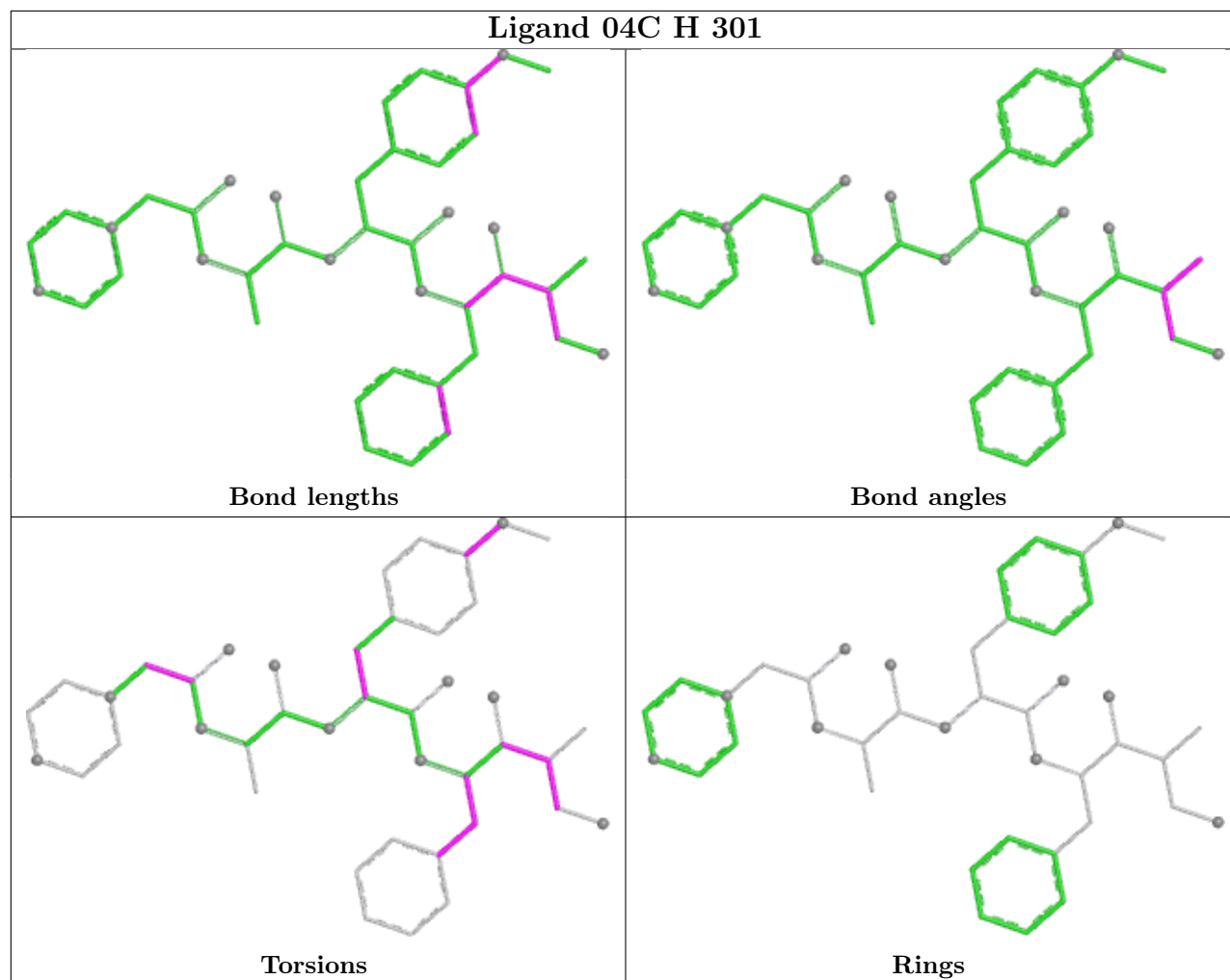
Ligand 04C 1 301



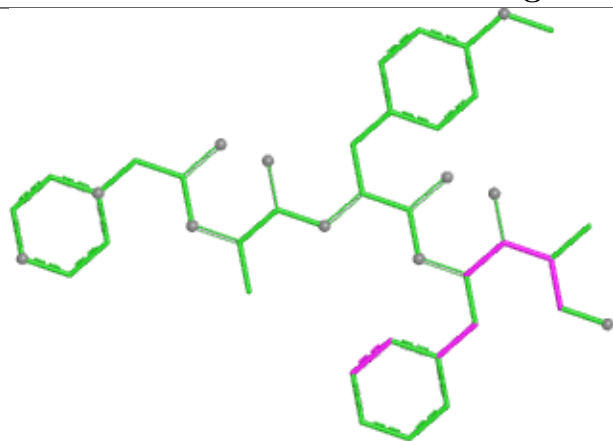
Ligand 04C K 301



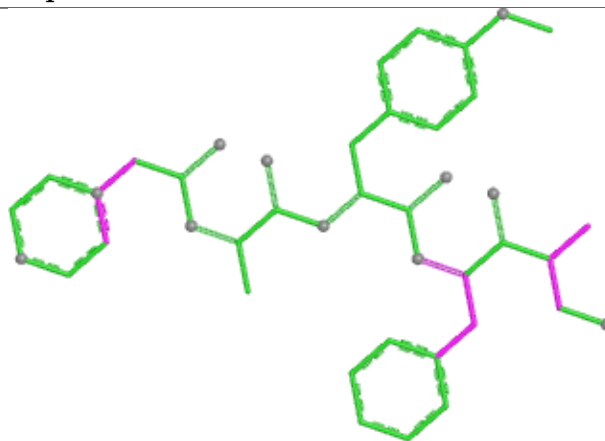
Ligand 04C H 301



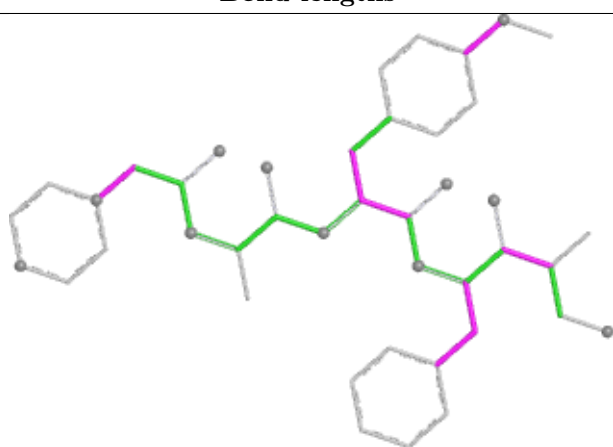
Ligand 04C p 301



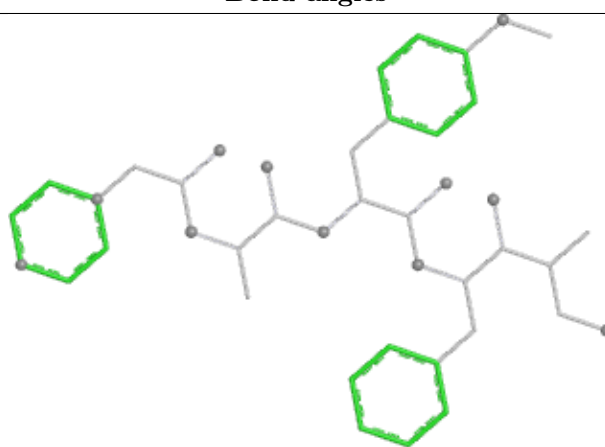
Bond lengths



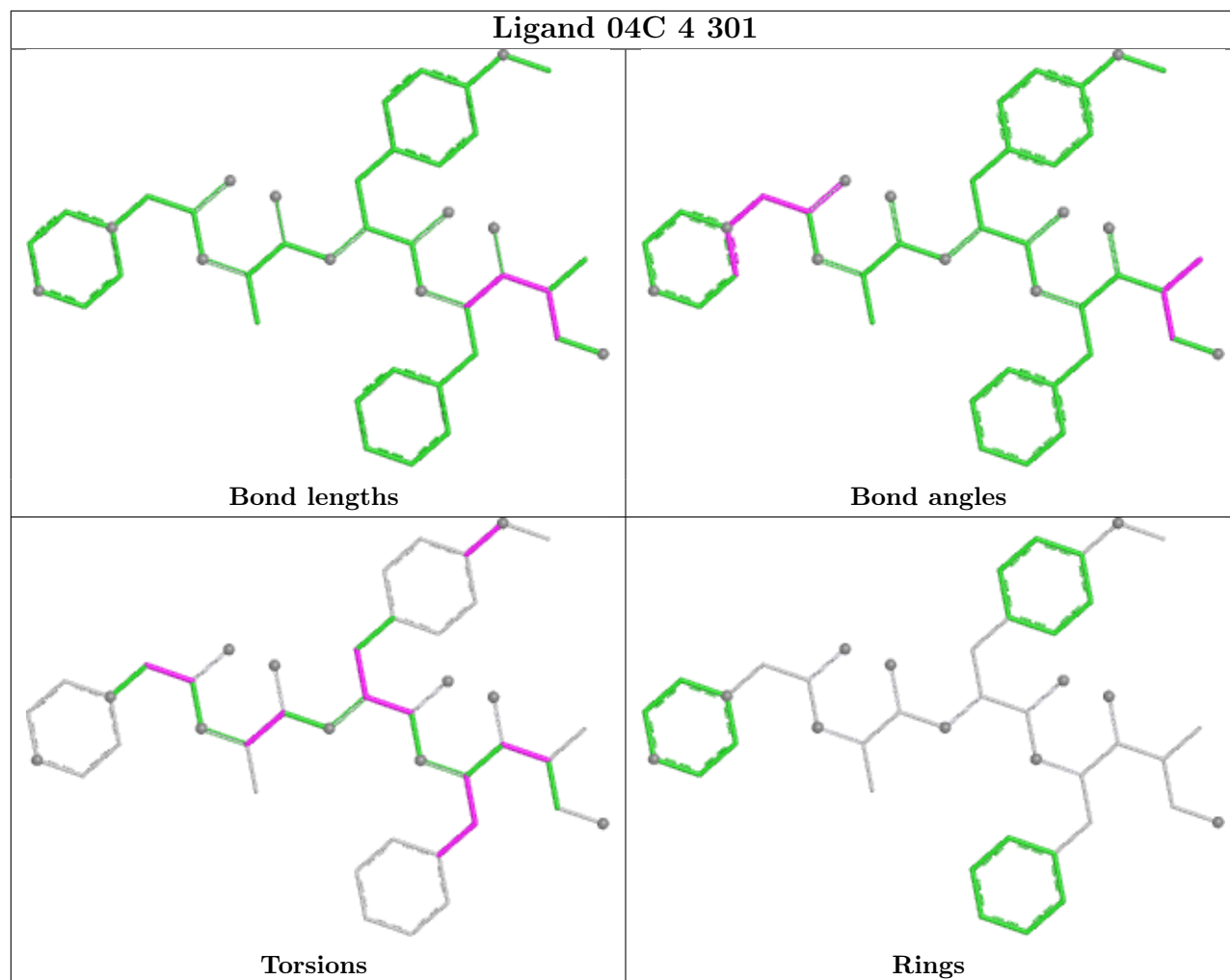
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	231/234 (98%)	-0.71	1 (0%) 88 85	42, 62, 99, 145	0
1	O	231/234 (98%)	-0.67	1 (0%) 88 85	40, 59, 95, 145	0
1	c	231/234 (98%)	-0.68	1 (0%) 88 85	44, 64, 99, 143	0
1	q	231/234 (98%)	-0.69	1 (0%) 88 85	39, 61, 97, 140	0
2	B	248/261 (95%)	-0.61	0 100 100	42, 69, 115, 156	0
2	P	248/261 (95%)	-0.66	0 100 100	34, 62, 108, 155	0
2	d	248/261 (95%)	-0.62	0 100 100	42, 71, 112, 161	0
2	r	248/261 (95%)	-0.64	2 (0%) 82 77	40, 63, 109, 143	0
3	C	239/248 (96%)	-0.40	1 (0%) 88 85	47, 83, 153, 182	0
3	Q	239/248 (96%)	-0.49	0 100 100	42, 74, 129, 163	0
3	e	239/248 (96%)	-0.45	0 100 100	51, 85, 148, 175	0
3	s	239/248 (96%)	-0.48	0 100 100	45, 75, 129, 164	0
4	D	233/241 (96%)	-0.64	0 100 100	50, 74, 104, 149	0
4	R	233/241 (96%)	-0.66	1 (0%) 88 85	43, 72, 108, 163	0
4	f	233/241 (96%)	-0.60	0 100 100	47, 75, 108, 158	0
4	t	233/241 (96%)	-0.57	2 (0%) 81 75	47, 73, 111, 171	0
5	E	238/263 (90%)	-0.50	0 100 100	45, 81, 135, 180	0
5	S	238/263 (90%)	-0.56	0 100 100	39, 65, 125, 160	0
5	g	238/263 (90%)	-0.48	0 100 100	48, 81, 136, 172	0
5	u	238/263 (90%)	-0.58	0 100 100	41, 65, 126, 156	0
6	F	244/255 (95%)	-0.48	1 (0%) 88 85	44, 76, 134, 167	0
6	T	244/255 (95%)	-0.65	2 (0%) 82 77	40, 64, 106, 159	0
6	h	244/255 (95%)	-0.46	1 (0%) 88 85	47, 77, 135, 156	0
6	v	244/255 (95%)	-0.63	2 (0%) 82 77	39, 65, 110, 158	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
7	G	243/246 (98%)	-0.58	0 100 100	42, 68, 108, 161	0
7	U	243/246 (98%)	-0.68	0 100 100	39, 59, 87, 121	0
7	i	243/246 (98%)	-0.58	0 100 100	44, 70, 108, 138	0
7	w	243/246 (98%)	-0.70	0 100 100	39, 59, 88, 122	0
8	H	220/234 (94%)	-0.75	0 100 100	24, 52, 91, 127	0
8	V	220/234 (94%)	-0.70	1 (0%) 87 83	23, 49, 89, 126	0
8	j	220/234 (94%)	-0.53	6 (2%) 56 47	27, 54, 113, 146	0
8	x	220/234 (94%)	-0.63	1 (0%) 87 83	33, 54, 91, 127	0
9	I	204/205 (99%)	-0.74	1 (0%) 87 83	40, 55, 87, 119	0
9	W	204/205 (99%)	-0.68	0 100 100	35, 54, 89, 122	0
9	k	204/205 (99%)	-0.70	0 100 100	40, 56, 88, 122	0
9	y	204/205 (99%)	-0.48	4 (1%) 65 56	41, 60, 89, 126	0
10	J	196/201 (97%)	-0.76	0 100 100	44, 59, 87, 114	0
10	X	196/201 (97%)	-0.79	0 100 100	40, 58, 85, 107	0
10	l	196/201 (97%)	-0.75	0 100 100	42, 59, 88, 112	0
10	z	196/201 (97%)	-0.76	0 100 100	40, 59, 86, 106	0
11	1	201/205 (98%)	-0.69	2 (0%) 79 73	36, 57, 88, 111	0
11	K	201/205 (98%)	-0.72	1 (0%) 87 83	38, 58, 92, 113	0
11	Y	201/205 (98%)	-0.71	1 (0%) 87 83	35, 56, 86, 109	0
11	m	201/205 (98%)	-0.70	1 (0%) 87 83	40, 59, 92, 117	0
12	2	213/213 (100%)	-0.74	1 (0%) 87 83	36, 57, 84, 135	0
12	L	213/213 (100%)	-0.80	0 100 100	40, 56, 90, 123	0
12	Z	213/213 (100%)	-0.77	0 100 100	37, 54, 86, 135	0
12	n	213/213 (100%)	-0.79	0 100 100	42, 57, 91, 132	0
13	3	216/219 (98%)	-0.73	0 100 100	34, 52, 79, 101	0
13	M	216/219 (98%)	-0.85	0 100 100	36, 53, 82, 115	0
13	a	216/219 (98%)	-0.80	0 100 100	33, 49, 79, 105	0
13	o	216/219 (98%)	-0.81	0 100 100	40, 56, 84, 123	0
14	4	202/205 (98%)	-0.77	0 100 100	31, 50, 99, 152	0
14	N	202/205 (98%)	-0.74	1 (0%) 87 83	30, 52, 91, 148	0
14	b	202/205 (98%)	-0.78	1 (0%) 87 83	30, 49, 95, 161	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
14	p	202/205 (98%)	-0.75	1 (0%) 87 83	32, 53, 92, 147	0
All	All	12512/12920 (96%)	-0.65	38 (0%) 90 87	23, 62, 111, 182	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	y	102	TYR	5.9
8	j	212	LEU	5.6
9	y	56	ALA	5.6
2	r	98	LEU	4.7
8	j	210	ALA	4.5
8	j	213	THR	4.4
8	j	209	THR	4.2
8	j	199	LEU	3.7
9	y	57	THR	3.6
6	T	3	ILE	3.2
4	t	233	ILE	3.2
14	p	201	THR	3.0
8	x	199	LEU	2.9
4	t	92	TRP	2.8
6	F	3	ILE	2.8
6	h	3	ILE	2.7
11	l	143	TYR	2.6
11	m	40	TYR	2.6
12	2	173	ARG	2.5
9	y	58	ASP	2.5
8	j	211	VAL	2.5
11	K	40	TYR	2.4
14	N	201	THR	2.4
8	V	199	LEU	2.3
1	O	1	ALA	2.2
4	R	233	ILE	2.2
6	T	186	CYS	2.2
2	r	248	ARG	2.1
6	v	3	ILE	2.1
6	v	5	THR	2.1
3	C	137	PHE	2.0
1	A	1	ALA	2.0
1	c	1	ALA	2.0
11	l	57	ARG	2.0
9	I	116	PHE	2.0
1	q	231	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
14	b	201	THR	2.0
11	Y	40	TYR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

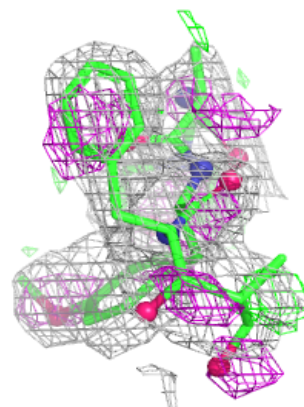
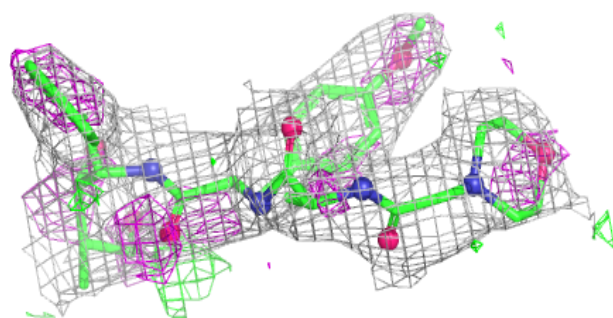
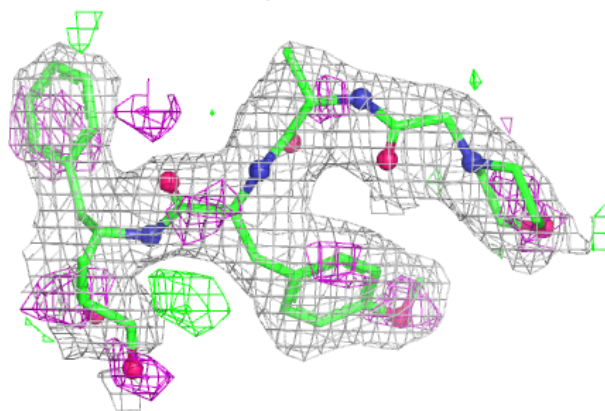
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	04C	N	301	42/42	0.91	0.09	24,34,58,70	0
15	04C	Y	301	42/42	0.91	0.08	24,41,70,74	0
15	04C	p	301	42/42	0.91	0.08	25,37,63,75	0
15	04C	1	301	42/42	0.91	0.08	24,39,71,77	0
15	04C	4	301	42/42	0.91	0.09	30,39,54,64	0
15	04C	j	301	42/42	0.92	0.08	33,37,50,53	0
15	04C	m	301	42/42	0.92	0.07	27,42,84,90	0
15	04C	H	301	42/42	0.92	0.08	30,37,50,51	0
15	04C	V	301	42/42	0.92	0.08	28,40,52,54	0
15	04C	K	301	42/42	0.92	0.08	24,41,79,87	0
15	04C	b	301	42/42	0.93	0.08	28,36,55,65	0
15	04C	x	301	42/42	0.93	0.08	31,40,52,58	0

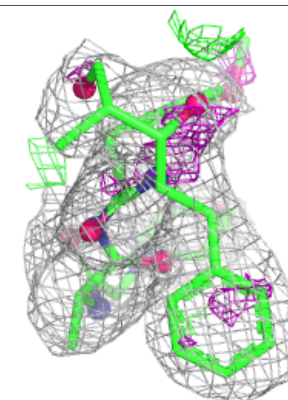
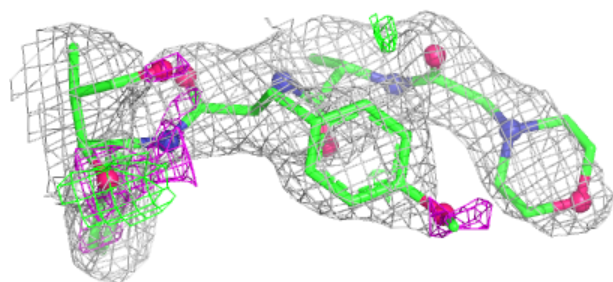
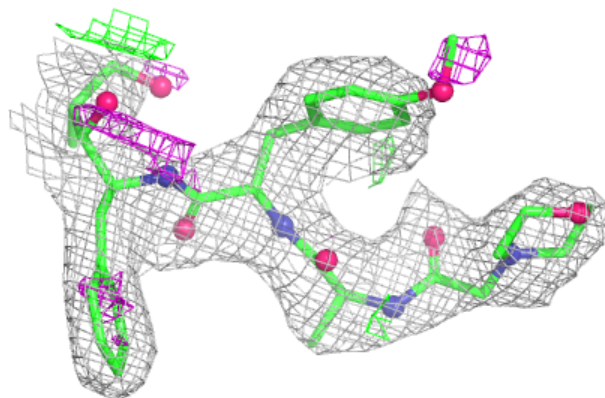
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 04C N 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

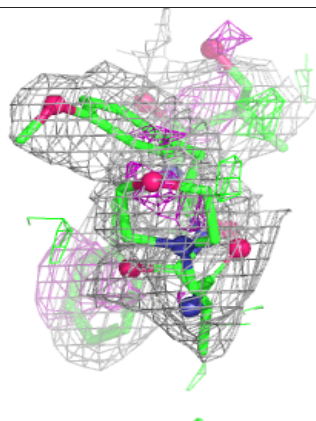
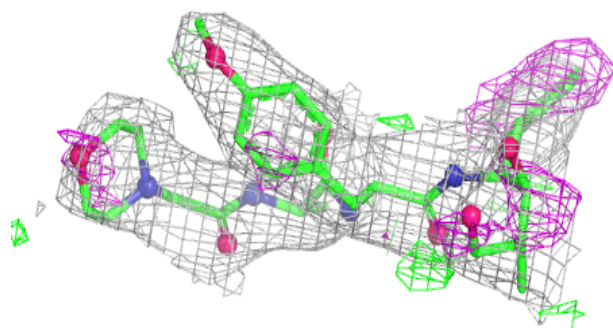
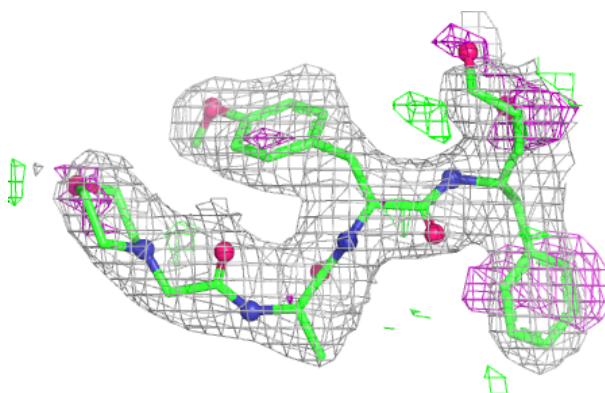
**Electron density around 04C Y 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



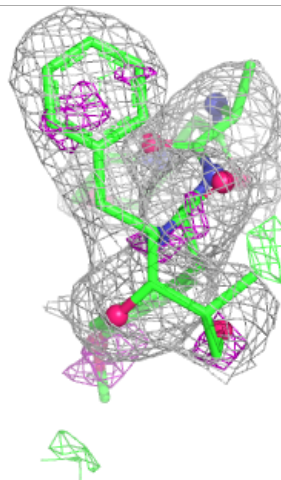
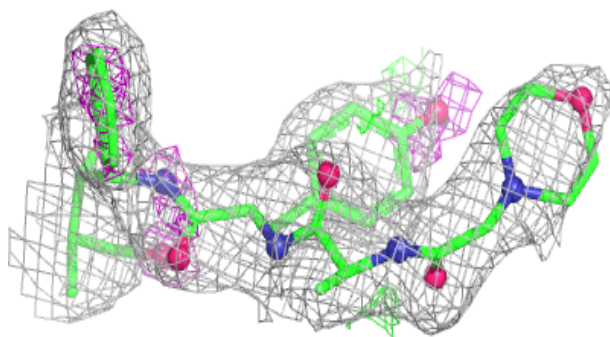
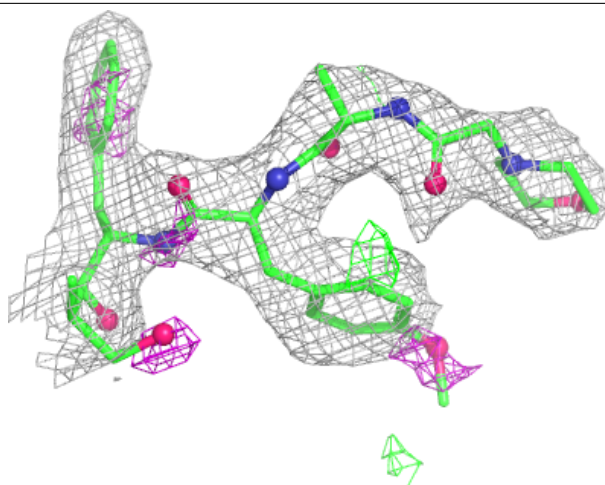
Electron density around 04C p 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



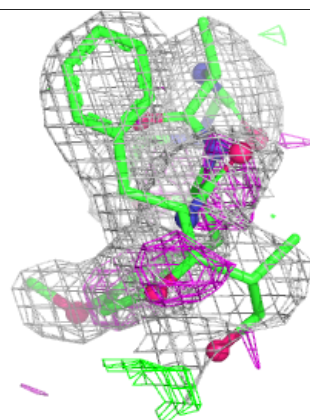
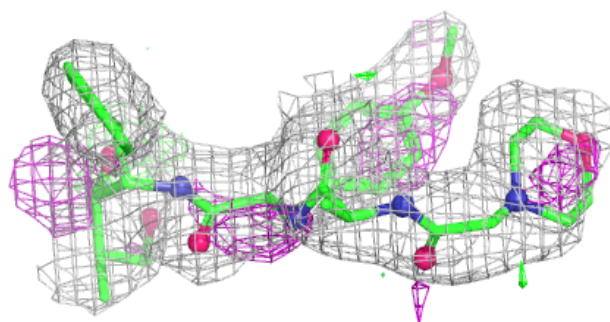
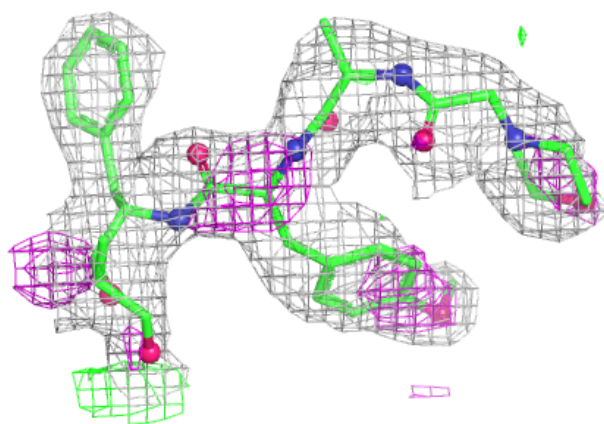
Electron density around 04C 1 301:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



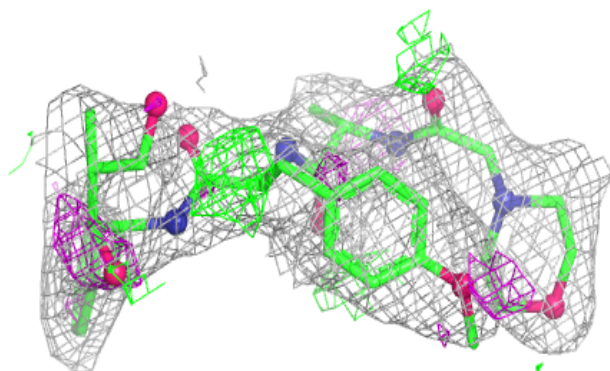
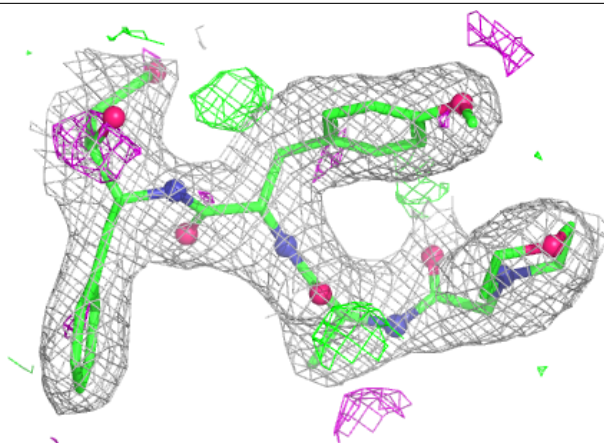
Electron density around 04C 4 301:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

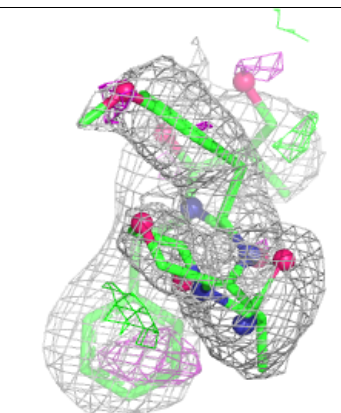
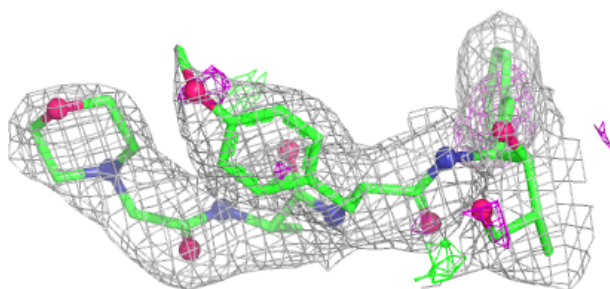
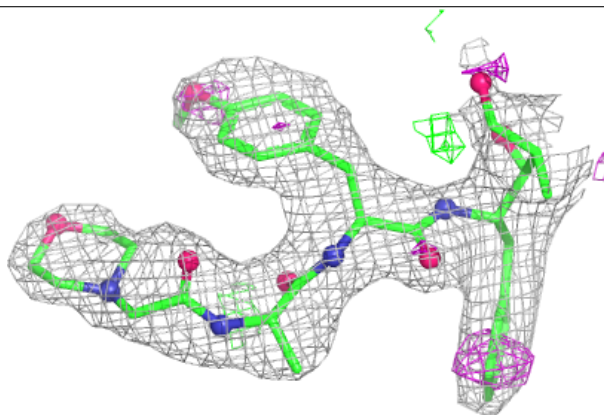


Electron density around 04C j 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

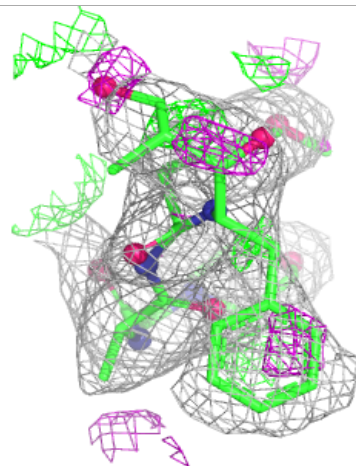
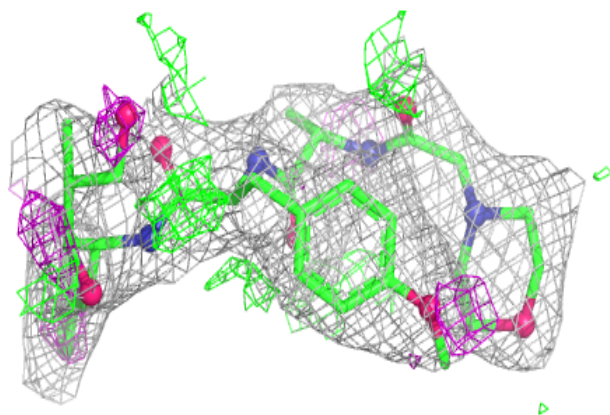
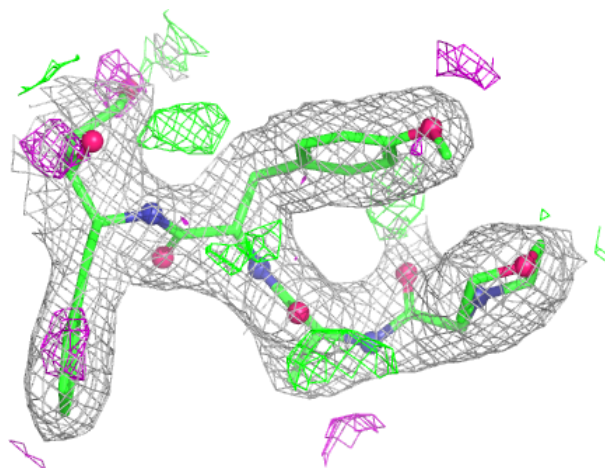
**Electron density around 04C m 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



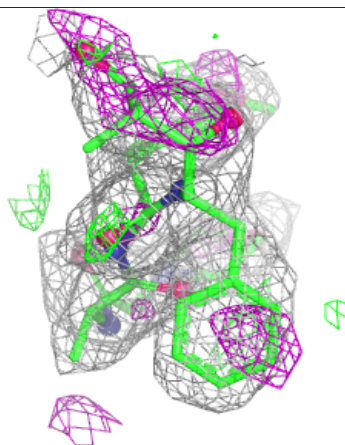
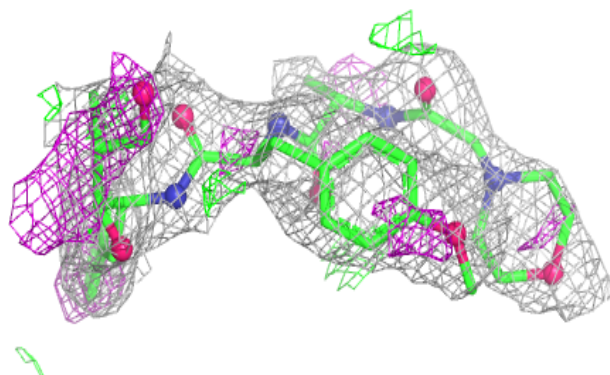
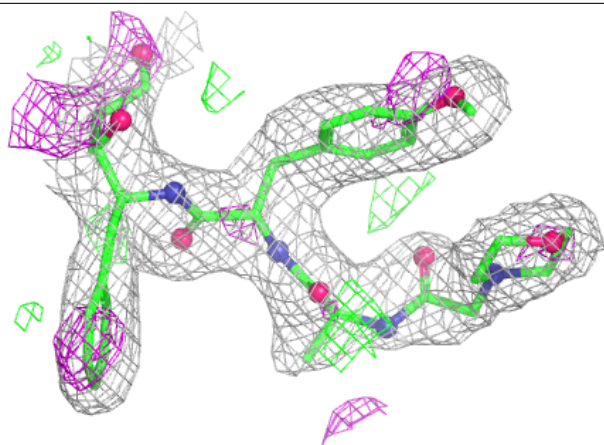
Electron density around 04C H 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



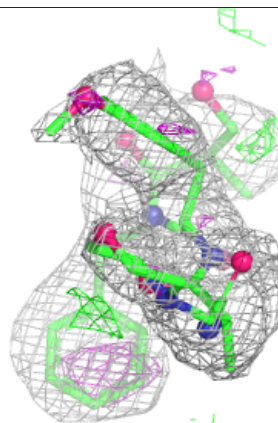
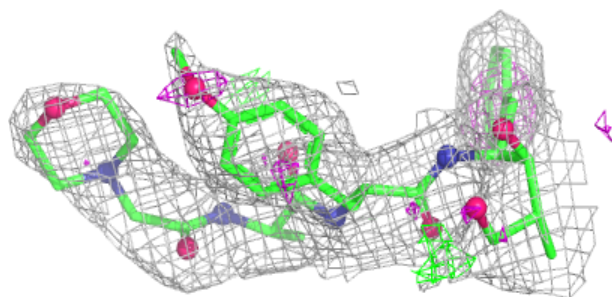
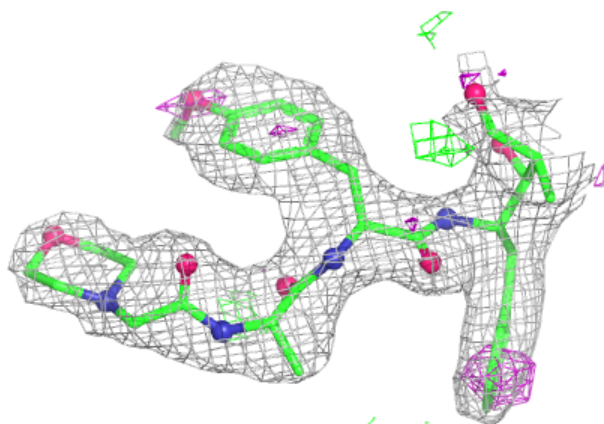
Electron density around 04C V 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



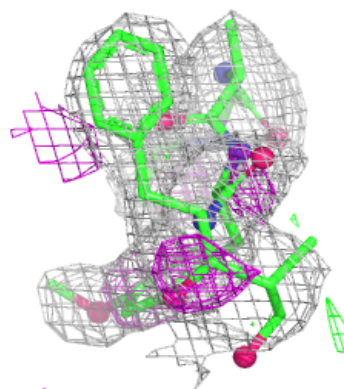
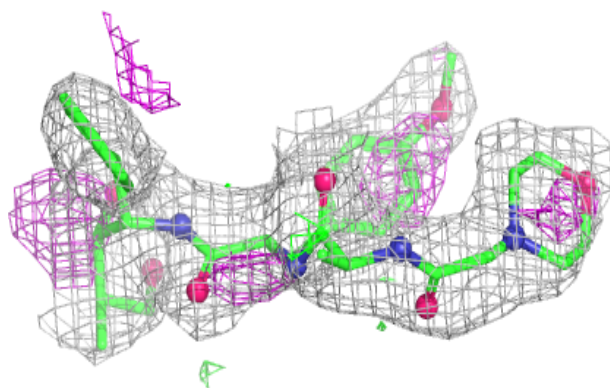
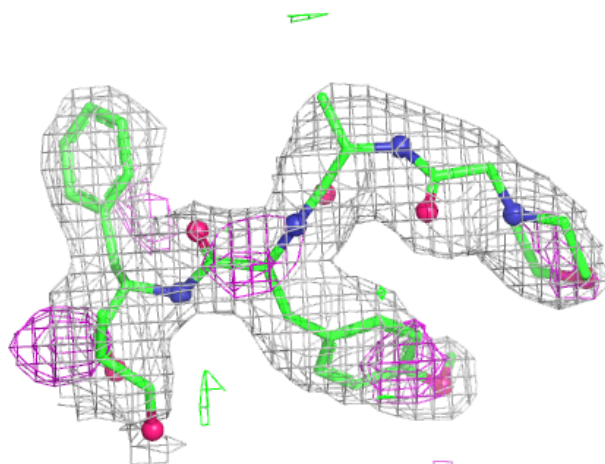
Electron density around 04C K 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



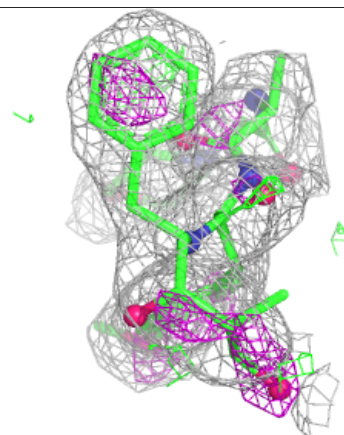
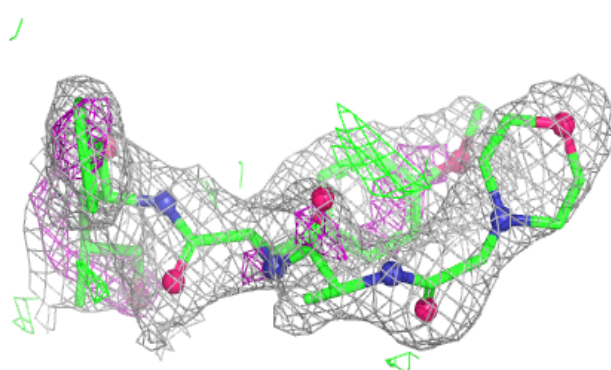
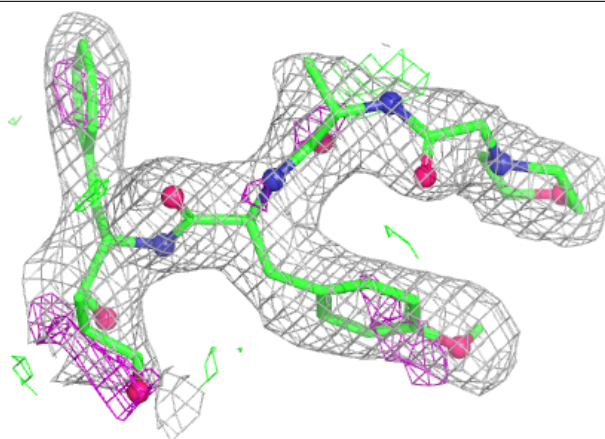
Electron density around 04C b 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 04C x 301:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.