Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:57 PM GMT

PDB ID	:	3UNB
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

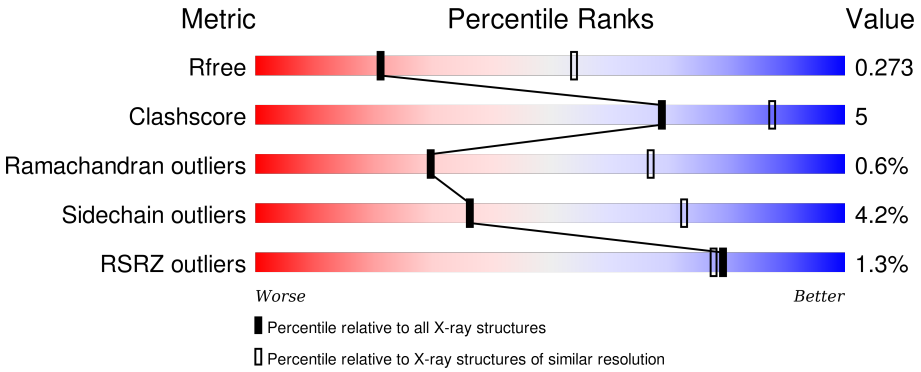
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	83% 15%
1	O	234	83% 15%
1	c	234	95%
1	q	234	94%
2	B	261	82% 12% 5%

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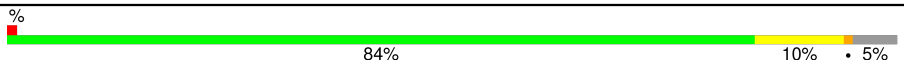
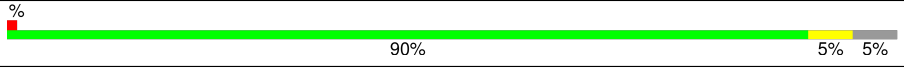
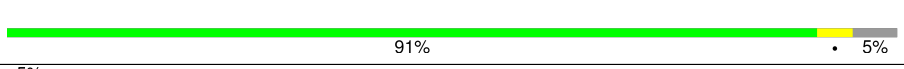
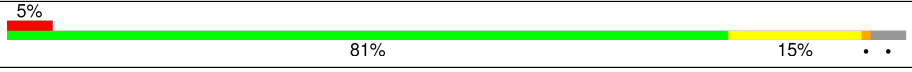
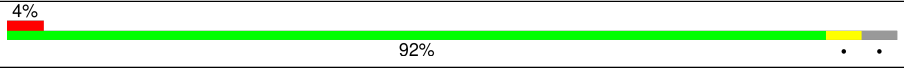
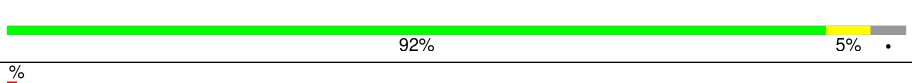
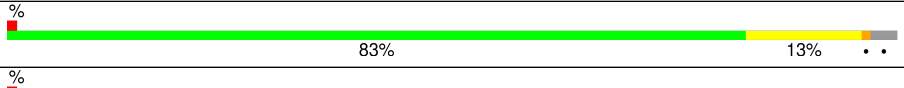
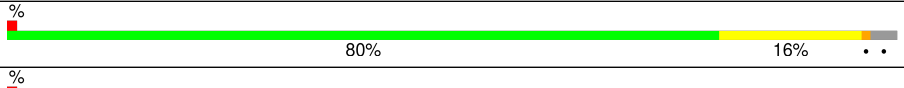
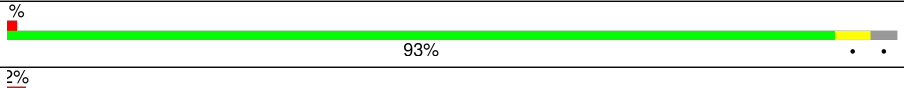
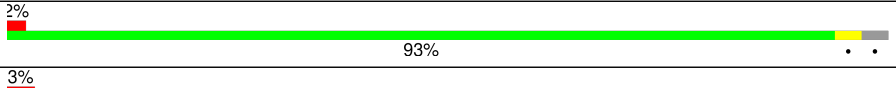
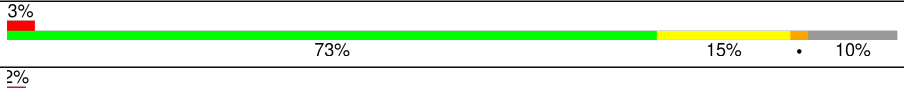
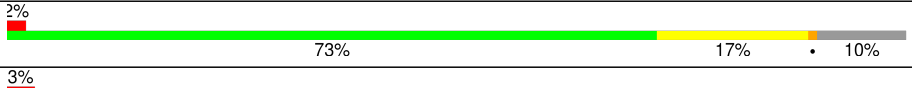
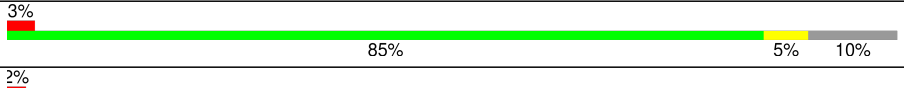
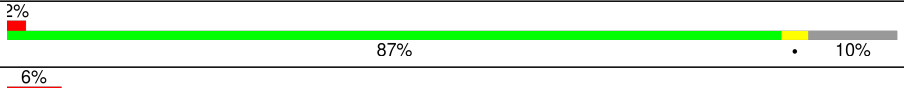
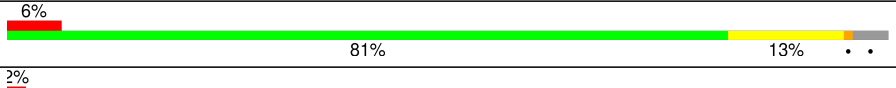
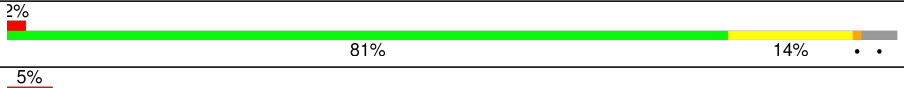
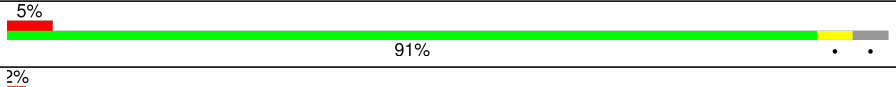
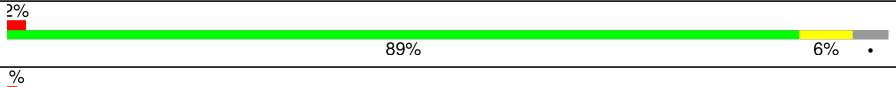
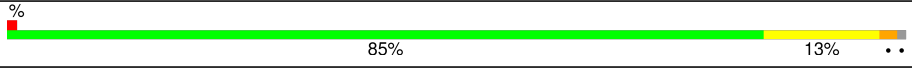
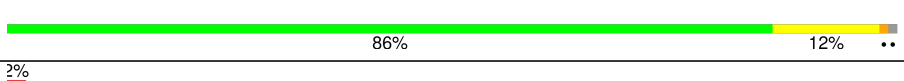
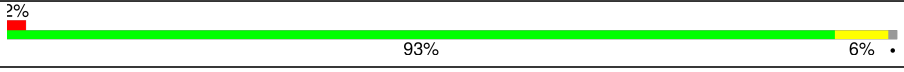
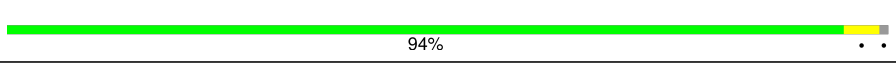
Mol	Chain	Length	Quality of chain
2	P	261	
2	d	261	
2	r	261	
3	C	248	
3	Q	248	
3	e	248	
3	s	248	
4	D	241	
4	R	241	
4	f	241	
4	t	241	
5	E	263	
5	S	263	
5	g	263	
5	u	263	
6	F	255	
6	T	255	
6	h	255	
6	v	255	
7	G	246	
7	U	246	
7	i	246	
7	w	246	
8	H	234	
8	V	234	

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Mol	Chain	Length	Quality of chain
8	j	234	4% 89% 5% 6%
8	x	234	89% 5% 6%
9	I	205	87% 12%
9	W	205	87% 12%
9	k	205	95%
9	y	205	2% 96%
10	J	201	88% 9%
10	X	201	85% 11%
10	l	201	95%
10	z	201	94%
11	1	205	82% 14%
11	K	205	85% 12%
11	Y	205	83% 14%
11	m	205	95%
12	2	213	87% 12%
12	L	213	91% 9%
12	Z	213	89% 11%
12	n	213	% 98%
13	3	219	82% 16%
13	M	219	88% 10%
13	a	219	95%
13	o	219	95%
14	4	205	% 93% 6%
14	N	205	2% 89% 9%
14	b	205	% 95%

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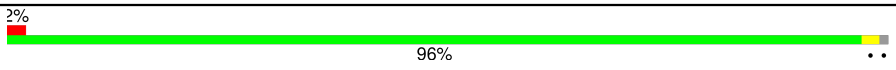
Mol	Chain	Length	Quality of chain
14	p	205	

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	C	N	O	S	0	0	0
			1881	1182	332	362	5			
3	Q	239	Total	C	N	O	S	0	0	0
			1881	1182	332	362	5			
3	e	239	Total	C	N	O	S	0	0	0
			1881	1182	332	362	5			
3	s	239	Total	C	N	O	S	0	0	0
			1881	1182	332	362	5			

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	C	N	O	S	0	0	0
			1778	1116	294	357	11			
4	R	233	Total	C	N	O	S	0	0	0
			1778	1116	294	357	11			
4	f	233	Total	C	N	O	S	0	0	0
			1778	1116	294	357	11			
4	t	233	Total	C	N	O	S	0	0	0
			1778	1116	294	357	11			

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

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

- 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			

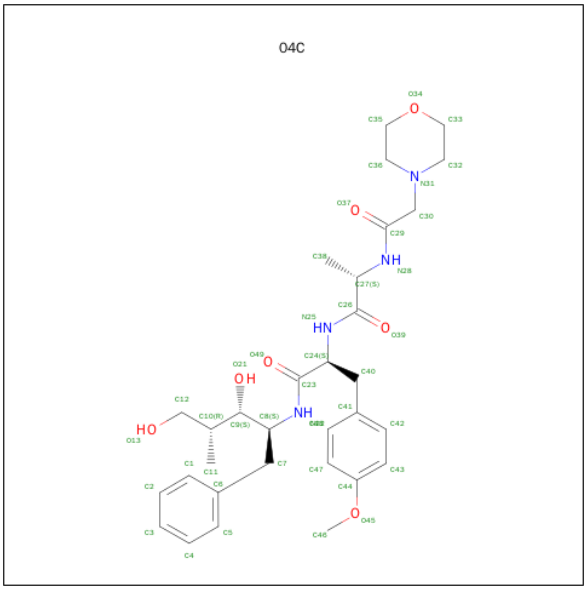
- Molecule 13 is a protein called Proteasome subunit beta type-4.

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 (three-letter code: 04C) (formula: $C_{31}H_{44}N_4O_7$).



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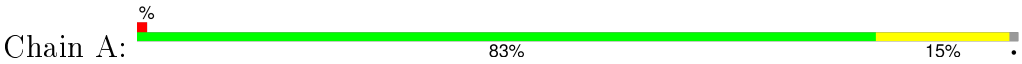
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	y	32	Total O 32 32	0	0
16	z	38	Total O 38 38	0	0
16	1	27	Total O 27 27	0	0
16	2	33	Total O 33 33	0	0
16	3	37	Total O 37 37	0	0
16	4	30	Total O 30 30	0	0

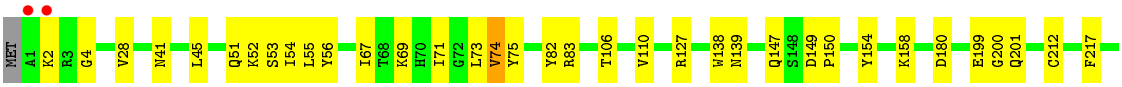
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (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

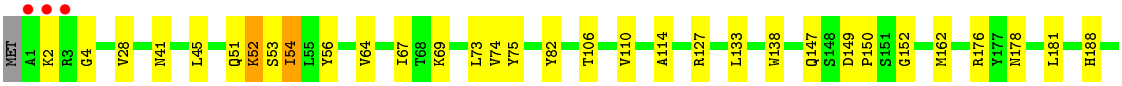
Chain A:

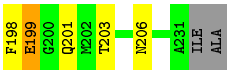




- Molecule 1: Proteasome subunit alpha type-2

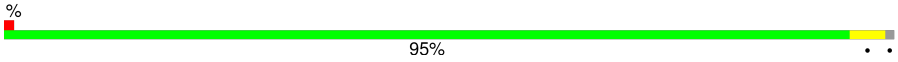
Chain O:

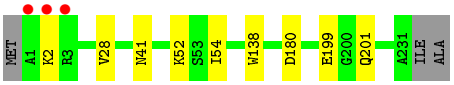




- Molecule 1: Proteasome subunit alpha type-2

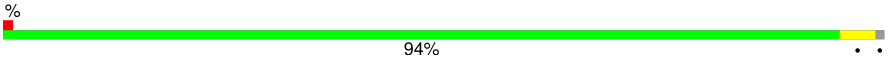
Chain c:

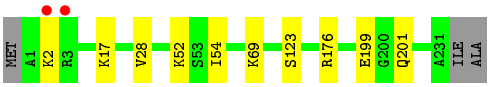




- Molecule 1: Proteasome subunit alpha type-2

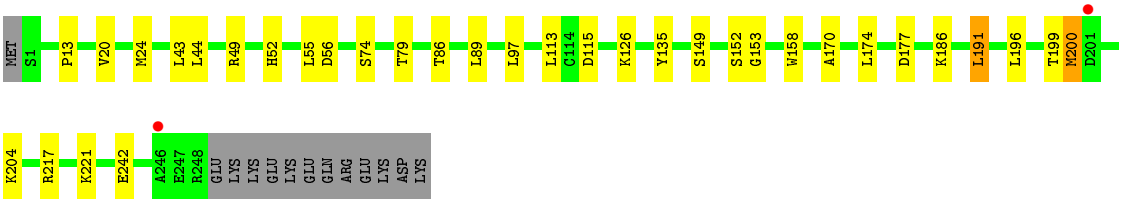
Chain q:



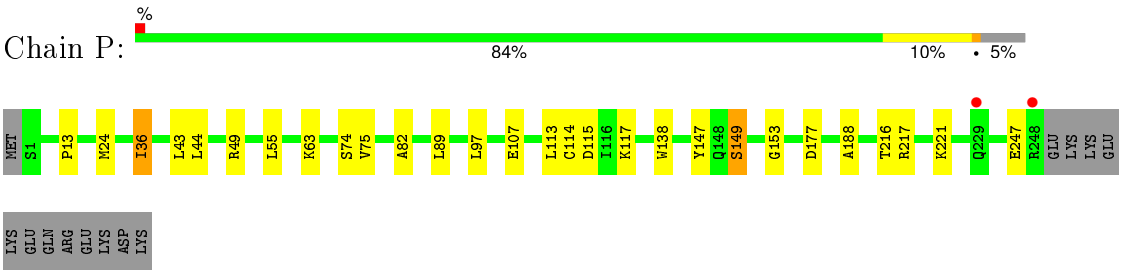


- Molecule 2: Proteasome subunit alpha type-4

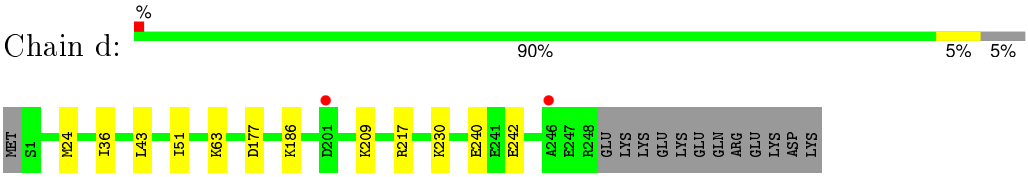
Chain B:



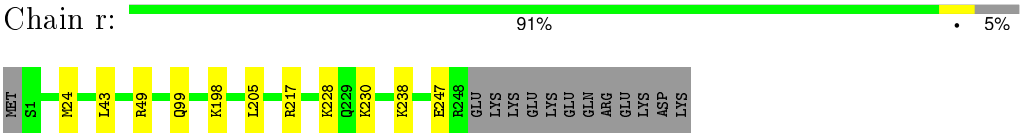
• Molecule 2: Proteasome subunit alpha type-4



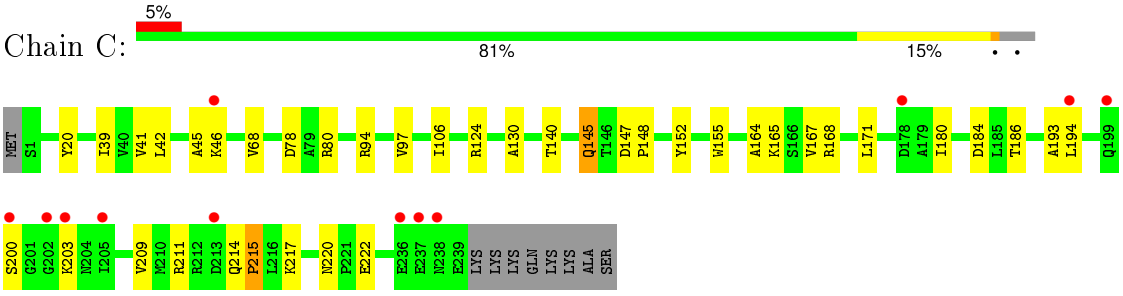
• Molecule 2: Proteasome subunit alpha type-4



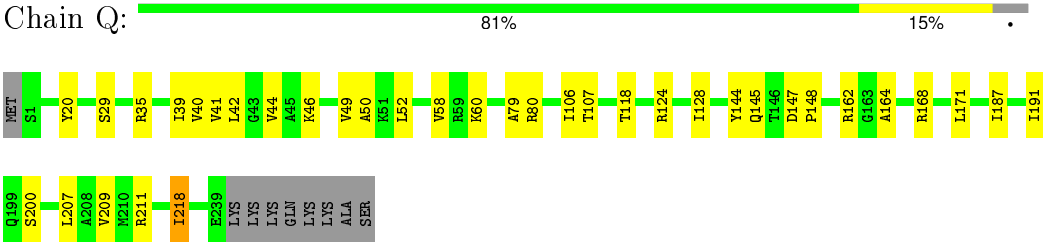
• Molecule 2: Proteasome subunit alpha type-4



• Molecule 3: Proteasome subunit alpha type-7

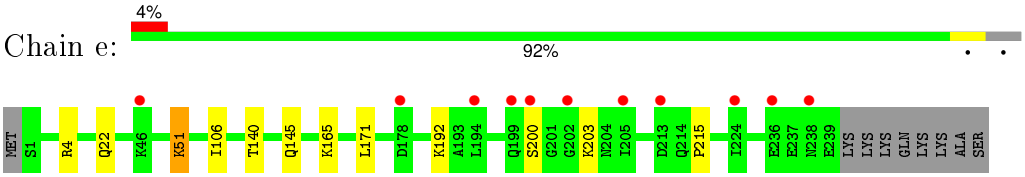


• Molecule 3: Proteasome subunit alpha type-7



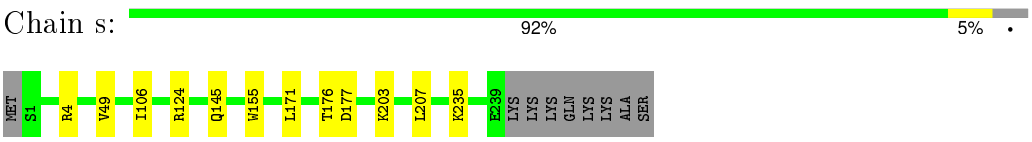
• Molecule 3: Proteasome subunit alpha type-7

Chain e:



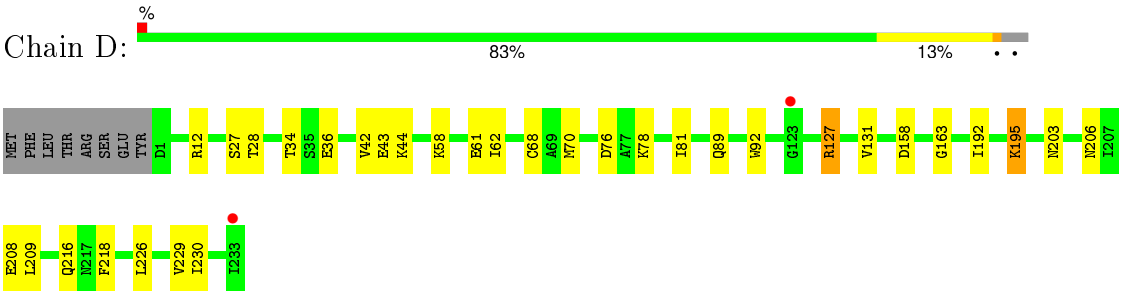
• Molecule 3: Proteasome subunit alpha type-7

Chain s:



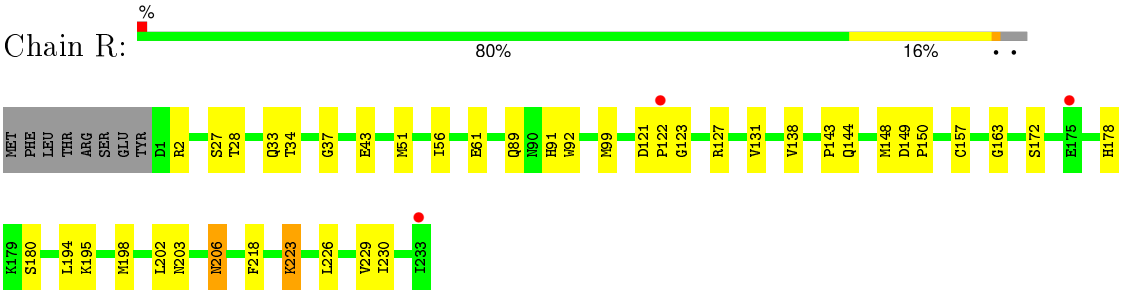
• Molecule 4: Proteasome subunit alpha type-5

Chain D:



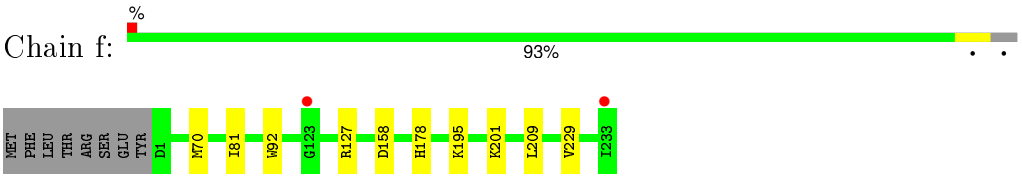
• Molecule 4: Proteasome subunit alpha type-5

Chain R:



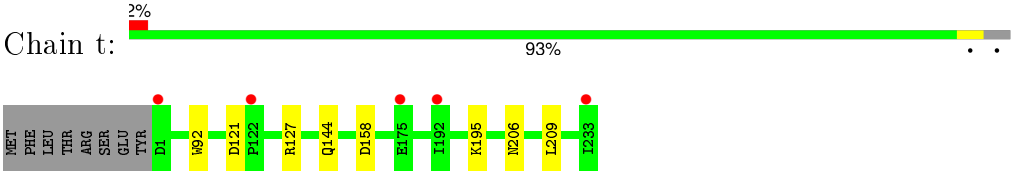
• Molecule 4: Proteasome subunit alpha type-5

Chain f:



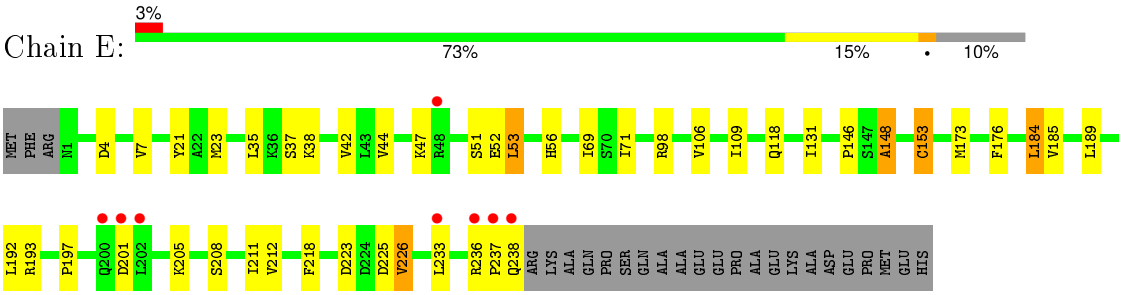
• Molecule 4: Proteasome subunit alpha type-5

Chain t:



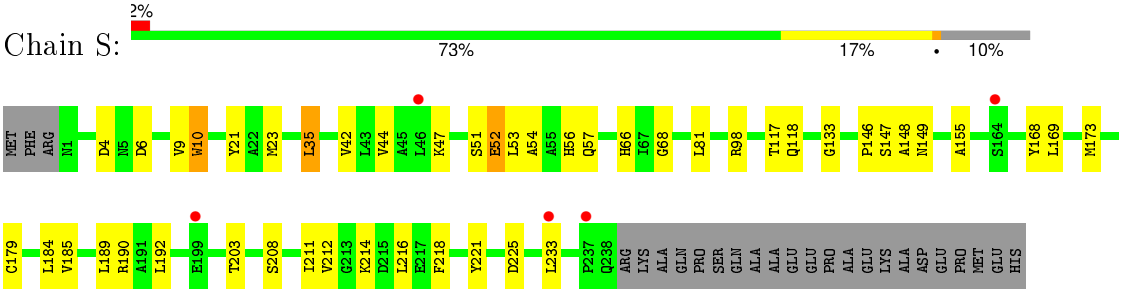
• Molecule 5: Proteasome subunit alpha type-1

Chain E:



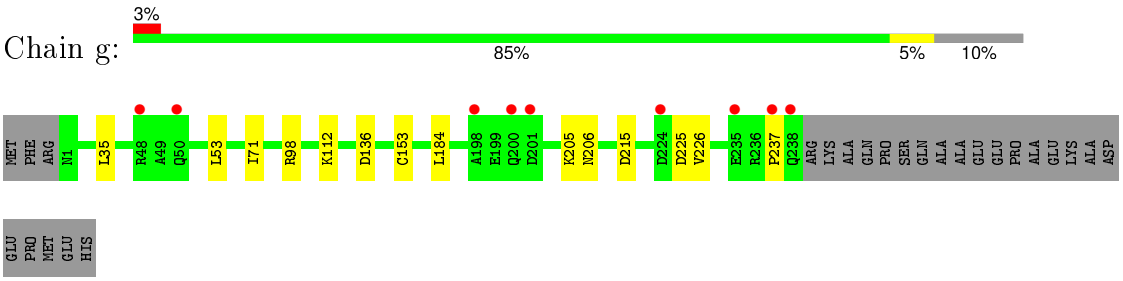
• Molecule 5: Proteasome subunit alpha type-1

Chain S:



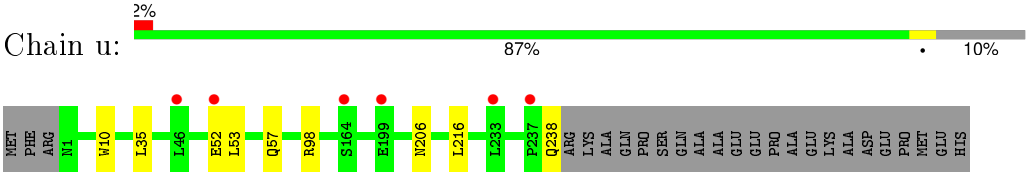
• Molecule 5: Proteasome subunit alpha type-1

Chain g:



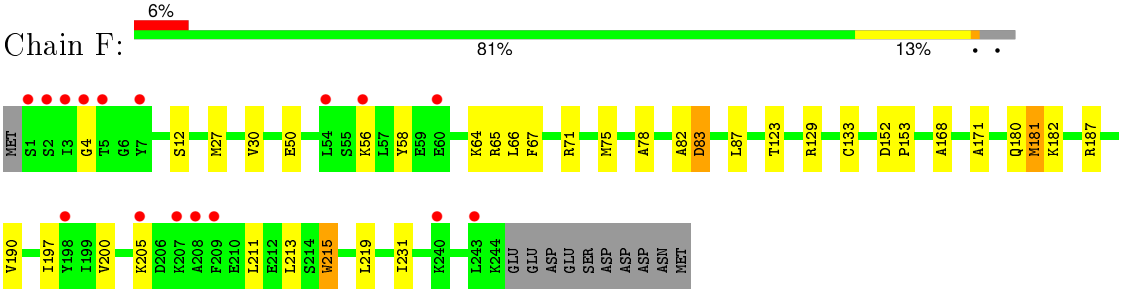
• Molecule 5: Proteasome subunit alpha type-1

Chain u:



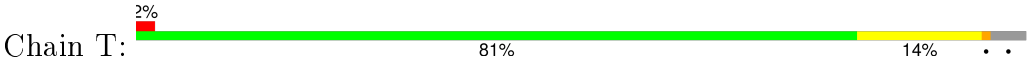
• Molecule 6: Proteasome subunit alpha type-3

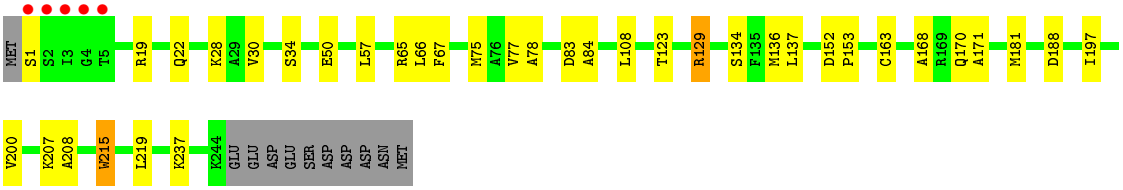
Chain F:



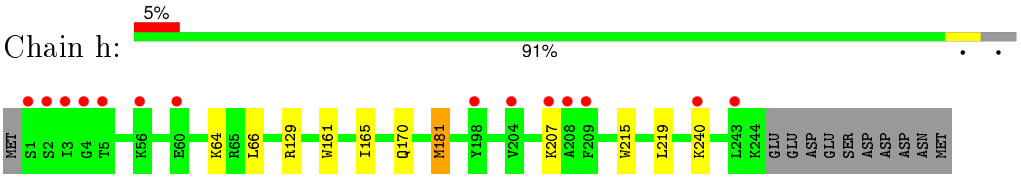
• Molecule 6: Proteasome subunit alpha type-3

Chain T:

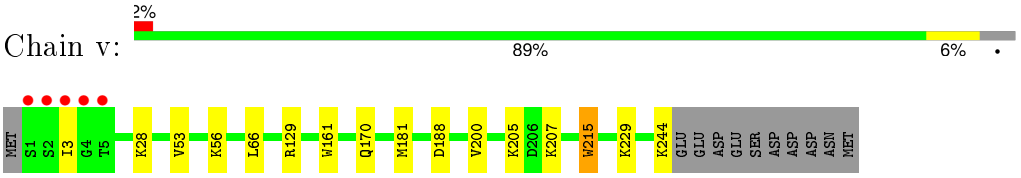




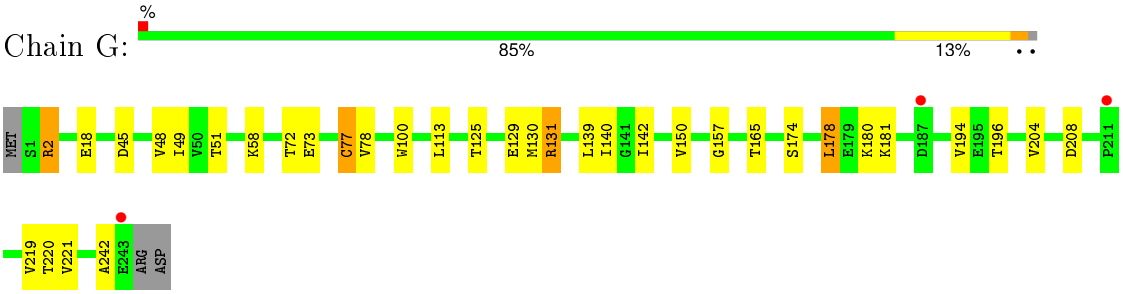
• Molecule 6: Proteasome subunit alpha type-3



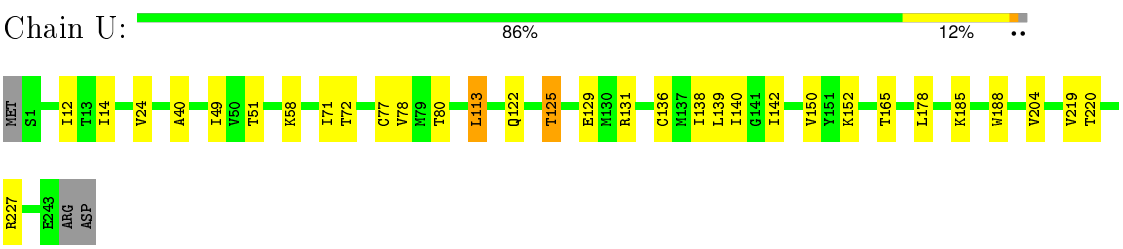
• Molecule 6: Proteasome subunit alpha type-3



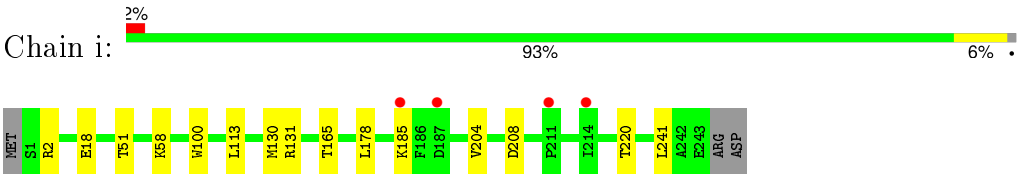
• Molecule 7: Proteasome subunit alpha type-6



• Molecule 7: Proteasome subunit alpha type-6

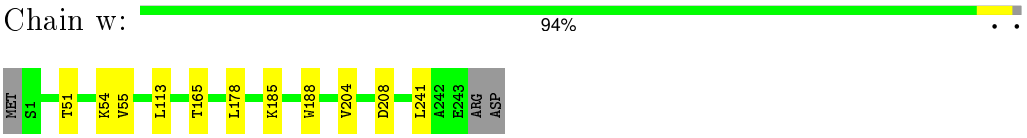


• Molecule 7: Proteasome subunit alpha type-6



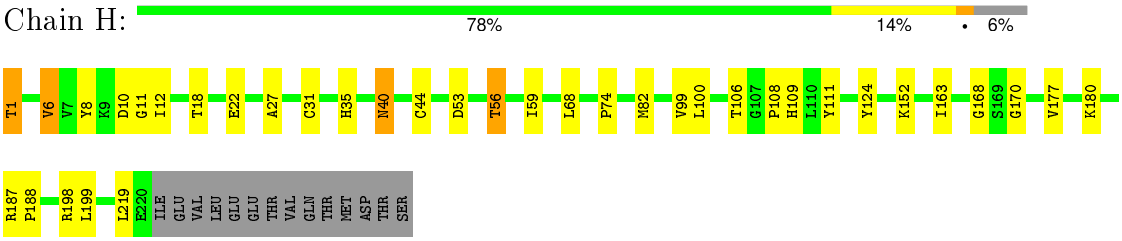
• Molecule 7: Proteasome subunit alpha type-6

Chain w:



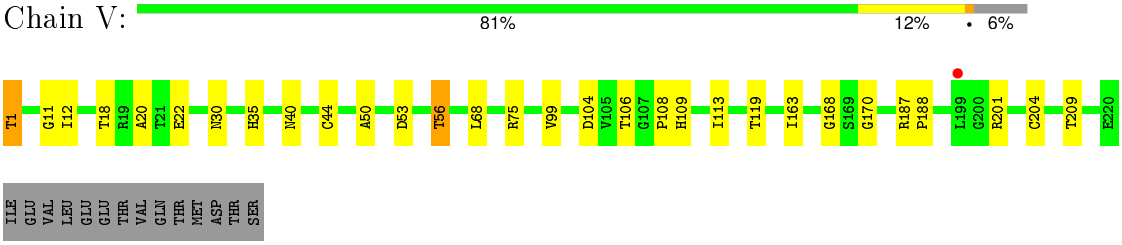
• Molecule 8: Proteasome subunit beta type-7

Chain H:



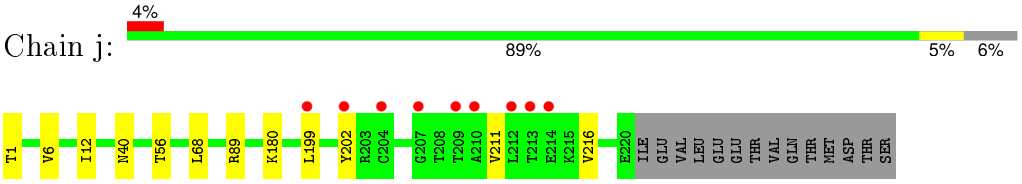
• Molecule 8: Proteasome subunit beta type-7

Chain V:



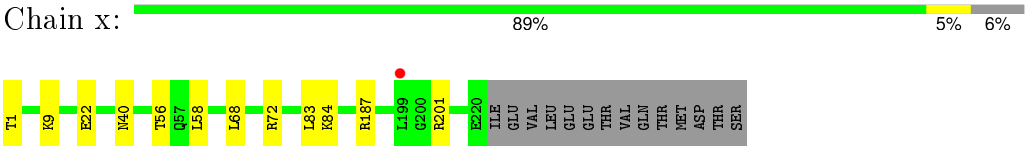
• Molecule 8: Proteasome subunit beta type-7

Chain j:



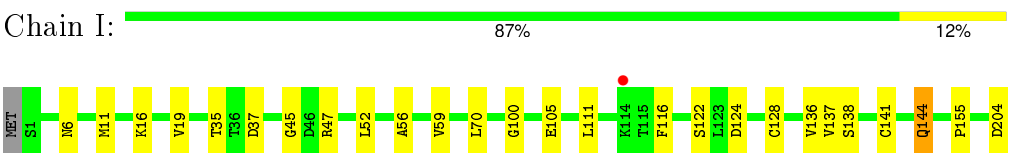
• Molecule 8: Proteasome subunit beta type-7

Chain x:



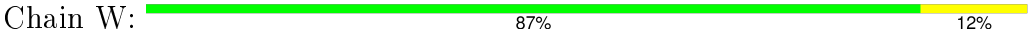
• Molecule 9: Proteasome subunit beta type-3

Chain I:



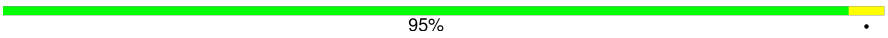
• Molecule 9: Proteasome subunit beta type-3

Chain W:



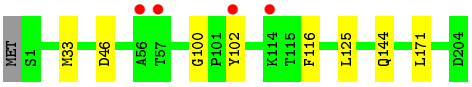
• Molecule 9: Proteasome subunit beta type-3

Chain k:



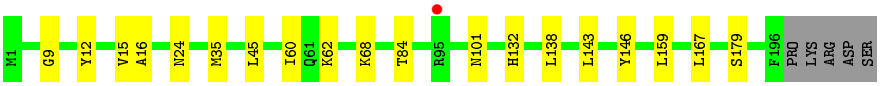
• Molecule 9: Proteasome subunit beta type-3

Chain y:



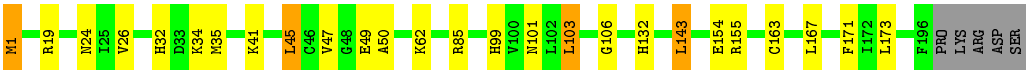
• Molecule 10: Proteasome subunit beta type-2

Chain J:



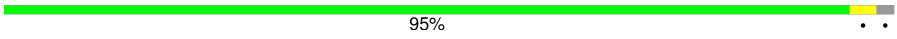
• Molecule 10: Proteasome subunit beta type-2

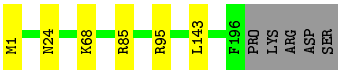
Chain X:



• Molecule 10: Proteasome subunit beta type-2

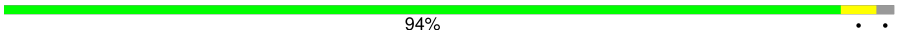
Chain l:

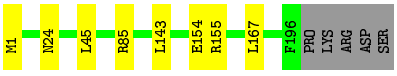




• Molecule 10: Proteasome subunit beta type-2

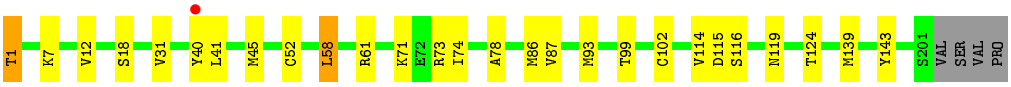
Chain z:





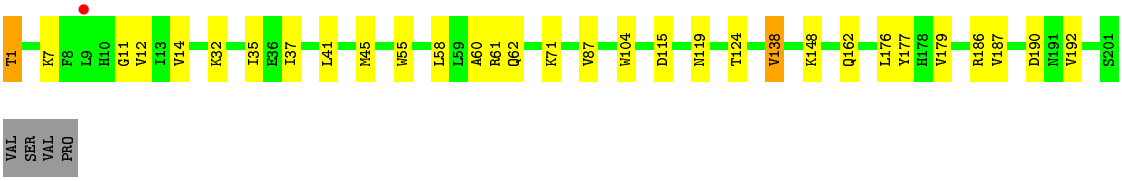
• Molecule 11: Proteasome subunit beta type-5

Chain K:



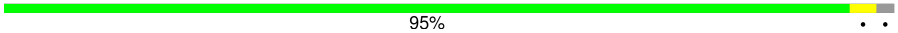
• Molecule 11: Proteasome subunit beta type-5

Chain Y:



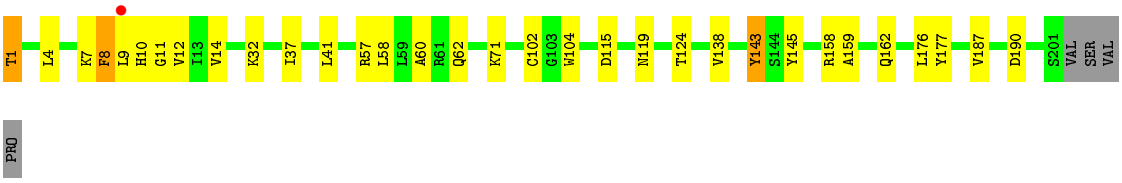
• Molecule 11: Proteasome subunit beta type-5

Chain m:



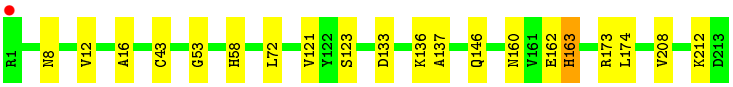
• Molecule 11: Proteasome subunit beta type-5

Chain 1:



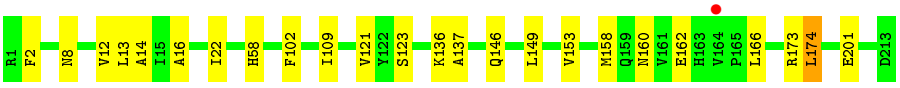
• Molecule 12: Proteasome subunit beta type-1

Chain L:



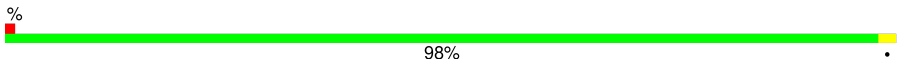
• Molecule 12: Proteasome subunit beta type-1

Chain Z:



• Molecule 12: Proteasome subunit beta type-1

Chain n:



• Molecule 12: Proteasome subunit beta type-1

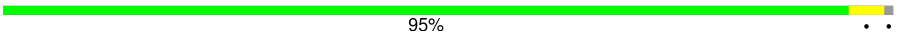
Chain 2:

• Molecule 13: Proteasome subunit beta type-4

Chain M:

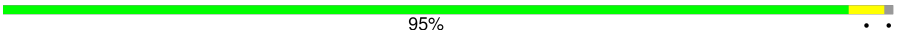
• Molecule 13: Proteasome subunit beta type-4

Chain a:



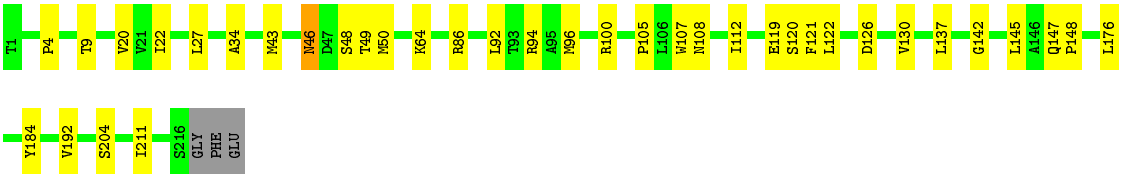
• Molecule 13: Proteasome subunit beta type-4

Chain o:



• Molecule 13: Proteasome subunit beta type-4

Chain 3:

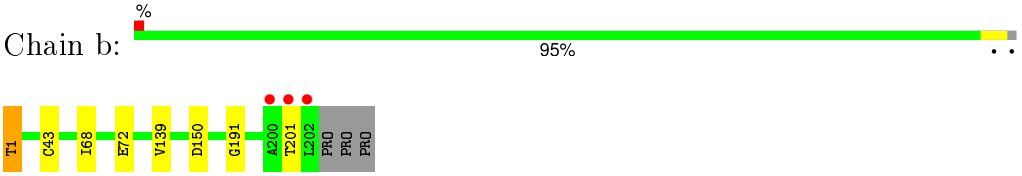


• Molecule 14: Proteasome subunit beta type-6

Chain N:

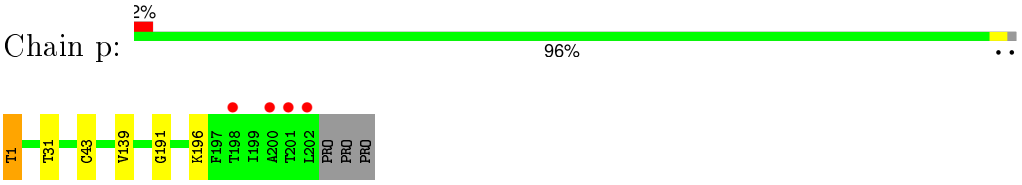
• Molecule 14: Proteasome subunit beta type-6

Chain b:



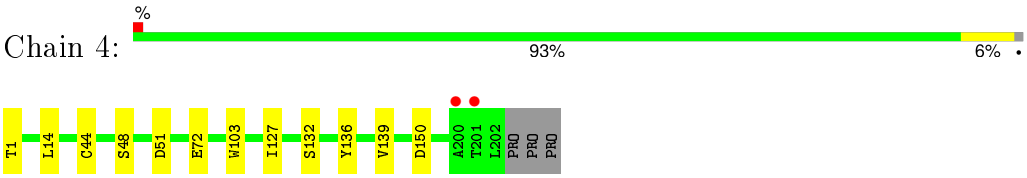
• Molecule 14: Proteasome subunit beta type-6

Chain p:



• Molecule 14: Proteasome subunit beta type-6

Chain 4:



4 Data and refinement statistics (i)

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 49.19 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.0 (15.00-2.90) 96.0 (49.19-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.57 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.6.0119	Depositor
R, R_{free}	0.230 , 0.273 0.230 , 0.273	Depositor DCC
R_{free} test set	15336 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	56.0	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 45.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Outliers	4 of 308934 reflections (0.001%)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.39	1/1845 (0.1%)	0.49	0/2498
1	O	0.39	1/1845 (0.1%)	0.48	0/2498
1	c	0.39	1/1845 (0.1%)	0.48	0/2498
1	q	0.39	0/1845	0.47	0/2498
2	B	0.37	1/1980 (0.1%)	0.48	0/2667
2	P	0.37	1/1980 (0.1%)	0.48	0/2667
2	d	0.37	0/1980	0.48	0/2667
2	r	0.37	0/1980	0.48	0/2667
3	C	0.33	0/1908	0.47	0/2576
3	Q	0.34	0/1908	0.48	0/2576
3	e	0.33	0/1908	0.47	0/2576
3	s	0.34	1/1908 (0.1%)	0.47	0/2576
4	D	0.36	1/1805 (0.1%)	0.47	0/2437
4	R	0.36	1/1805 (0.1%)	0.46	0/2437
4	f	0.36	1/1805 (0.1%)	0.47	0/2437
4	t	0.37	0/1805	0.47	0/2437
5	E	0.37	0/1907	0.49	0/2578
5	S	0.38	1/1907 (0.1%)	0.51	0/2578
5	g	0.37	0/1907	0.48	0/2578
5	u	0.38	1/1907 (0.1%)	0.50	0/2578
6	F	0.39	1/1938 (0.1%)	0.48	0/2608
6	T	0.38	1/1938 (0.1%)	0.48	0/2608
6	h	0.38	1/1938 (0.1%)	0.48	0/2608
6	v	0.39	2/1938 (0.1%)	0.48	0/2608
7	G	0.37	1/1924 (0.1%)	0.48	0/2600
7	U	0.38	1/1924 (0.1%)	0.49	0/2600
7	i	0.37	1/1924 (0.1%)	0.48	0/2600
7	w	0.38	1/1924 (0.1%)	0.48	0/2600
8	H	0.35	0/1683	0.51	1/2276 (0.0%)
8	V	0.37	1/1683 (0.1%)	0.51	0/2276
8	j	0.33	0/1683	0.52	0/2276
8	x	0.36	1/1683 (0.1%)	0.52	1/2276 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
9	I	0.34	0/1621	0.49	0/2185
9	W	0.35	0/1621	0.49	0/2185
9	k	0.34	0/1621	0.48	0/2185
9	y	0.35	0/1621	0.50	0/2185
10	J	0.33	0/1602	0.49	0/2167
10	X	0.33	0/1602	0.49	0/2167
10	l	0.33	0/1602	0.49	0/2167
10	z	0.33	0/1602	0.49	0/2167
11	1	0.44	1/1588 (0.1%)	0.50	0/2145
11	K	0.44	1/1588 (0.1%)	0.50	0/2145
11	Y	0.46	2/1588 (0.1%)	0.48	0/2145
11	m	0.45	1/1588 (0.1%)	0.50	0/2145
12	2	0.32	0/1685	0.48	0/2271
12	L	0.33	0/1685	0.48	0/2271
12	Z	0.33	0/1685	0.48	0/2271
12	n	0.33	0/1685	0.47	0/2271
13	3	0.40	0/1718	0.50	0/2325
13	M	0.41	3/1718 (0.2%)	0.50	0/2325
13	a	0.41	1/1718 (0.1%)	0.51	0/2325
13	o	0.40	1/1718 (0.1%)	0.48	0/2325
14	4	0.39	1/1546 (0.1%)	0.48	0/2094
14	N	0.39	2/1546 (0.1%)	0.48	0/2094
14	b	0.39	1/1546 (0.1%)	0.49	0/2094
14	p	0.39	1/1546 (0.1%)	0.48	0/2094
All	All	0.37	37/99000 (0.0%)	0.49	2/133708 (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 (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Y	1	THR	C-N	7.39	1.51	1.34
11	m	1	THR	C-N	7.02	1.50	1.34
11	K	1	THR	C-N	6.13	1.48	1.34
8	V	1	THR	C-N	6.04	1.48	1.34
8	x	1	THR	C-N	6.00	1.47	1.34
14	p	1	THR	C-N	5.49	1.46	1.34
7	G	100	TRP	CD2-CE2	5.19	1.47	1.41
14	b	1	THR	C-N	5.16	1.46	1.34
13	M	91	TRP	CD2-CE2	5.12	1.47	1.41
3	s	155	TRP	CD2-CE2	5.12	1.47	1.41
11	Y	55	TRP	CD2-CE2	5.10	1.47	1.41
14	N	1	THR	C-N	5.10	1.45	1.34
5	S	10	TRP	CD2-CE2	5.09	1.47	1.41
11	1	1	THR	C-N	5.09	1.45	1.34
7	U	188	TRP	CD2-CE2	5.09	1.47	1.41
4	R	92	TRP	CD2-CE2	5.08	1.47	1.41
14	4	103	TRP	CD2-CE2	5.07	1.47	1.41
4	f	92	TRP	CD2-CE2	5.06	1.47	1.41
1	A	138	TRP	CD2-CE2	5.05	1.47	1.41
4	D	92	TRP	CD2-CE2	5.05	1.47	1.41
6	F	215	TRP	CD2-CE2	5.04	1.47	1.41
6	T	215	TRP	CD2-CE2	5.03	1.47	1.41
7	i	100	TRP	CD2-CE2	5.03	1.47	1.41
14	N	103	TRP	CD2-CE2	5.03	1.47	1.41
13	M	209	TRP	CD2-CE2	5.03	1.47	1.41
6	v	215	TRP	CD2-CE2	5.03	1.47	1.41
6	v	161	TRP	CD2-CE2	5.02	1.47	1.41
13	o	91	TRP	CD2-CE2	5.02	1.47	1.41
6	h	161	TRP	CD2-CE2	5.02	1.47	1.41
13	M	107	TRP	CD2-CE2	5.02	1.47	1.41
1	O	138	TRP	CD2-CE2	5.02	1.47	1.41
1	c	138	TRP	CD2-CE2	5.01	1.47	1.41
2	P	138	TRP	CD2-CE2	5.01	1.47	1.41
13	a	209	TRP	CD2-CE2	5.01	1.47	1.41
5	u	10	TRP	CD2-CE2	5.01	1.47	1.41
2	B	158	TRP	CD2-CE2	5.00	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	w	188	TRP	CD2-CE2	5.00	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	1	THR	C-N-CA	6.26	137.36	121.70
8	x	1	THR	C-N-CA	5.11	134.48	121.70

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	1	1	THR	Peptide
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

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	21	0
1	O	1806	0	1805	21	0
1	c	1806	0	1805	0	0
1	q	1806	0	1805	0	0
2	B	1950	0	1973	13	0
2	P	1950	0	1973	13	0
2	d	1950	0	1973	0	0
2	r	1950	0	1973	0	0
3	C	1881	0	1907	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Q	1881	0	1907	20	0
3	e	1881	0	1907	0	0
3	s	1881	0	1907	0	0
4	D	1778	0	1767	14	0
4	R	1778	0	1767	19	0
4	f	1778	0	1767	0	0
4	t	1778	0	1767	0	0
5	E	1872	0	1859	22	0
5	S	1872	0	1859	25	0
5	g	1872	0	1859	0	0
5	u	1872	0	1859	0	0
6	F	1903	0	1894	20	0
6	T	1903	0	1894	21	0
6	h	1903	0	1894	0	0
6	v	1903	0	1894	0	0
7	G	1890	0	1900	17	0
7	U	1890	0	1900	16	0
7	i	1890	0	1900	0	0
7	w	1890	0	1900	0	0
8	H	1656	0	1682	23	0
8	V	1656	0	1683	15	0
8	j	1656	0	1682	0	0
8	x	1656	0	1683	0	0
9	I	1592	0	1612	13	0
9	W	1592	0	1612	15	0
9	k	1592	0	1612	0	0
9	y	1592	0	1612	0	0
10	J	1570	0	1573	12	0
10	X	1570	0	1573	13	0
10	l	1570	0	1573	0	0
10	z	1570	0	1573	0	0
11	1	1557	0	1523	14	0
11	K	1557	0	1524	14	0
11	Y	1557	0	1523	12	0
11	m	1557	0	1524	0	0
12	2	1654	0	1652	16	0
12	L	1654	0	1652	9	0
12	Z	1654	0	1652	12	0
12	n	1654	0	1652	0	0
13	3	1685	0	1664	23	0
13	M	1685	0	1664	11	0
13	a	1685	0	1664	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	o	1685	0	1664	0	0
14	4	1519	0	1485	5	0
14	N	1519	0	1486	9	0
14	b	1519	0	1486	0	0
14	p	1519	0	1485	0	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	0	0
15	j	42	0	42	0	0
15	m	42	0	42	0	0
15	p	42	0	42	0	0
15	x	42	0	42	0	0
16	1	27	0	0	1	0
16	2	33	0	0	0	0
16	3	37	0	0	2	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	0	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	0	0
16	h	19	0	0	0	0
16	i	29	0	0	0	0
16	j	25	0	0	0	0
16	k	30	0	0	0	0
16	l	22	0	0	0	0
16	m	20	0	0	0	0
16	n	29	0	0	0	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	0	0
16	y	32	0	0	0	0
16	z	38	0	0	0	0
All	All	99236	0	97694	443	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 (443) 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
8:V:187:ARG:HB3	8:V:188:PRO:HD3	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:4:GLY:HA2	7:G:129:GLU:HG2	1.61	0.82
5:S:47:LYS:HE3	5:S:208:SER:HB2	1.63	0.81
12:L:123:SER:HB3	12:L:136:LYS:HG2	1.63	0.78
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
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
4:D:34:THR:HG22	4:D:36:GLU:H	1.54	0.73
13:M:46:ASN:HD22	13:M:48:SER:H	1.37	0.71
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
12:2:13:LEU:HD11	12:2:149:LEU:HD11	1.74	0.70
3:C:45:ALA:HB2	3:C:194:LEU:HD22	1.74	0.69
1:O:67:ILE:HD11	1:O:73:LEU:HD12	1.74	0.69
7:U:122:GLN:O	7:U:125:THR:HG22	1.93	0.69
13:M:122:LEU:HG	13:M:137:LEU:HD12	1.75	0.68
12:L:162:GLU:O	12:L:163:HIS:HB2	1.94	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
1:A:127:ARG:HH21	7:G:125:THR:HG22	1.59	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
7:U:142:ILE:HG12	7:U:219:VAL:HG12	1.77	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
15:H:301:04C:H8	15:H:301:04C:H24	1.77	0.65
12:Z:13:LEU:HD11	12:Z:149:LEU:HD11	1.78	0.65
7:G:2:ARG:H	7:G:18:GLU:HG2	1.61	0.65
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
6:T:65:ARG:HH21	6:T:78:ALA:HA	1.63	0.64
8:V:44:CYS:HB2	8:V:99:VAL:HB	1.79	0.63
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
15:V:301:04C:H24	15:V:301:04C:H8	1.81	0.61
5:E:44:VAL:HG12	5:E:192:LEU:HD22	1.83	0.60
1:O:75:TYR:HB3	1:O:82:TYR:CD1	2.36	0.60
7:U:77:CYS:HB3	7:U:139:LEU:HD23	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:46:LYS:HE2	3:Q:162:ARG:HB3	1.83	0.60
4:D:226:LEU:O	4:D:230:ILE:HG12	2.01	0.60
13:3:46:ASN:HD21	13:3:49:THR:HG22	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
11:1:115:ASP:HB2	11:1:119:ASN:HB2	1.84	0.59
13:M:46:ASN:HD21	13:M:49:THR:HG23	1.66	0.59
11:K:115:ASP:HB2	11:K:119:ASN:HB2	1.85	0.59
8:H:40:ASN:H	8:H:40:ASN:HD22	1.50	0.59
7:U:49:ILE:HG21	7:U:78:VAL:HB	1.82	0.59
13:3:145:LEU:HG	16:3:333:HOH:O	2.03	0.58
12:L:16:ALA:HB2	12:L:121:VAL:HG23	1.84	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
4:D:27:SER:HB2	4:D:43:GLU:HG3	1.86	0.58
3:Q:44:VAL:HG21	3:Q:60:LYS:HB2	1.85	0.58
11:K:87:VAL:HG11	11:K:116:SER:HA	1.84	0.58
1:O:51:GLN:O	1:O:52:LYS:CB	2.52	0.57
3:C:152:TYR:HE2	4:D:78:LYS:HE2	1.69	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
9:W:144:GLN:HE21	9:W:144:GLN:H	1.51	0.57
10:X:99:HIS:HB3	16:X:306:HOH:O	2.03	0.57
9:W:6:ASN:ND2	9:W:56:ALA:H	2.03	0.57
13:3:46:ASN:HD22	13:3:48:SER:H	1.53	0.57
5:S:51:SER:O	5:S:53:LEU:N	2.38	0.57
11:Y:138:VAL:HG11	11:Y:162:GLN:HG3	1.86	0.57
5:S:118:GLN:HG3	6:T:129:ARG:HG3	1.87	0.57
2:P:44:LEU:HD13	2:P:74:SER:HB2	1.87	0.57
9:W:167:SER:O	9:W:171:LEU:HB2	2.05	0.56
7:U:142:ILE:HG12	7:U:219:VAL:CG1	2.35	0.56
4:R:202:LEU:HD21	4:R:230:ILE:HD12	1.86	0.56
6:F:168:ALA:HB3	6:F:200:VAL:HG13	1.86	0.56
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
12:L:12:VAL:HG21	12:L:53:GLY:HA3	1.88	0.55
14:N:16:ALA:HB2	14:N:121:VAL:HG23	20.64	0.55
11:1:7:LYS:HE2	11:1:124:THR:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:204:ASP:HB3	11:Y:192:VAL:HG11	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
13:M:27:LEU:HD11	13:M:34:ALA:HB1	1.89	0.55
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
5:E:47:LYS:CE	5:E:208:SER:HB2	2.38	0.54
8:H:152:LYS:HE2	8:H:177:VAL:HG21	1.88	0.54
12:2:145:LEU:HD22	12:2:178:VAL:HB	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
2:B:196:LEU:O	2:B:200:MET:HB2	2.08	0.53
3:Q:118:THR:O	4:R:127:ARG:NH1	2.41	0.53
2:P:153:GLY:O	3:Q:80:ARG:NH2	2.42	0.53
14:N:20:THR:HG22	14:N:31:THR:OG1	2.09	0.53
7:G:181:LYS:HD3	7:G:196:THR:HG23	1.91	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
10:X:35:MET:HG2	10:X:45:LEU:HD13	1.89	0.53
8:V:209:THR:HG21	9:W:167:SER:HB3	1.91	0.53
11:K:7:LYS:HB3	11:K:12:VAL:HG22	1.91	0.53
7:G:140:ILE:HG22	7:G:150:VAL:HG22	1.91	0.53
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
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
12:Z:136:LYS:HA	12:Z:146:GLN:NE2	2.25	0.52
8:V:168:GLY:O	15:V:301:04C:H33	2.10	0.52
11:1:176:LEU:HB3	11:1:187:VAL:HB	1.90	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
7:U:136:CYS:SG	7:U:152:LYS:HE2	2.49	0.52
1:O:127:ARG:HH21	7:U:125:THR:HG23	1.73	0.52
3:C:152:TYR:CE2	4:D:78:LYS:HE2	2.45	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
5:S:44:VAL:HG12	5:S:192:LEU:HD22	1.91	0.52
3:Q:29:SER:HB2	3:Q:60:LYS:HE2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:3:46:ASN:ND2	13:3:49:THR:HG22	2.24	0.51
2:P:117:LYS:HZ3	2:P:149:SER:HB3	1.75	0.51
5:S:10:TRP:H	6:T:22:GLN:HE22	1.58	0.51
5:S:23:MET:HA	5:S:146:PRO:HG2	1.92	0.51
12:2:8:ASN:ND2	12:2:58:HIS:H	2.09	0.51
12:L:137:ALA:H	12:L:146:GLN:HE21	1.57	0.51
8:H:22:GLU:HG2	8:H:27:ALA:HB2	1.92	0.51
6:T:34:SER:HB2	6:T:50:GLU:HG3	1.92	0.51
8:V:106:THR:HB	8:V:109:HIS:HE2	1.76	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
6:T:83:ASP:OD2	6:T:129:ARG:NH2	2.44	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
12:2:159:GLN:HG2	12:2:160:ASN:H	1.76	0.51
14:N:152:CYS:O	14:N:156:THR:HG22	2.11	0.51
11:Y:176:LEU:HB3	11:Y:187:VAL:HB	1.92	0.51
4:D:76:ASP:OD2	4:D:127:ARG:NH2	2.44	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
10:X:103:LEU:HD13	10:X:132:HIS:HD2	1.76	0.51
9:I:35:THR:HG22	9:I:37:ASP:H	1.75	0.51
8:V:187:ARG:HB3	8:V:188:PRO:CD	2.36	0.50
3:Q:50:ALA:C	3:Q:52:LEU:H	2.14	0.50
12:L:123:SER:CB	12:L:136:LYS:HG2	2.36	0.50
10:J:167:LEU:HB3	12:2:187:VAL:CG1	111.08	0.50
1:A:45:LEU:HB3	1:A:74:VAL:HG21	1.93	0.50
9:W:44:MET:HE3	9:W:70:LEU:HD22	1.93	0.50
6:F:87:LEU:HD12	6:F:133:CYS:SG	2.52	0.50
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.94	0.50
6:T:30:VAL:HG21	6:T:134:SER:HB2	1.94	0.50
8:V:18:THR:HB	8:V:30:ASN:HA	1.93	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
2:P:75:VAL:HG11	2:P:82:ALA:CB	2.42	0.50
4:R:203:ASN:H	4:R:206:ASN:ND2	2.10	0.49
3:Q:107:THR:HG21	3:Q:144:TYR:HB3	1.94	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:14:VAL:HB	11:Y:177:TYR:HB2	1.95	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
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
3:Q:195:LEU:HA	3:Q:198:VAL:HG12	1.94	0.49
2:P:89:LEU:HG	2:P:113:LEU:HD13	1.95	0.49
13:3:46:ASN:ND2	13:3:48:SER:H	2.10	0.49
14:N:30:VAL:O	14:N:30:VAL:HG13	2.12	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
1:O:51:GLN:HG3	1:O:56:TYR:HB2	1.94	0.49
13:3:50:MET:CE	13:3:192:VAL:HG23	2.43	0.49
5:S:35:LEU:HD13	5:S:184:LEU:HD22	1.94	0.49
3:Q:35:ARG:HA	3:Q:40:VAL:HG13	1.95	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
5:E:42:VAL:HG22	5:E:211:ILE:HG12	1.96	0.48
5:S:4:ASP:HB2	5:S:21:TYR:HE1	1.77	0.48
1:O:188:HIS:HD2	16:O:325:HOH:O	1.96	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
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
14:4:48:SER:HB2	15:4:301:04C:H25	1.95	0.48
5:S:233:LEU:HD23	5:S:233:LEU:H	1.79	0.48
5:S:4:ASP:HB2	5:S:21:TYR:CE1	2.49	0.48
3:C:145:GLN:HG2	3:C:155:TRP:NE1	2.29	0.48
3:C:164:ALA:O	3:C:168:ARG:HB2	2.14	0.48
1:A:106:THR:O	1:A:110:VAL:HG23	2.13	0.47
11:1:14:VAL:HB	11:1:177:TYR:HB2	1.96	0.47
5:E:148:ALA:HB3	6:F:82:ALA:HB1	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
15:4:301:04C:H8	15:4:301:04C:H22	1.97	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
6:T:67:PHE:HB2	6:T:75:MET:HB3	1.95	0.47
11:K:18:SER:O	11:K:31:VAL:HG22	2.14	0.47
6:T:1:SER:HB3	6:T:19:ARG:HH22	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1:138:VAL:CG2	11:1:159:ALA:HA	2.44	0.47
6:T:207:LYS:HG2	6:T:208:ALA:H	1.79	0.47
4:D:192:ILE:O	4:D:195:LYS:HG3	2.15	0.47
13:3:27:LEU:HD22	13:3:184:TYR:HB2	1.95	0.47
12:2:159:GLN:NE2	12:2:159:GLN:H	2.12	0.47
10:J:167:LEU:HB3	12:2:187:VAL:HG13	111.00	0.47
2:P:75:VAL:HG11	2:P:82:ALA:HB2	1.96	0.47
3:C:94:ARG:HB3	10:J:62:LYS:HE2	1.96	0.47
12:Z:14:ALA:HA	12:Z:22:ILE:O	2.14	0.47
8:V:35:HIS:CG	8:V:56:THR:HG21	2.49	0.47
1:O:198:PHE:O	1:O:199:GLU:HG2	2.14	0.47
5:E:223:ASP:O	5:E:226:VAL:HG12	2.14	0.47
2:P:115:ASP:OD1	3:Q:80:ARG:NH1	2.47	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
12:2:1:ARG:HD3	12:2:2:PHE:H	1.79	0.47
9:I:144:GLN:HE21	9:I:144:GLN:H	1.61	0.47
1:A:51:GLN:O	1:A:52:LYS:HG2	2.15	0.47
8:H:219:LEU:HD13	9:I:47:ARG:HD3	1.97	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
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
12:2:16:ALA:HB2	12:2:121:VAL:HG23	1.96	0.47
7:U:12:ILE:HG13	7:U:14:ILE:HG12	1.97	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
4:R:157:CYS:HA	5:S:54:ALA:HA	1.97	0.46
5:E:118:GLN:HG3	6:F:129:ARG:HG3	1.97	0.46
2:P:107:GLU:HG3	2:P:147:TYR:OH	2.15	0.46
8:H:106:THR:HB	8:H:109:HIS:HE2	1.81	0.46
3:Q:58:VAL:O	3:Q:58:VAL:HG12	2.16	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
3:C:41:VAL:HB	3:C:209:VAL:HG12	1.98	0.46
12:Z:16:ALA:HB2	12:Z:121:VAL:HG23	1.97	0.46
6:F:190:VAL:HG13	6:F:213:LEU:HD22	1.97	0.46
8:H:40:ASN:H	8:H:40:ASN:ND2	2.13	0.46
6:F:27:MET:O	6:F:30:VAL:HG12	2.16	0.46
5:E:106:VAL:HA	5:E:109:ILE:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:171:PHE:CE2	10:X:173:LEU:HB2	2.51	0.46
14:N:14:LEU:HD23	14:N:44:CYS:SG	2.55	0.46
9:I:6:ASN:ND2	9:I:56:ALA:H	2.14	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
13:3:126:ASP:HB2	13:3:130:VAL:HB	1.98	0.46
13:3:211:ILE:H	13:3:211:ILE:HD12	1.80	0.46
3:Q:147:ASP:HB2	3:Q:148:PRO:HD2	1.98	0.46
13:3:92:LEU:CD2	13:3:112:ILE:HD11	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
11:1:11:GLY:HA2	11:1:104:TRP:HZ3	1.80	0.45
5:S:117:THR:O	6:T:129:ARG:NH1	2.48	0.45
2:B:170:ALA:HB2	2:B:199:THR:HG21	1.98	0.45
5:S:212:VAL:HB	5:S:218:PHE:HD1	1.80	0.45
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.97	0.45
6:T:136:MET:CE	6:T:163:CYS:HB3	2.46	0.45
4:D:28:THR:HA	4:D:163:GLY:HA3	1.99	0.45
4:R:223:LYS:H	4:R:223:LYS:HD2	1.81	0.45
1:A:53:SER:C	1:A:55:LEU:H	2.20	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
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
12:Z:149:LEU:HD23	12:Z:174:LEU:HD22	1.99	0.45
10:X:1:MET:HB2	16:X:308:HOH:O	2.17	0.45
1:O:106:THR:O	1:O:110:VAL:HG23	2.17	0.45
12:Z:137:ALA:H	12:Z:146:GLN:HE21	1.65	0.44
10:X:101:ASN:HB3	10:X:132:HIS:CE1	2.51	0.44
9:W:137:VAL:HG11	9:W:145:MET:HB3	2.00	0.44
11:Y:35:ILE:HB	11:Y:45:MET:HE3	1.99	0.44
5:S:68:GLY:HA3	5:S:218:PHE:CZ	2.52	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
5:S:47:LYS:CB	5:S:56:HIS:HB3	2.43	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
4:D:44:LYS:HE3	4:D:208:GLU:HG3	1.99	0.44
9:W:35:THR:HG22	9:W:37:ASP:H	1.83	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

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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
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
5:S:42:VAL:HG22	5:S:211:ILE:HG12	2.00	0.44
12:L:136:LYS:HA	12:L:146:GLN:NE2	2.33	0.44
6:T:34:SER:OG	6:T:65:ARG:NH1	2.51	0.44
11:Y:37:ILE:HG23	11:Y:60:ALA:HA	2.00	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
9:W:64:GLN:HE22	10:X:85:ARG:NH1	2.16	0.44
13:M:59:ASP:HB3	13:M:108:ASN:HD21	1.82	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:I:52:LEU:HB2	9:I:59:VAL:HG13	1.99	0.44
13:M:27:LEU:HD22	13:M:184:TYR:HB2	1.99	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
6:T:50:GLU:HB3	6:T:197:ILE:HG23	2.00	0.43
12:2:43:CYS:HB3	12:2:196:CYS:SG	2.58	0.43
11:1:9:LEU:HB2	11:1:145:TYR:CE2	2.53	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
13:M:46:ASN:ND2	13:M:49:THR:HG23	2.33	0.43
5:S:155:ALA:HB3	6:T:57:LEU:HD22	2.01	0.43
1:O:114:ALA:HB1	1:O:152:GLY:O	2.18	0.43
6:F:197:ILE:HG21	6:F:211:LEU:HD13	1.98	0.43
5:S:6:ASP:HB2	5:S:9:VAL:HG23	2.00	0.43
8:H:168:GLY:O	15:H:301:04C:H33	2.18	0.43
1:A:51:GLN:HG3	1:A:56:TYR:HB2	2.00	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:F:152:ASP:HB2	6:F:153:PRO:HD2	2.00	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
4:D:89:GLN:HB3	11:K:61:ARG:HG3	2.01	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
14:4:127:ILE:HD11	14:4:136:TYR:CE2	2.54	0.43
12:Z:123:SER:HB3	12:Z:136:LYS:HG2	2.00	0.43
11:Y:11:GLY:HA2	11:Y:104:TRP:HZ3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:147:ASP:HB2	3:C:148:PRO:HD2	2.00	0.43
5:E:4:ASP:HB2	5:E:21:TYR:HE1	1.84	0.43
3:C:220:ASN:ND2	3:C:222:GLU:HB2	2.34	0.43
8:V:20:ALA:HB2	15:V:301:04C:H42	2.00	0.43
12:2:12:VAL:HG13	12:2:109:ILE:HD12	2.00	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
6:T:50:GLU:O	6:T:50:GLU:HG3	2.19	0.43
3:Q:44:VAL:HG21	3:Q:187:ILE:HA	14.08	0.43
13:3:147:GLN:HB3	13:3:148:PRO:HD3	2.01	0.43
1:O:149:ASP:HB2	1:O:150:PRO:CD	2.48	0.42
11:K:7:LYS:HE2	11:K:124:THR:HA	2.00	0.42
11:Y:7:LYS:HE2	11:Y:124:THR:HA	2.01	0.42
4:R:34:THR:HG22	4:R:37:GLY:O	2.19	0.42
8:H:6:VAL:HG23	8:H:124:TYR:HB3	2.01	0.42
3:Q:218:ILE:H	3:Q:218:ILE:HG13	1.57	0.42
6:F:123:THR:O	7:G:131:ARG:NH1	2.52	0.42
7:U:40:ALA:HB2	7:U:49:ILE:HD13	2.00	0.42
10:X:143:LEU:HD13	10:X:163:CYS:SG	2.59	0.42
6:T:136:MET:HE1	6:T:163:CYS:HB3	2.02	0.42
13:3:86:ARG:HG3	13:3:121:PHE:CE1	2.55	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
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
13:3:96:MET:HE1	13:3:108:ASN:HB2	2.01	0.42
13:3:122:LEU:HG	13:3:137:LEU:HD12	2.00	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
3:C:180:ILE:HA	3:C:186:THR:HG22	2.02	0.42
13:M:20:VAL:HG11	13:M:122:LEU:HD13	2.00	0.42
13:3:46:ASN:HD22	13:3:46:ASN:C	2.23	0.42
7:U:49:ILE:CG2	7:U:78:VAL:HB	2.47	0.42
3:Q:41:VAL:HB	3:Q:209:VAL:HG12	2.01	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
5:E:51:SER:O	5:E:53:LEU:N	2.52	0.42
1:O:147:GLN:HG3	1:O:162:MET:CE	2.50	0.42
8:H:100:LEU:HB3	8:H:111:TYR:HB2	2.01	0.42
10:X:49:GLU:HB2	10:X:99:HIS:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:130:ALA:O	3:C:145:GLN:HA	2.20	0.42
13:M:96:MET:HE1	13:M:108:ASN:HB2	2.02	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
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
5:S:168:TYR:OH	5:S:190:ARG:HD2	2.20	0.41
11:1:37:ILE:HG23	11:1:60:ALA:HA	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
12:2:14:ALA:HA	12:2:22:ILE:O	2.19	0.41
15:H:301:04C:H41	15:H:301:04C:H29	1.84	0.41
5:S:221:TYR:HD2	5:S:225:ASP:HB3	1.86	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
4:R:61:GLU:HB3	4:R:218:PHE:CD2	2.55	0.41
5:E:153:CYS:HB3	6:F:58:TYR:HD2	1.85	0.41
8:V:50:ALA:HB2	9:W:128:CYS:HB2	2.02	0.41
8:H:11:GLY:HA2	8:H:108:PRO:HB3	2.01	0.41
7:G:48:VAL:HG11	7:G:194:VAL:HA	2.01	0.41
2:B:52:HIS:H	2:B:55:LEU:HD12	1.84	0.41
14:N:18:SER:HB2	14:N:30:VAL:HA	2.01	0.41
10:J:138:LEU:HD21	10:X:26:VAL:HG12	2.01	0.41
7:U:140:ILE:HG22	7:U:150:VAL:HG22	2.01	0.41
14:N:174:ILE:HB	14:N:189:LEU:HB2	2.02	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
10:X:19:ARG:HA	10:X:32:HIS:O	2.21	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
6:F:187:ARG:NH2	6:F:231:ILE:HG23	2.36	0.41
11:1:8:PHE:CE1	11:1:10:HIS:HB2	2.55	0.41
15:N:301:04C:H22	15:N:301:04C:H8	2.03	0.41
2:P:13:PRO:HA	3:Q:20:TYR:CE2	2.55	0.41
3:C:39:ILE:HG22	3:C:211:ARG:HG2	2.01	0.41
1:A:212:CYS:HB2	1:A:217:PHE:HD1	1.86	0.41
13:3:22:ILE:HB	13:3:50:MET:HE3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:114:CYS:HB3	2:P:153:GLY:O	2.21	0.41
13:3:43:MET:SD	13:3:64:LYS:HG3	2.61	0.41
7:G:174:SER:O	7:G:178:LEU:HD22	2.21	0.41
3:Q:79:ALA:HA	3:Q:128:ILE:HD13	2.02	0.41
6:F:65:ARG:NH1	6:F:78:ALA:HA	2.27	0.41
1:A:67:ILE:HD11	1:A:73:LEU:CG	2.48	0.41
11:1:4:LEU:HD21	11:1:159:ALA:HB3	2.03	0.41
14:4:127:ILE:HD12	14:4:132:SER:HB2	2.02	0.41
5:S:169:LEU:O	5:S:173:MET:HB3	2.21	0.41
5:E:201:ASP:HB3	5:E:236:ARG:HH11	1.84	0.41
5:S:66:HIS:O	5:S:133:GLY:HA2	2.21	0.41
8:H:187:ARG:CB	8:H:188:PRO:HD3	2.40	0.40
1:O:45:LEU:HD13	1:O:74:VAL:HG23	2.03	0.40
5:E:193:ARG:HD3	5:E:236:ARG:HD3	2.03	0.40
6:T:77:VAL:HG11	6:T:84:ALA:HB1	2.03	0.40
13:3:105:PRO:HB2	16:3:334:HOH:O	2.20	0.40
9:W:144:GLN:HE21	9:W:144:GLN:N	2.18	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
10:X:32:HIS:ND1	10:X:34:LYS:HE3	2.36	0.40
11:K:58:LEU:HD12	11:K:86:MET:SD	2.61	0.40
3:Q:187:ILE:O	3:Q:191:ILE:HD12	3.01	0.40
11:1:7:LYS:HB3	11:1:12:VAL:HG22	2.02	0.40
7:G:49:ILE:CG2	7:G:78:VAL:HB	2.52	0.40
4:R:121:ASP:HB3	4:R:122:PRO:HD2	2.03	0.40
5:S:147:SER:C	5:S:149:ASN:H	2.25	0.40
4:R:51:MET:SD	4:R:56:ILE:HD11	2.61	0.40
1:O:73:LEU:HD21	1:O:133:LEU:HB3	2.03	0.40
9:I:144:GLN:HE21	9:I:144:GLN:N	2.19	0.40
4:D:61:GLU:HB3	4:D:218:PHE:CD2	2.57	0.40
11:1:158:ARG:HE	11:1:162: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%)	7	26
1	O	229/234 (98%)	215 (94%)	9 (4%)	5 (2%)	8	31
1	c	229/234 (98%)	217 (95%)	7 (3%)	5 (2%)	8	31
1	q	229/234 (98%)	216 (94%)	9 (4%)	4 (2%)	11	38
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%)	39	74
3	C	237/248 (96%)	220 (93%)	15 (6%)	2 (1%)	24	60
3	Q	237/248 (96%)	227 (96%)	8 (3%)	2 (1%)	24	60
3	e	237/248 (96%)	224 (94%)	10 (4%)	3 (1%)	15	46
3	s	237/248 (96%)	225 (95%)	11 (5%)	1 (0%)	39	74
4	D	231/241 (96%)	222 (96%)	9 (4%)	0	100	100
4	R	231/241 (96%)	220 (95%)	10 (4%)	1 (0%)	39	74
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%)	15	46
5	S	236/263 (90%)	219 (93%)	15 (6%)	2 (1%)	24	60
5	g	236/263 (90%)	220 (93%)	15 (6%)	1 (0%)	39	74
5	u	236/263 (90%)	221 (94%)	14 (6%)	1 (0%)	39	74
6	F	242/255 (95%)	232 (96%)	8 (3%)	2 (1%)	24	60
6	T	242/255 (95%)	234 (97%)	8 (3%)	0	100	100
6	h	242/255 (95%)	235 (97%)	5 (2%)	2 (1%)	24	60
6	v	242/255 (95%)	233 (96%)	7 (3%)	2 (1%)	24	60
7	G	241/246 (98%)	235 (98%)	3 (1%)	3 (1%)	16	48
7	U	241/246 (98%)	235 (98%)	6 (2%)	0	100	100
7	i	241/246 (98%)	234 (97%)	5 (2%)	2 (1%)	24	60
7	w	241/246 (98%)	234 (97%)	6 (2%)	1 (0%)	39	74
8	H	218/234 (93%)	213 (98%)	5 (2%)	0	100	100
8	V	218/234 (93%)	210 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	j	218/234 (93%)	212 (97%)	6 (3%)	0	100	100
8	x	218/234 (93%)	210 (96%)	7 (3%)	1 (0%)	34	71
9	I	202/205 (98%)	188 (93%)	9 (4%)	5 (2%)	7	27
9	W	202/205 (98%)	189 (94%)	12 (6%)	1 (0%)	34	71
9	k	202/205 (98%)	187 (93%)	12 (6%)	3 (2%)	13	42
9	y	202/205 (98%)	183 (91%)	16 (8%)	3 (2%)	13	42
10	J	194/201 (96%)	187 (96%)	6 (3%)	1 (0%)	34	71
10	X	194/201 (96%)	188 (97%)	4 (2%)	2 (1%)	19	54
10	l	194/201 (96%)	186 (96%)	7 (4%)	1 (0%)	34	71
10	z	194/201 (96%)	186 (96%)	7 (4%)	1 (0%)	34	71
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
11	m	199/205 (97%)	192 (96%)	7 (4%)	0	100	100
12	2	211/213 (99%)	204 (97%)	5 (2%)	2 (1%)	21	57
12	L	211/213 (99%)	204 (97%)	6 (3%)	1 (0%)	34	71
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%)	34	71
13	M	214/219 (98%)	203 (95%)	10 (5%)	1 (0%)	34	71
13	a	214/219 (98%)	202 (94%)	11 (5%)	1 (0%)	34	71
13	o	214/219 (98%)	206 (96%)	7 (3%)	1 (0%)	34	71
14	4	200/205 (98%)	193 (96%)	7 (4%)	0	100	100
14	N	200/205 (98%)	191 (96%)	8 (4%)	1 (0%)	34	71
14	b	200/205 (98%)	189 (94%)	10 (5%)	1 (0%)	34	71
14	p	200/205 (98%)	188 (94%)	11 (6%)	1 (0%)	34	71
All	All	12400/12920 (96%)	11841 (96%)	482 (4%)	77 (1%)	30	67

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	181	MET
14	N	191	GLY

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	184 (97%)	5 (3%)	54 85
1	O	189/191 (99%)	185 (98%)	4 (2%)	61 88
1	c	189/191 (99%)	186 (98%)	3 (2%)	70 91
1	q	189/191 (99%)	183 (97%)	6 (3%)	46 81
2	B	208/221 (94%)	194 (93%)	14 (7%)	20 50
2	P	208/221 (94%)	195 (94%)	13 (6%)	22 54
2	d	208/221 (94%)	196 (94%)	12 (6%)	25 58
2	r	208/221 (94%)	198 (95%)	10 (5%)	31 67
3	C	202/210 (96%)	191 (95%)	11 (5%)	27 62
3	Q	202/210 (96%)	195 (96%)	7 (4%)	43 78
3	e	202/210 (96%)	192 (95%)	10 (5%)	30 65
3	s	202/210 (96%)	192 (95%)	10 (5%)	30 65
4	D	195/203 (96%)	185 (95%)	10 (5%)	29 65
4	R	195/203 (96%)	185 (95%)	10 (5%)	29 65
4	f	195/203 (96%)	186 (95%)	9 (5%)	33 69
4	t	195/203 (96%)	187 (96%)	8 (4%)	37 73
5	E	204/224 (91%)	192 (94%)	12 (6%)	24 58
5	S	204/224 (91%)	195 (96%)	9 (4%)	35 70
5	g	204/224 (91%)	191 (94%)	13 (6%)	22 53
5	u	204/224 (91%)	197 (97%)	7 (3%)	44 79
6	F	200/211 (95%)	192 (96%)	8 (4%)	38 74
6	T	200/211 (95%)	190 (95%)	10 (5%)	30 65
6	h	200/211 (95%)	191 (96%)	9 (4%)	34 70
6	v	200/211 (95%)	187 (94%)	13 (6%)	21 52
7	G	207/210 (99%)	196 (95%)	11 (5%)	28 63
7	U	207/210 (99%)	195 (94%)	12 (6%)	25 58
7	i	207/210 (99%)	195 (94%)	12 (6%)	25 58
7	w	207/210 (99%)	198 (96%)	9 (4%)	35 71
8	H	181/195 (93%)	174 (96%)	7 (4%)	39 75
8	V	181/195 (93%)	174 (96%)	7 (4%)	39 75
8	j	181/195 (93%)	170 (94%)	11 (6%)	23 56
8	x	181/195 (93%)	171 (94%)	10 (6%)	27 61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	I	174/175 (99%)	171 (98%)	3 (2%)	68 91
9	W	174/175 (99%)	170 (98%)	4 (2%)	58 87
9	k	174/175 (99%)	168 (97%)	6 (3%)	44 79
9	y	174/175 (99%)	169 (97%)	5 (3%)	50 83
10	J	166/171 (97%)	164 (99%)	2 (1%)	78 94
10	X	166/171 (97%)	157 (95%)	9 (5%)	27 62
10	l	166/171 (97%)	161 (97%)	5 (3%)	48 83
10	z	166/171 (97%)	159 (96%)	7 (4%)	36 73
11	1	157/161 (98%)	147 (94%)	10 (6%)	22 53
11	K	157/161 (98%)	152 (97%)	5 (3%)	46 81
11	Y	157/161 (98%)	147 (94%)	10 (6%)	22 53
11	m	157/161 (98%)	151 (96%)	6 (4%)	40 76
12	2	178/178 (100%)	173 (97%)	5 (3%)	51 84
12	L	178/178 (100%)	170 (96%)	8 (4%)	34 70
12	Z	178/178 (100%)	171 (96%)	7 (4%)	39 75
12	n	178/178 (100%)	173 (97%)	5 (3%)	51 84
13	3	178/180 (99%)	173 (97%)	5 (3%)	51 84
13	M	178/180 (99%)	172 (97%)	6 (3%)	44 79
13	a	178/180 (99%)	172 (97%)	6 (3%)	44 79
13	o	178/180 (99%)	172 (97%)	6 (3%)	44 79
14	4	159/162 (98%)	156 (98%)	3 (2%)	65 89
14	N	159/162 (98%)	156 (98%)	3 (2%)	65 89
14	b	159/162 (98%)	153 (96%)	6 (4%)	40 76
14	p	159/162 (98%)	155 (98%)	4 (2%)	55 85
All	All	10392/10768 (96%)	9954 (96%)	438 (4%)	36 73

All (438) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	28	VAL
1	A	69	LYS
1	A	74	VAL
1	A	229	LEU

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Mol	Chain	Res	Type
2	B	24	MET
2	B	43	LEU
2	B	49	ARG
2	B	79	THR
2	B	97	LEU
2	B	126	LYS
2	B	177	ASP
2	B	186	LYS
2	B	191	LEU
2	B	200	MET
2	B	204	LYS
2	B	217	ARG
2	B	221	LYS
2	B	242	GLU
3	C	42	LEU
3	C	46	LYS
3	C	78	ASP
3	C	124	ARG
3	C	140	THR
3	C	145	GLN
3	C	165	LYS
3	C	171	LEU
3	C	184	ASP
3	C	203	LYS
3	C	217	LYS
4	D	12	ARG
4	D	70	MET
4	D	81	ILE
4	D	127	ARG
4	D	131	VAL
4	D	158	ASP
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	38	LYS
5	E	53	LEU
5	E	71	ILE
5	E	98	ARG
5	E	153	CYS

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Mol	Chain	Res	Type
5	E	184	LEU
5	E	205	LYS
5	E	225	ASP
5	E	226	VAL
5	E	238	GLN
6	F	56	LYS
6	F	66	LEU
6	F	71	ARG
6	F	83	ASP
6	F	181	MET
6	F	205	LYS
6	F	215	TRP
6	F	219	LEU
7	G	51	THR
7	G	58	LYS
7	G	77	CYS
7	G	113	LEU
7	G	130	MET
7	G	131	ARG
7	G	165	THR
7	G	178	LEU
7	G	180	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	180	LYS
8	H	198	ARG
9	I	19	VAL
9	I	70	LEU
9	I	144	GLN
10	J	68	LYS
10	J	143	LEU
11	K	41	LEU
11	K	58	LEU
11	K	71	LYS
11	K	73	ARG
11	K	93	MET
12	L	43	CYS

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Mol	Chain	Res	Type
12	L	72	LEU
12	L	133	ASP
12	L	160	ASN
12	L	173	ARG
12	L	174	LEU
12	L	208	VAL
12	L	212	LYS
13	M	46	ASN
13	M	49	THR
13	M	94	ARG
13	M	100	ARG
13	M	152	GLU
13	M	195	LYS
14	N	20	THR
14	N	139	VAL
14	N	201	THR
1	O	2	LYS
1	O	28	VAL
1	O	69	LYS
1	O	176	ARG
2	P	24	MET
2	P	36	ILE
2	P	43	LEU
2	P	49	ARG
2	P	55	LEU
2	P	63	LYS
2	P	97	LEU
2	P	149	SER
2	P	177	ASP
2	P	216	THR
2	P	217	ARG
2	P	221	LYS
2	P	247	GLU
3	Q	42	LEU
3	Q	106	ILE
3	Q	124	ARG
3	Q	145	GLN
3	Q	171	LEU
3	Q	207	LEU
3	Q	218	ILE
4	R	2	ARG
4	R	33	GLN

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Mol	Chain	Res	Type
4	R	131	VAL
4	R	144	GLN
4	R	148	MET
4	R	172	SER
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	203	THR
5	S	214	LYS
5	S	216	LEU
6	T	28	LYS
6	T	66	LEU
6	T	129	ARG
6	T	170	GLN
6	T	181	MET
6	T	188	ASP
6	T	200	VAL
6	T	215	TRP
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
7	U	227	ARG
8	V	12	ILE
8	V	22	GLU
8	V	40	ASN

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Mol	Chain	Res	Type
8	V	56	THR
8	V	68	LEU
8	V	201	ARG
8	V	204	CYS
9	W	101	PRO
9	W	114	LYS
9	W	117	LYS
9	W	144	GLN
10	X	1	MET
10	X	45	LEU
10	X	47	VAL
10	X	62	LYS
10	X	103	LEU
10	X	143	LEU
10	X	154	GLU
10	X	155	ARG
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	186	ARG
11	Y	190	ASP
12	Z	2	PHE
12	Z	102	PHE
12	Z	158	MET
12	Z	160	ASN
12	Z	162	GLU
12	Z	174	LEU
12	Z	201	GLU
13	a	37	ARG
13	a	46	ASN
13	a	94	ARG
13	a	100	ARG
13	a	119	GLU
13	a	182	ARG
14	b	43	CYS
14	b	68	ILE

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Mol	Chain	Res	Type
14	b	72	GLU
14	b	139	VAL
14	b	150	ASP
14	b	201	THR
1	c	2	LYS
1	c	28	VAL
1	c	52	LYS
2	d	24	MET
2	d	36	ILE
2	d	43	LEU
2	d	51	ILE
2	d	63	LYS
2	d	177	ASP
2	d	186	LYS
2	d	209	LYS
2	d	217	ARG
2	d	230	LYS
2	d	240	GLU
2	d	242	GLU
3	e	4	ARG
3	e	22	GLN
3	e	51	LYS
3	e	106	ILE
3	e	140	THR
3	e	145	GLN
3	e	165	LYS
3	e	171	LEU
3	e	192	LYS
3	e	203	LYS
4	f	70	MET
4	f	81	ILE
4	f	127	ARG
4	f	158	ASP
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	71	ILE
5	g	98	ARG

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Mol	Chain	Res	Type
5	g	112	LYS
5	g	136	ASP
5	g	153	CYS
5	g	184	LEU
5	g	205	LYS
5	g	206	ASN
5	g	215	ASP
5	g	225	ASP
5	g	226	VAL
6	h	64	LYS
6	h	66	LEU
6	h	129	ARG
6	h	165	ILE
6	h	170	GLN
6	h	181	MET
6	h	215	TRP
6	h	219	LEU
6	h	240	LYS
7	i	18	GLU
7	i	51	THR
7	i	58	LYS
7	i	113	LEU
7	i	130	MET
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	180	LYS
8	j	199	LEU
8	j	202	TYR
8	j	211	VAL
8	j	216	VAL
9	k	16	LYS

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Mol	Chain	Res	Type
9	k	114	LYS
9	k	136	VAL
9	k	144	GLN
9	k	152	LEU
9	k	174	VAL
10	l	1	MET
10	l	68	LYS
10	l	85	ARG
10	l	95	ARG
10	l	143	LEU
11	m	8	PHE
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	133	ASP
12	n	160	ASN
12	n	174	LEU
13	o	46	ASN
13	o	49	THR
13	o	94	ARG
13	o	100	ARG
13	o	152	GLU
13	o	195	LYS
14	p	31	THR
14	p	43	CYS
14	p	139	VAL
14	p	196	LYS
1	q	2	LYS
1	q	17	LYS
1	q	28	VAL
1	q	69	LYS
1	q	123	SER
1	q	176	ARG
2	r	24	MET
2	r	43	LEU
2	r	49	ARG
2	r	99	GLN
2	r	198	LYS

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Mol	Chain	Res	Type
2	r	217	ARG
2	r	228	LYS
2	r	230	LYS
2	r	238	LYS
2	r	247	GLU
3	s	4	ARG
3	s	106	ILE
3	s	124	ARG
3	s	145	GLN
3	s	171	LEU
3	s	176	THR
3	s	177	ASP
3	s	203	LYS
3	s	207	LEU
3	s	235	LYS
4	t	92	TRP
4	t	121	ASP
4	t	127	ARG
4	t	144	GLN
4	t	158	ASP
4	t	195	LYS
4	t	206	ASN
4	t	209	LEU
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	66	LEU
6	v	129	ARG
6	v	170	GLN
6	v	181	MET
6	v	188	ASP
6	v	200	VAL
6	v	205	LYS
6	v	215	TRP
6	v	229	LYS

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Mol	Chain	Res	Type
6	v	244	LYS
7	w	51	THR
7	w	54	LYS
7	w	55	VAL
7	w	113	LEU
7	w	165	THR
7	w	178	LEU
7	w	185	LYS
7	w	204	VAL
7	w	241	LEU
8	x	9	LYS
8	x	22	GLU
8	x	40	ASN
8	x	56	THR
8	x	58	LEU
8	x	68	LEU
8	x	72	ARG
8	x	83	LEU
8	x	84	LYS
8	x	201	ARG
9	y	33	MET
9	y	102	TYR
9	y	125	LEU
9	y	144	GLN
9	y	171	LEU
10	z	1	MET
10	z	45	LEU
10	z	85	ARG
10	z	143	LEU
10	z	154	GLU
10	z	155	ARG
10	z	167	LEU
11	1	8	PHE
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	143	TYR
11	1	190	ASP

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Mol	Chain	Res	Type
12	2	1	ARG
12	2	102	PHE
12	2	159	GLN
12	2	162	GLU
12	2	166	LEU
13	3	46	ASN
13	3	94	ARG
13	3	100	ARG
13	3	119	GLU
13	3	204	SER
14	4	72	GLU
14	4	139	VAL
14	4	150	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (160) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	139	ASN
2	B	94	GLN
2	B	108	GLN
2	B	122	GLN
2	B	154	ASN
3	C	22	GLN
3	C	91	GLN
4	D	196	GLN
4	D	216	GLN
5	E	2	GLN
5	E	28	GLN
5	E	57	GLN
5	E	143	GLN
6	F	147	GLN
6	F	180	GLN
7	G	126	GLN
8	H	30	ASN
8	H	40	ASN
8	H	62	ASN
8	H	66	HIS
9	I	6	ASN
9	I	64	GLN
9	I	144	GLN
10	J	55	GLN

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Mol	Chain	Res	Type
11	K	29	GLN
11	K	178	HIS
12	L	8	ASN
12	L	108	ASN
12	L	146	GLN
12	L	151	ASN
12	L	163	HIS
13	M	46	ASN
13	M	81	HIS
13	M	104	ASN
13	M	108	ASN
14	N	123	GLN
1	O	111	GLN
1	O	139	ASN
2	P	94	GLN
2	P	101	GLN
2	P	108	GLN
2	P	122	GLN
2	P	197	ASN
3	Q	22	GLN
4	R	91	HIS
4	R	178	HIS
4	R	196	GLN
4	R	206	ASN
5	S	180	ASN
6	T	22	GLN
7	U	91	GLN
7	U	126	GLN
8	V	30	ASN
8	V	40	ASN
8	V	66	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	61	GLN
10	X	132	HIS
11	Y	29	GLN
11	Y	62	GLN
11	Y	162	GLN

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Mol	Chain	Res	Type
11	Y	178	HIS
12	Z	8	ASN
12	Z	108	ASN
12	Z	146	GLN
12	Z	152	GLN
13	a	46	ASN
13	a	81	HIS
13	a	157	GLN
14	b	53	GLN
14	b	123	GLN
1	c	111	GLN
1	c	139	ASN
2	d	94	GLN
2	d	197	ASN
3	e	91	GLN
3	e	220	ASN
4	f	91	HIS
4	f	96	ASN
4	f	203	ASN
5	g	28	GLN
5	g	40	HIS
5	g	57	GLN
5	g	143	GLN
5	g	187	HIS
5	g	206	ASN
6	h	180	GLN
7	i	91	GLN
7	i	99	ASN
7	i	126	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	64	GLN
9	k	144	GLN
9	k	172	ASN
10	l	55	GLN
10	l	132	HIS
11	m	175	ASN
11	m	178	HIS

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Mol	Chain	Res	Type
12	n	8	ASN
12	n	108	ASN
12	n	146	GLN
12	n	163	HIS
13	o	46	ASN
13	o	69	GLN
13	o	104	ASN
13	o	108	ASN
13	o	147	GLN
13	o	157	GLN
14	p	123	GLN
1	q	111	GLN
1	q	139	ASN
2	r	87	ASN
2	r	94	GLN
2	r	99	GLN
2	r	101	GLN
2	r	122	GLN
2	r	197	ASN
3	s	22	GLN
4	t	91	HIS
4	t	196	GLN
4	t	206	ASN
5	u	40	HIS
5	u	143	GLN
5	u	206	ASN
7	w	126	GLN
8	x	30	ASN
8	x	40	ASN
8	x	66	HIS
8	x	116	HIS
9	y	6	ASN
9	y	39	GLN
9	y	64	GLN
9	y	71	ASN
9	y	144	GLN
10	z	55	GLN
10	z	61	GLN
10	z	71	ASN
10	z	132	HIS
11	1	29	GLN
11	1	162	GLN

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Mol	Chain	Res	Type
12	2	8	ASN
12	2	36	HIS
12	2	108	ASN
12	2	146	GLN
12	2	151	ASN
12	2	159	GLN
13	3	46	ASN
13	3	108	ASN
14	4	123	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 carbohydrates 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	1	301	11	43,44,44	1.80	7 (16%)	55,58,58	0.99	4 (7%)
15	04C	4	301	14	43,44,44	1.21	2 (4%)	55,58,58	1.01	3 (5%)
15	04C	H	301	8	43,44,44	1.30	5 (11%)	55,58,58	0.88	3 (5%)
15	04C	K	301	11	43,44,44	1.22	3 (6%)	55,58,58	1.22	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	04C	N	301	14	43,44,44	1.20	3 (6%)	55,58,58	1.10	3 (5%)
15	04C	V	301	8	43,44,44	1.24	4 (9%)	55,58,58	0.90	3 (5%)
15	04C	Y	301	11	43,44,44	1.33	4 (9%)	55,58,58	1.10	3 (5%)
15	04C	b	301	14	43,44,44	1.16	2 (4%)	55,58,58	1.02	3 (5%)
15	04C	j	301	8	43,44,44	1.26	4 (9%)	55,58,58	0.85	0
15	04C	m	301	11	43,44,44	1.22	3 (6%)	55,58,58	1.11	2 (3%)
15	04C	p	301	14	43,44,44	1.24	3 (6%)	55,58,58	1.13	4 (7%)
15	04C	x	301	8	43,44,44	1.21	3 (6%)	55,58,58	0.93	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	1	301	11	-	0/44/52/52	0/3/3/3
15	04C	4	301	14	-	0/44/52/52	0/3/3/3
15	04C	H	301	8	-	0/44/52/52	0/3/3/3
15	04C	K	301	11	-	0/44/52/52	0/3/3/3
15	04C	N	301	14	-	0/44/52/52	0/3/3/3
15	04C	V	301	8	-	0/44/52/52	0/3/3/3
15	04C	Y	301	11	-	0/44/52/52	0/3/3/3
15	04C	b	301	14	-	0/44/52/52	0/3/3/3
15	04C	j	301	8	-	0/44/52/52	0/3/3/3
15	04C	m	301	11	-	0/44/52/52	0/3/3/3
15	04C	p	301	14	-	0/44/52/52	0/3/3/3
15	04C	x	301	8	-	0/44/52/52	0/3/3/3

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	1	301	04C	O45-C44	-8.26	1.19	1.37
15	H	301	04C	O45-C44	-2.46	1.32	1.37
15	1	301	04C	C40-C41	2.15	1.56	1.51
15	1	301	04C	C5-C6	2.17	1.43	1.38
15	1	301	04C	C48-C41	2.20	1.43	1.38
15	H	301	04C	C5-C6	2.21	1.43	1.38
15	x	301	04C	C5-C6	2.23	1.43	1.38
15	V	301	04C	C47-C44	2.27	1.43	1.38
15	j	301	04C	C2-C3	2.33	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	K	301	04C	C5-C6	2.34	1.43	1.38
15	V	301	04C	C5-C6	2.36	1.43	1.38
15	N	301	04C	C7-C6	2.42	1.57	1.51
15	m	301	04C	C5-C6	2.48	1.44	1.38
15	H	301	04C	C47-C44	2.53	1.43	1.38
15	1	301	04C	C12-C10	2.69	1.56	1.52
15	Y	301	04C	C5-C6	2.71	1.44	1.38
15	N	301	04C	C12-C10	2.72	1.56	1.52
15	j	301	04C	C10-C9	2.77	1.58	1.53
15	x	301	04C	C10-C9	2.79	1.58	1.53
15	Y	301	04C	C12-C10	2.80	1.56	1.52
15	Y	301	04C	O45-C44	2.80	1.43	1.37
15	b	301	04C	C12-C10	2.83	1.56	1.52
15	p	301	04C	C12-C10	2.90	1.56	1.52
15	p	301	04C	C7-C6	2.90	1.58	1.51
15	K	301	04C	C12-C10	2.93	1.56	1.52
15	b	301	04C	C10-C9	2.94	1.59	1.53
15	N	301	04C	C10-C9	2.96	1.59	1.53
15	m	301	04C	C10-C9	2.97	1.59	1.53
15	m	301	04C	C12-C10	2.99	1.56	1.52
15	Y	301	04C	C10-C9	3.00	1.59	1.53
15	V	301	04C	C10-C9	3.00	1.59	1.53
15	4	301	04C	C10-C9	3.02	1.59	1.53
15	1	301	04C	C10-C9	3.09	1.59	1.53
15	p	301	04C	C10-C9	3.13	1.59	1.53
15	4	301	04C	C12-C10	3.13	1.56	1.52
15	K	301	04C	C10-C9	3.15	1.59	1.53
15	H	301	04C	C10-C9	3.17	1.59	1.53
15	x	301	04C	C12-C10	3.19	1.56	1.52
15	V	301	04C	C12-C10	3.20	1.56	1.52
15	j	301	04C	C12-C10	3.24	1.56	1.52
15	1	301	04C	C47-C44	3.25	1.45	1.38
15	j	301	04C	C5-C6	3.27	1.45	1.38
15	H	301	04C	C12-C10	3.35	1.56	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	K	301	04C	C11-C10-C12	-5.39	102.76	109.86
15	p	301	04C	C11-C10-C12	-4.87	103.44	109.86
15	m	301	04C	C11-C10-C12	-4.73	103.62	109.86
15	N	301	04C	C11-C10-C12	-4.72	103.63	109.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b	301	04C	C11-C10-C12	-4.35	104.13	109.86
15	4	301	04C	C11-C10-C12	-3.90	104.72	109.86
15	V	301	04C	C11-C10-C12	-3.52	105.22	109.86
15	N	301	04C	C7-C8-N22	-3.40	106.42	110.14
15	x	301	04C	C11-C10-C12	-3.13	105.73	109.86
15	p	301	04C	C7-C8-N22	-2.85	107.02	110.14
15	b	301	04C	C7-C8-N22	-2.76	107.12	110.14
15	4	301	04C	C7-C8-N22	-2.53	107.37	110.14
15	1	301	04C	C11-C10-C12	-2.52	106.54	109.86
15	x	301	04C	C7-C8-N22	-2.50	107.40	110.14
15	Y	301	04C	C41-C40-C24	-2.43	106.34	113.41
15	H	301	04C	C7-C8-N22	-2.28	107.65	110.14
15	V	301	04C	C7-C8-N22	-2.15	107.79	110.14
15	Y	301	04C	C7-C8-C9	-2.14	106.40	111.14
15	H	301	04C	C11-C10-C12	-2.10	107.09	109.86
15	1	301	04C	C7-C8-N22	-2.04	107.91	110.14
15	N	301	04C	C30-N31-C32	2.03	114.07	111.07
15	H	301	04C	C30-N31-C36	2.04	114.08	111.07
15	V	301	04C	C32-N31-C36	2.06	113.36	108.90
15	1	301	04C	C32-N31-C36	2.06	113.36	108.90
15	b	301	04C	C32-N31-C36	2.13	113.50	108.90
15	4	301	04C	C30-N31-C32	2.21	114.33	111.07
15	p	301	04C	C30-N31-C32	2.21	114.33	111.07
15	x	301	04C	C32-N31-C36	2.31	113.90	108.90
15	p	301	04C	C6-C7-C8	2.77	117.90	113.48
15	1	301	04C	C6-C7-C8	3.66	119.31	113.48
15	m	301	04C	C30-N31-C36	4.17	117.23	111.07
15	K	301	04C	C30-N31-C36	4.46	117.66	111.07
15	Y	301	04C	C6-C7-C8	4.87	121.23	113.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

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

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.35	2 (0%) 85 84	42, 62, 99, 145	0
1	O	231/234 (98%)	-0.34	3 (1%) 79 78	40, 59, 95, 145	0
1	c	231/234 (98%)	-0.34	3 (1%) 79 78	44, 64, 99, 143	0
1	q	231/234 (98%)	-0.34	2 (0%) 85 84	39, 61, 97, 140	0
2	B	248/261 (95%)	-0.31	2 (0%) 87 86	42, 69, 115, 156	0
2	P	248/261 (95%)	-0.29	2 (0%) 87 86	34, 62, 108, 155	0
2	d	248/261 (95%)	-0.26	2 (0%) 87 86	42, 71, 112, 161	0
2	r	248/261 (95%)	-0.28	0 100 100	40, 63, 109, 143	0
3	C	239/248 (96%)	0.17	12 (5%) 32 26	47, 83, 153, 182	0
3	Q	239/248 (96%)	-0.06	0 100 100	42, 74, 129, 163	0
3	e	239/248 (96%)	0.17	11 (4%) 36 30	51, 85, 148, 175	0
3	s	239/248 (96%)	-0.05	0 100 100	45, 75, 129, 164	0
4	D	233/241 (96%)	-0.29	2 (0%) 85 84	50, 74, 104, 149	0
4	R	233/241 (96%)	-0.25	3 (1%) 79 78	43, 72, 108, 163	0
4	f	233/241 (96%)	-0.29	2 (0%) 85 84	47, 75, 108, 158	0
4	t	233/241 (96%)	-0.22	5 (2%) 67 62	47, 73, 111, 171	0
5	E	238/263 (90%)	0.01	8 (3%) 49 41	45, 81, 135, 180	0
5	S	238/263 (90%)	-0.09	5 (2%) 67 62	39, 65, 125, 160	0
5	g	238/263 (90%)	0.05	9 (3%) 44 37	48, 81, 136, 172	0
5	u	238/263 (90%)	-0.06	6 (2%) 61 55	41, 65, 126, 156	0
6	F	244/255 (95%)	-0.00	16 (6%) 22 16	44, 76, 134, 167	0
6	T	244/255 (95%)	-0.20	5 (2%) 68 64	40, 64, 106, 159	0
6	h	244/255 (95%)	0.03	14 (5%) 27 21	47, 77, 135, 156	0
6	v	244/255 (95%)	-0.20	5 (2%) 68 64	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%)	-0.14	3 (1%) 81 78	42, 68, 108, 161	0
7	U	243/246 (98%)	-0.36	0 100 100	39, 59, 87, 121	0
7	i	243/246 (98%)	-0.12	4 (1%) 74 72	44, 70, 108, 138	0
7	w	243/246 (98%)	-0.39	0 100 100	39, 59, 88, 122	0
8	H	220/234 (94%)	-0.30	0 100 100	24, 52, 91, 127	0
8	V	220/234 (94%)	-0.36	1 (0%) 91 90	23, 49, 89, 126	0
8	j	220/234 (94%)	-0.10	9 (4%) 41 34	27, 54, 113, 146	0
8	x	220/234 (94%)	-0.29	1 (0%) 91 90	33, 54, 91, 127	0
9	I	204/205 (99%)	-0.33	1 (0%) 91 90	40, 55, 87, 119	0
9	W	204/205 (99%)	-0.35	0 100 100	35, 54, 89, 122	0
9	k	204/205 (99%)	-0.31	0 100 100	40, 56, 88, 122	0
9	y	204/205 (99%)	-0.16	4 (1%) 68 64	41, 60, 89, 126	0
10	J	196/201 (97%)	-0.36	1 (0%) 91 90	44, 59, 87, 114	0
10	X	196/201 (97%)	-0.41	0 100 100	40, 58, 85, 107	0
10	l	196/201 (97%)	-0.37	0 100 100	42, 59, 88, 112	0
10	z	196/201 (97%)	-0.37	0 100 100	40, 59, 86, 106	0
11	1	201/205 (98%)	-0.32	1 (0%) 91 90	36, 57, 88, 111	0
11	K	201/205 (98%)	-0.38	1 (0%) 91 90	38, 58, 92, 113	0
11	Y	201/205 (98%)	-0.33	1 (0%) 91 90	35, 56, 86, 109	0
11	m	201/205 (98%)	-0.34	1 (0%) 91 90	40, 59, 92, 117	0
12	2	213/213 (100%)	-0.30	1 (0%) 91 90	36, 57, 84, 135	0
12	L	213/213 (100%)	-0.24	1 (0%) 91 90	40, 56, 90, 123	0
12	Z	213/213 (100%)	-0.35	1 (0%) 91 90	37, 54, 86, 135	0
12	n	213/213 (100%)	-0.21	2 (0%) 85 84	42, 57, 91, 132	0
13	3	216/219 (98%)	-0.29	0 100 100	34, 52, 79, 101	0
13	M	216/219 (98%)	-0.37	0 100 100	36, 53, 82, 115	0
13	a	216/219 (98%)	-0.36	0 100 100	33, 49, 79, 105	0
13	o	216/219 (98%)	-0.31	0 100 100	40, 56, 84, 123	0
14	4	202/205 (98%)	-0.38	2 (0%) 84 82	31, 50, 99, 152	0
14	N	202/205 (98%)	-0.25	4 (1%) 68 64	30, 52, 91, 148	0
14	b	202/205 (98%)	-0.38	3 (1%) 76 74	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%)	-0.24	4 (1%) 68 64	32, 53, 92, 147	0
All	All	12512/12920 (96%)	-0.24	165 (1%) 79 78	23, 62, 111, 182	0

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	t	233	ILE	9.3
6	T	1	SER	8.8
6	v	1	SER	8.6
8	j	212	LEU	7.3
14	N	201	THR	6.6
6	F	3	ILE	5.9
4	R	122	PRO	5.7
4	R	233	ILE	5.6
14	p	201	THR	5.5
6	T	2	SER	5.5
4	D	233	ILE	5.0
5	E	237	PRO	4.9
4	f	233	ILE	4.8
6	F	2	SER	4.8
6	h	1	SER	4.8
8	j	213	THR	4.7
14	p	198	THR	4.4
1	O	2	LYS	4.4
14	b	201	THR	4.4
6	h	60	GLU	4.3
4	t	122	PRO	4.1
14	p	200	ALA	4.1
6	v	2	SER	4.0
1	O	3	ARG	3.9
3	e	202	GLY	3.9
5	S	237	PRO	3.8
3	C	202	GLY	3.8
7	i	211	PRO	3.8
6	h	2	SER	3.8
8	j	209	THR	3.7
14	b	200	ALA	3.7
5	u	237	PRO	3.7
8	j	207	GLY	3.6
6	T	3	ILE	3.6
1	A	1	ALA	3.6
7	G	211	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
6	F	4	GLY	3.6
6	T	5	THR	3.5
1	q	2	LYS	3.5
14	N	200	ALA	3.5
1	c	1	ALA	3.5
8	j	210	ALA	3.5
11	Y	9	LEU	3.5
8	x	199	LEU	3.4
2	P	248	ARG	3.4
6	F	5	THR	3.4
8	j	202	TYR	3.3
6	F	56	LYS	3.3
6	F	205	LYS	3.3
5	g	237	PRO	3.3
6	v	4	GLY	3.3
5	g	201	ASP	3.3
6	F	60	GLU	3.3
6	v	3	ILE	3.2
6	h	207	LYS	3.2
11	1	9	LEU	3.2
14	N	198	THR	3.2
14	4	201	THR	3.2
3	C	200	SER	3.2
8	V	199	LEU	3.2
6	h	5	THR	3.1
7	i	185	LYS	3.1
5	E	201	ASP	3.1
6	h	56	LYS	3.0
6	h	4	GLY	3.0
3	C	236	GLU	3.0
2	d	201	ASP	3.0
6	F	1	SER	3.0
3	C	199	GLN	3.0
9	y	102	TYR	3.0
5	u	199	GLU	2.9
3	e	205	ILE	2.9
3	C	203	LYS	2.9
6	h	240	LYS	2.9
4	D	123	GLY	2.9
4	f	123	GLY	2.8
11	K	40	TYR	2.8
5	E	238	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
8	j	199	LEU	2.7
3	C	213	ASP	2.7
1	O	1	ALA	2.7
1	A	2	LYS	2.7
6	v	5	THR	2.7
3	e	200	SER	2.7
6	T	4	GLY	2.7
3	e	199	GLN	2.7
1	q	3	ARG	2.6
3	e	213	ASP	2.6
12	n	162	GLU	2.6
7	G	187	ASP	2.6
3	e	236	GLU	2.6
1	c	2	LYS	2.6
5	g	224	ASP	2.6
1	c	3	ARG	2.6
5	g	238	GLN	2.6
6	F	208	ALA	2.6
2	B	201	ASP	2.6
6	h	208	ALA	2.5
6	F	207	LYS	2.5
6	F	209	PHE	2.5
5	E	202	LEU	2.5
5	u	46	LEU	2.5
5	u	233	LEU	2.5
7	i	187	ASP	2.5
9	I	114	LYS	2.5
14	p	202	LEU	2.5
6	h	198	TYR	2.4
11	m	40	TYR	2.4
6	h	243	LEU	2.4
5	S	199	GLU	2.4
9	y	56	ALA	2.4
3	e	238	ASN	2.4
14	b	202	LEU	2.4
2	P	229	GLN	2.4
9	y	114	LYS	2.4
8	j	214	GLU	2.4
3	C	194	LEU	2.4
5	E	200	GLN	2.4
6	F	7	TYR	2.4
6	F	240	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
3	e	194	LEU	2.3
3	C	238	ASN	2.3
4	R	175	GLU	2.3
5	S	233	LEU	2.3
5	E	236	ARG	2.3
6	F	198	TYR	2.3
3	C	205	ILE	2.3
3	C	237	GLU	2.3
9	y	57	THR	2.3
4	t	1	ASP	2.3
12	L	1	ARG	2.3
5	u	52	GLU	2.3
7	G	243	GLU	2.3
12	n	1	ARG	2.3
8	j	204	CYS	2.2
12	2	164	VAL	2.2
3	C	178	ASP	2.2
5	S	164	SER	2.2
3	e	178	ASP	2.2
5	g	200	GLN	2.2
6	h	204	VAL	2.2
3	e	46	LYS	2.2
5	S	46	LEU	2.2
4	t	175	GLU	2.2
6	F	54	LEU	2.2
10	J	95	ARG	2.2
12	Z	164	VAL	2.2
2	B	246	ALA	2.1
5	g	50	GLN	2.1
3	C	46	LYS	2.1
14	N	202	LEU	2.1
6	h	3	ILE	2.1
5	g	48	ARG	2.1
5	g	235	GLU	2.1
4	t	192	ILE	2.1
2	d	246	ALA	2.1
6	F	243	LEU	2.1
5	E	233	LEU	2.0
6	h	209	PHE	2.0
5	E	48	ARG	2.0
7	i	214	ILE	2.0
3	e	224	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
5	g	198	ALA	2.0
14	4	200	ALA	2.0
5	u	164	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
15	04C	Y	301	42/42	0.94	0.19	1.50	24,41,70,74	0
15	04C	1	301	42/42	0.94	0.19	1.44	24,39,71,77	0
15	04C	K	301	42/42	0.95	0.17	0.90	24,41,79,87	0
15	04C	m	301	42/42	0.94	0.17	0.82	27,42,84,90	0
15	04C	p	301	42/42	0.93	0.18	0.64	25,37,63,75	0
15	04C	4	301	42/42	0.92	0.17	0.62	30,39,54,64	0
15	04C	N	301	42/42	0.94	0.18	0.60	24,34,58,70	0
15	04C	b	301	42/42	0.94	0.17	0.45	28,36,55,65	0
15	04C	x	301	42/42	0.96	0.17	0.29	31,40,52,58	0
15	04C	V	301	42/42	0.95	0.16	-0.02	28,40,52,54	0
15	04C	H	301	42/42	0.94	0.14	-0.68	30,37,50,51	0
15	04C	j	301	42/42	0.95	0.15	-0.89	33,37,50,53	0

6.5 Other polymers (i)

There are no such residues in this entry.