



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:54 PM UTC

PDB ID : 3UNE / pdb_00003une
Title : Mouse constitutive 20S proteasome
Authors : Huber, E.; Basler, M.; Schwab, R.; Heinemeyer, W.; Kirk, C.; Groettrup, M.; Groll, M.
Deposited on : 2011-11-15
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

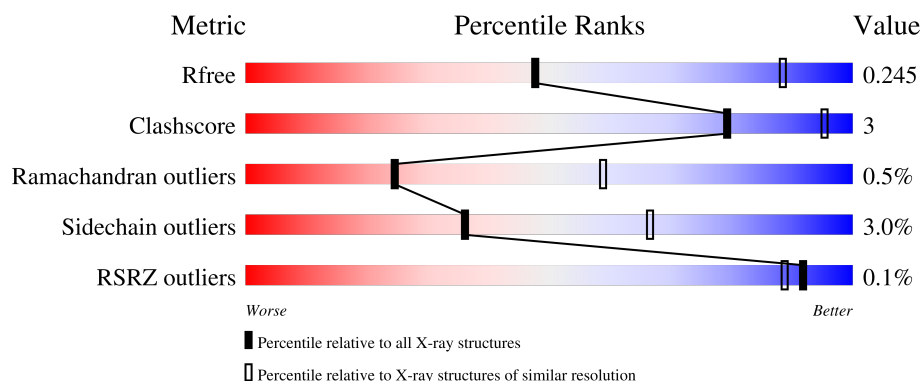
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



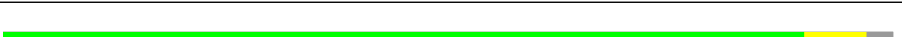
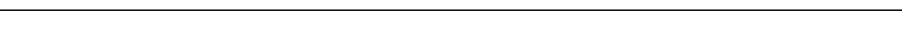
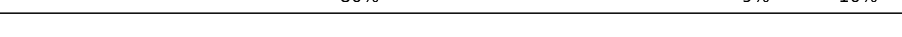
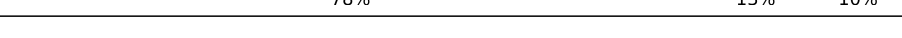
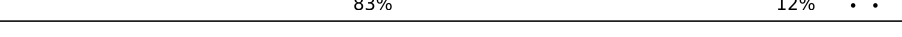
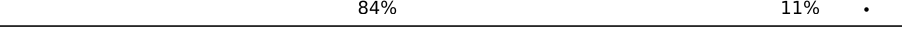
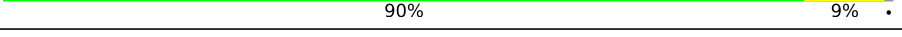
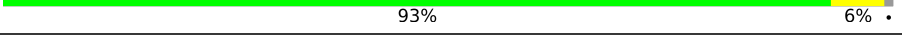
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	234	81%18%.
1	O	234	83%16%
1	c	234	85%13%.
1	q	234	84%15%
2	B	261	89%7%5%

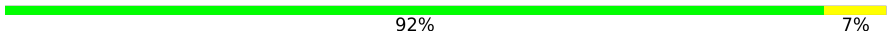
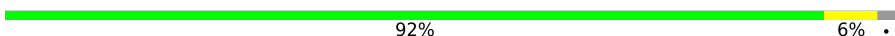
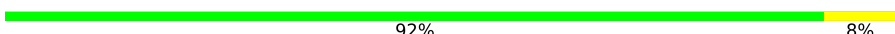
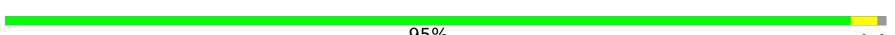
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Mol	Chain	Length	Quality of chain
2	P	261	 89% 7% 5%
2	d	261	 86% 8% 5%
2	r	261	 89% 7% 5%
3	C	248	 87% 10% .
3	Q	248	 85% 11% .
3	e	248	 83% 12% . .
3	s	248	 85% 10% . .
4	D	241	 86% 11% .
4	R	241	 86% 10% .
4	f	241	 88% 9% .
4	t	241	 90% 7% .
5	E	263	 82% 8% . 10%
5	S	263	 77% 13% . 10%
5	g	263	 80% 9% . 10%
5	u	263	 78% 13% 10%
6	F	255	 85% 11% .
6	T	255	 83% 12% . .
6	h	255	 87% 7% . .
6	v	255	 84% 11% .
7	G	246	 90% 9% .
7	U	246	 92% 7% .
7	i	246	 93% 6% .
7	w	246	 89% 10% .
8	H	234	 81% 13% 6%
8	V	234	 83% 10% . 6%

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Mol	Chain	Length	Quality of chain
8	j	234	 84%10%6%
8	x	234	 83%11%6%
9	I	205	 85%13%.
9	W	205	 92%7%
9	k	205	 90%10%
9	y	205	 86%12%.
10	J	201	 91%6%..
10	X	201	 92%6%.
10	l	201	 94%. .
10	z	201	 87%10%..
11	1	205	 91%7%.
11	K	205	 91%7%.
11	Y	205	 92%6%.
11	m	205	 90%8%.
12	2	213	 90%10%
12	L	213	 86%14%
12	Z	213	 92%8%
12	n	213	 88%12%
13	3	219	 90%7%..
13	M	219	 88%11%.
13	a	219	 89%9%.
13	o	219	 88%10%..
14	4	205	 93%5%.
14	N	205	 92%6%.
14	b	205	 95%..

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Mol	Chain	Length	Quality of chain
14	p	205	 94%5% •

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 97956 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	233	Total	C	N	O	S	0	0	0
			1817	1159	311	341	6			
1	O	233	Total	C	N	O	S	0	0	0
			1817	1159	311	341	6			
1	c	233	Total	C	N	O	S	0	0	0
			1817	1159	311	341	6			
1	q	233	Total	C	N	O	S	0	0	0
			1817	1159	311	341	6			

- 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			

- 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	244	Total	C	N	O	S	0	0	0
			1895	1202	316	364	13			
7	U	244	Total	C	N	O	S	0	0	0
			1895	1202	316	364	13			
7	i	244	Total	C	N	O	S	0	0	0
			1895	1202	316	364	13			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	w	244	Total	C	N	O	S	0	0	0
			1895	1202	316	364	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			
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			

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

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	12	Total	O	0	0
			12	12		
15	B	11	Total	O	0	0
			11	11		
15	C	7	Total	O	0	0
			7	7		
15	D	5	Total	O	0	0
			5	5		
15	E	8	Total	O	0	0
			8	8		
15	F	11	Total	O	0	0
			11	11		
15	G	11	Total	O	0	0
			11	11		
15	H	17	Total	O	0	0
			17	17		
15	I	12	Total	O	0	0
			12	12		
15	J	13	Total	O	0	0
			13	13		
15	K	11	Total	O	0	0
			11	11		
15	L	18	Total	O	0	0
			18	18		
15	M	15	Total	O	0	0
			15	15		
15	N	13	Total	O	0	0
			13	13		
15	O	18	Total	O	0	0
			18	18		
15	P	24	Total	O	0	0
			24	24		
15	Q	12	Total	O	0	0
			12	12		
15	R	12	Total	O	0	0
			12	12		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	S	19	Total O 19 19	0	0
15	T	13	Total O 13 13	0	0
15	U	21	Total O 21 21	0	0
15	V	19	Total O 19 19	0	0
15	W	21	Total O 21 21	0	0
15	X	8	Total O 8 8	0	0
15	Y	8	Total O 8 8	0	0
15	Z	16	Total O 16 16	0	0
15	a	16	Total O 16 16	0	0
15	b	20	Total O 20 20	0	0
15	c	15	Total O 15 15	0	0
15	d	9	Total O 9 9	0	0
15	e	3	Total O 3 3	0	0
15	f	3	Total O 3 3	0	0
15	g	7	Total O 7 7	0	0
15	h	7	Total O 7 7	0	0
15	i	10	Total O 10 10	0	0
15	j	13	Total O 13 13	0	0
15	k	11	Total O 11 11	0	0
15	l	8	Total O 8 8	0	0
15	m	11	Total O 11 11	0	0

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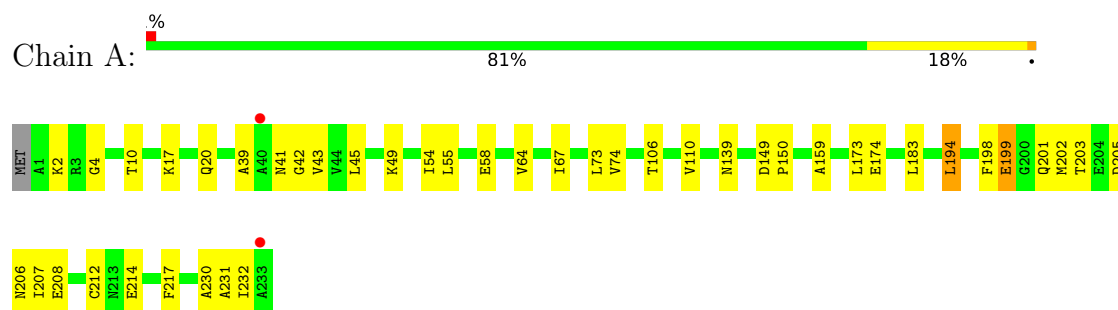
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	n	13	Total 13	O 13	0	0
15	o	11	Total 11	O 11	0	0
15	p	6	Total 6	O 6	0	0
15	q	3	Total 3	O 3	0	0
15	r	10	Total 10	O 10	0	0
15	s	7	Total 7	O 7	0	0
15	t	6	Total 6	O 6	0	0
15	u	7	Total 7	O 7	0	0
15	v	11	Total 11	O 11	0	0
15	w	10	Total 10	O 10	0	0
15	x	6	Total 6	O 6	0	0
15	y	10	Total 10	O 10	0	0
15	z	6	Total 6	O 6	0	0
15	1	12	Total 12	O 12	0	0
15	2	17	Total 17	O 17	0	0
15	3	10	Total 10	O 10	0	0
15	4	7	Total 7	O 7	0	0

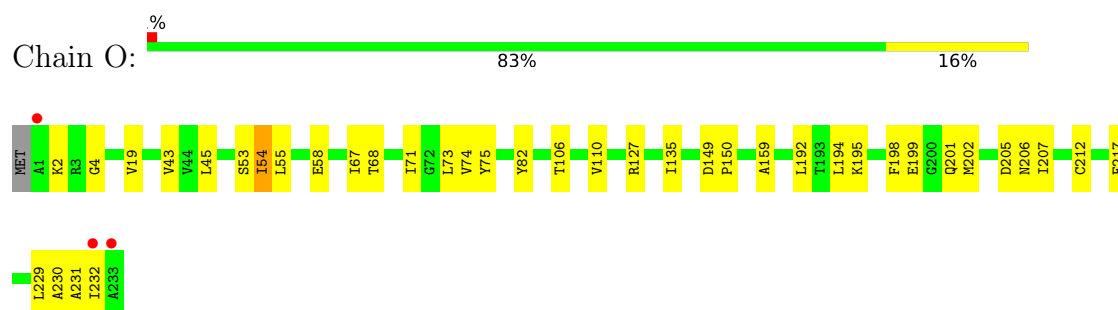
3 Residue-property plots [i](#)

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

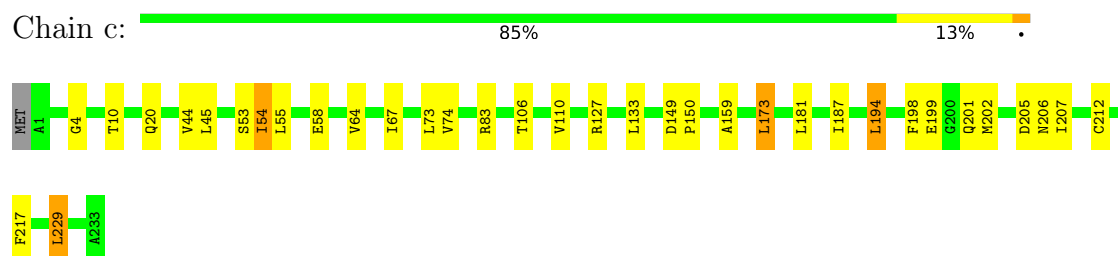
- Molecule 1: Proteasome subunit alpha type-2



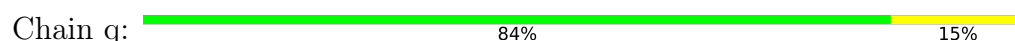
- Molecule 1: Proteasome subunit alpha type-2

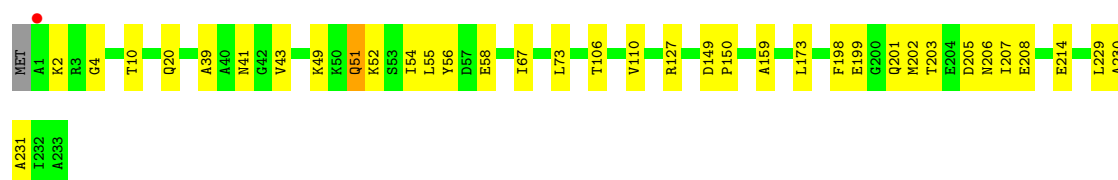


- Molecule 1: Proteasome subunit alpha type-2



- Molecule 1: Proteasome subunit alpha type-2





- Molecule 2: Proteasome subunit alpha type-4

Chain B: 89% 7% 5%



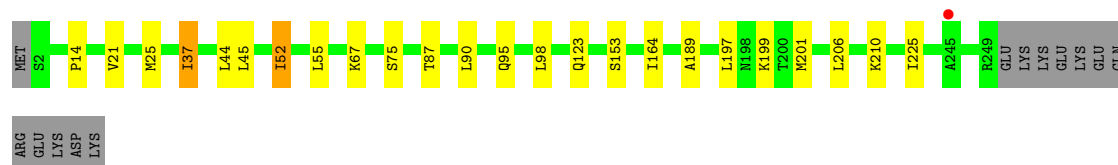
- Molecule 2: Proteasome subunit alpha type-4

Chain P: 89% 7% 5%



- Molecule 2: Proteasome subunit alpha type-4

Chain d: 86% 8% 5%



- Molecule 2: Proteasome subunit alpha type-4

Chain r: 89% 7% 5%



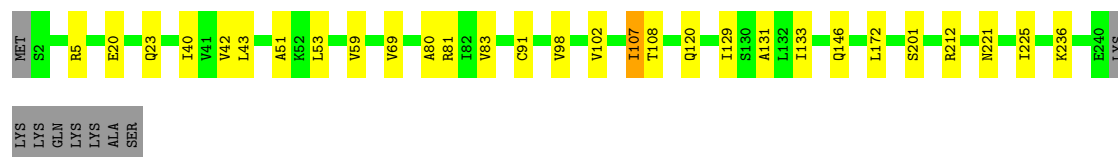
- Molecule 3: Proteasome subunit alpha type-7

Chain C: 87% 10% 3%



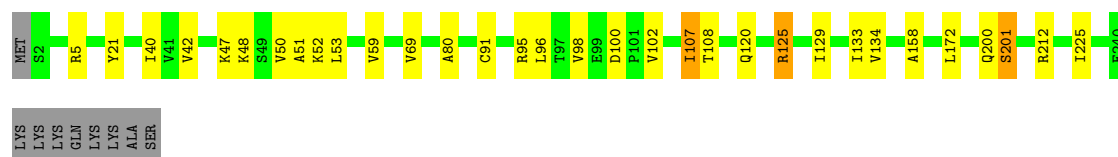
- Molecule 3: Proteasome subunit alpha type-7

Chain Q: 85% 11% 4%



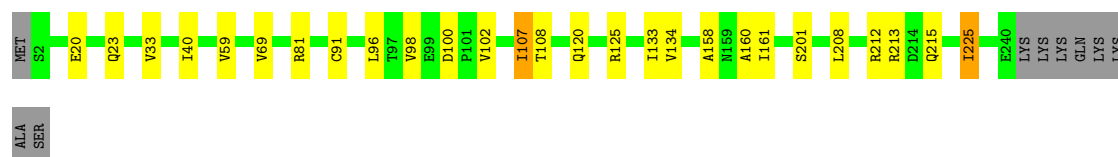
• Molecule 3: Proteasome subunit alpha type-7

Chain e: 83% 12% . .



• Molecule 3: Proteasome subunit alpha type-7

Chain s: 85% 10% . .



• Molecule 4: Proteasome subunit alpha type-5

Chain D: 86% 11% .



• Molecule 4: Proteasome subunit alpha type-5

Chain R: 86% 10% .



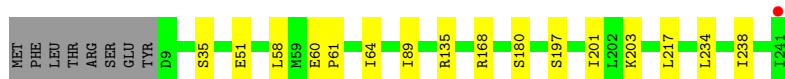
• Molecule 4: Proteasome subunit alpha type-5

Chain f: 88% 9% .



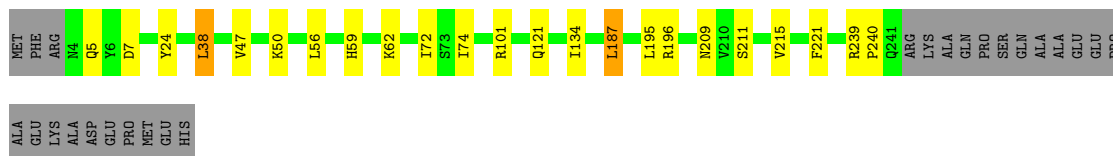
• Molecule 4: Proteasome subunit alpha type-5

Chain t: 90% 7% .



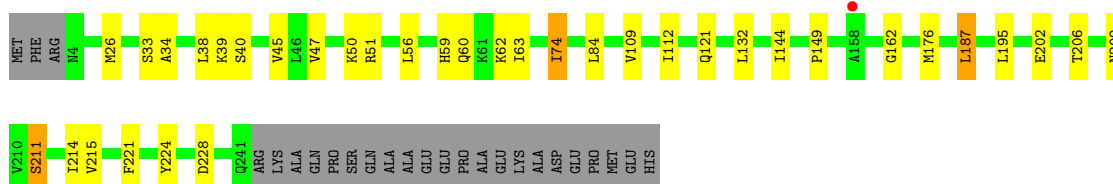
• Molecule 5: Proteasome subunit alpha type-1

Chain E: 82% 8% 10%



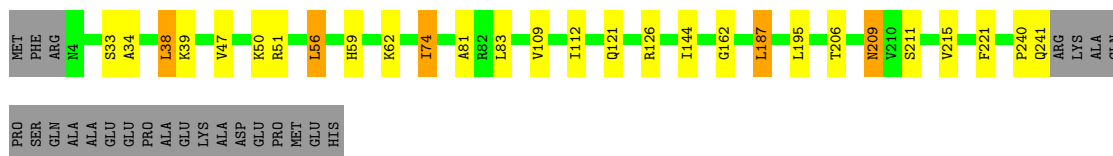
• Molecule 5: Proteasome subunit alpha type-1

Chain S: 77% 13% 10%



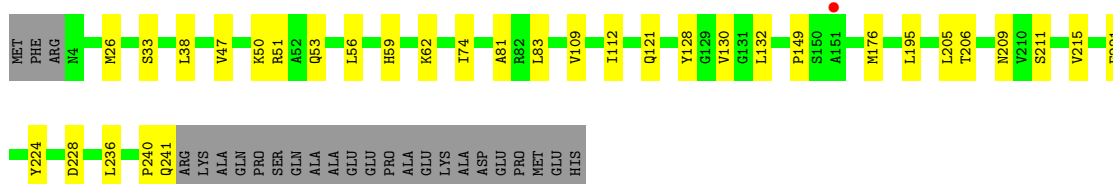
• Molecule 5: Proteasome subunit alpha type-1

Chain g: 80% 9% 10%



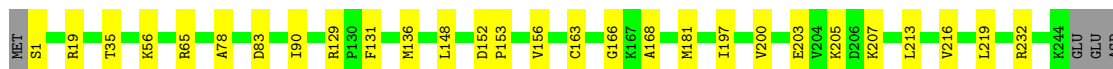
• Molecule 5: Proteasome subunit alpha type-1

Chain u: 78% 13% 10%



• Molecule 6: Proteasome subunit alpha type-3

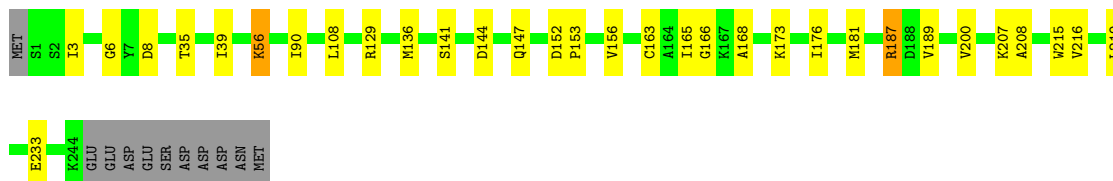
Chain F: 85% 11% 4%



GLU
SER
ASP
ASP
ASP
ASN
MET

• Molecule 6: Proteasome subunit alpha type-3

Chain T:  83% 12% . .



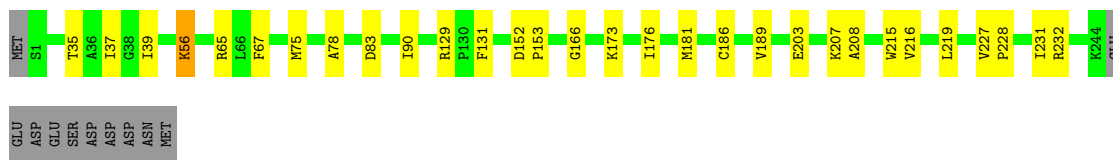
• Molecule 6: Proteasome subunit alpha type-3

Chain h:  87% 7% . .



• Molecule 6: Proteasome subunit alpha type-3

Chain v:  84% 11% .

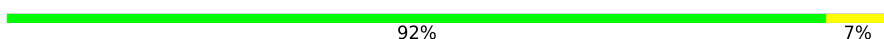


• Molecule 7: Proteasome subunit alpha type-6

Chain G:  90% 9% .

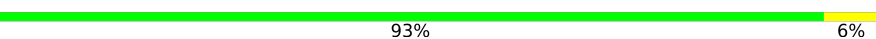


• Molecule 7: Proteasome subunit alpha type-6

Chain U:  92% 7% .



• Molecule 7: Proteasome subunit alpha type-6

Chain i:  93% 6% .



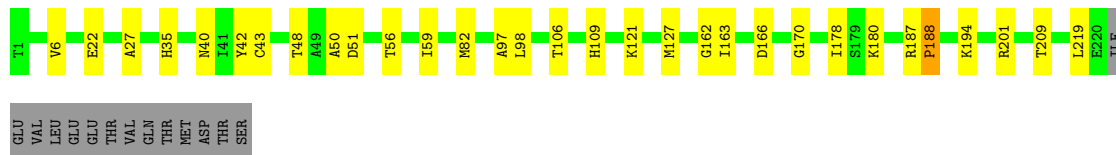
- Molecule 7: Proteasome subunit alpha type-6

Chain w:  89% 10%



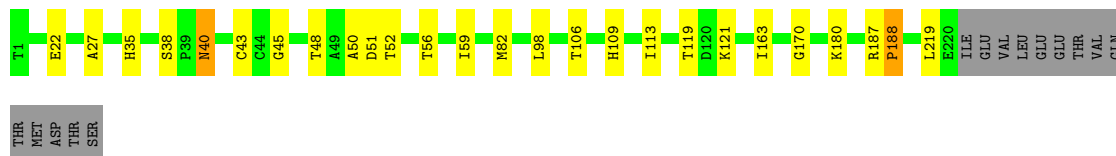
- Molecule 8: Proteasome subunit beta type-7

Chain H:  81% 13% 6%



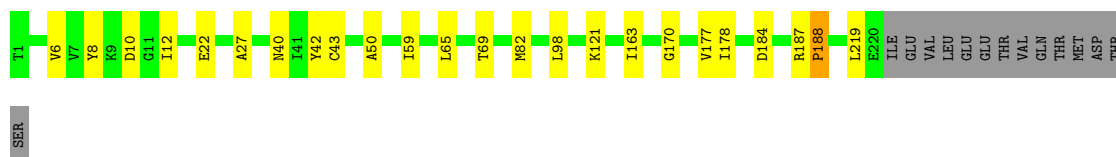
- Molecule 8: Proteasome subunit beta type-7

Chain V:  83% 10% 6%



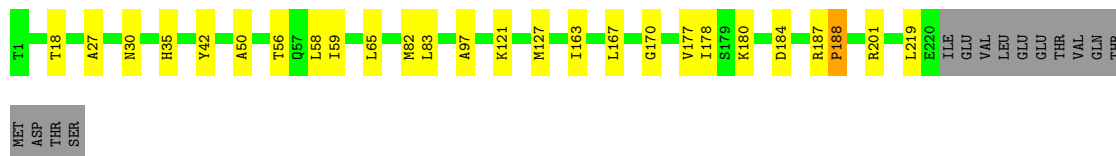
- Molecule 8: Proteasome subunit beta type-7

Chain j:  84% 10% 6%



- Molecule 8: Proteasome subunit beta type-7

Chain x:  83% 11% 6%



- Molecule 9: Proteasome subunit beta type-3

Chain I:  85% 13%



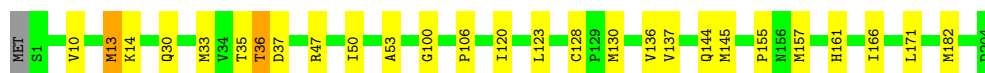
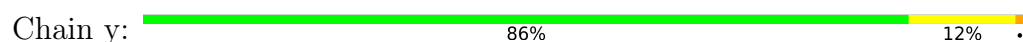
- Molecule 9: Proteasome subunit beta type-3



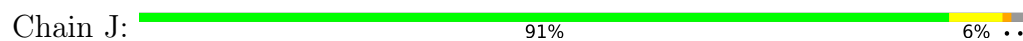
- Molecule 9: Proteasome subunit beta type-3



- Molecule 9: Proteasome subunit beta type-3



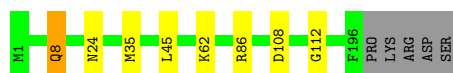
- Molecule 10: Proteasome subunit beta type-2



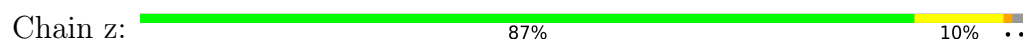
- Molecule 10: Proteasome subunit beta type-2

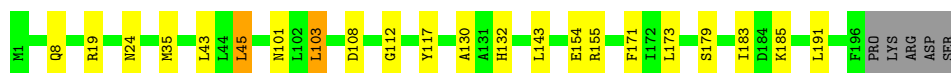


- Molecule 10: Proteasome subunit beta type-2



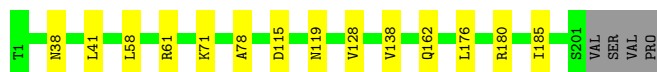
- Molecule 10: Proteasome subunit beta type-2





- Molecule 11: Proteasome subunit beta type-5

Chain K: 91% 7%



- Molecule 11: Proteasome subunit beta type-5

Chain Y: 92% 6%



- Molecule 11: Proteasome subunit beta type-5

Chain m: 90% 8%



- Molecule 11: Proteasome subunit beta type-5

Chain 1: 91% 7%



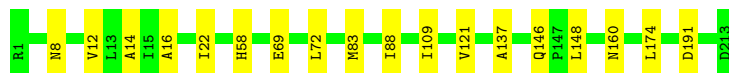
- Molecule 12: Proteasome subunit beta type-1

Chain L: 86% 14%



- Molecule 12: Proteasome subunit beta type-1

Chain Z: 92% 8%

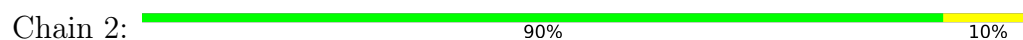


- Molecule 12: Proteasome subunit beta type-1

Chain n: 88% 12%



- Molecule 12: Proteasome subunit beta type-1



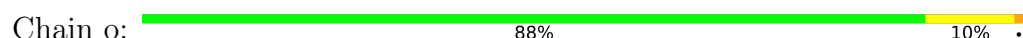
- Molecule 13: Proteasome subunit beta type-4



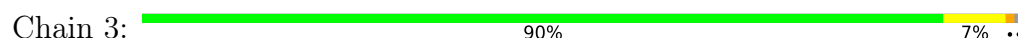
- Molecule 13: Proteasome subunit beta type-4



- Molecule 13: Proteasome subunit beta type-4



- Molecule 13: Proteasome subunit beta type-4



- Molecule 14: Proteasome subunit beta type-6



- Molecule 14: Proteasome subunit beta type-6





- Molecule 14: Proteasome subunit beta type-6



- Molecule 14: Proteasome subunit beta type-6



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	170.97Å 201.30Å 226.01Å 90.00° 108.07° 90.00°	Depositor
Resolution (Å)	15.00 – 3.20 15.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.1 (15.00-3.20) 97.3 (15.00-3.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.6.0119	Depositor
R, R_{free}	0.220 , 0.246 0.221 , 0.245	Depositor DCC
R_{free} test set	11753 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	84.9	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 69.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	97956	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.52	0/1856	0.76	0/2512
1	O	0.52	0/1856	0.76	0/2512
1	c	0.52	0/1856	0.76	0/2512
1	q	0.52	0/1856	0.75	0/2512
2	B	0.49	0/1980	0.73	0/2667
2	P	0.49	0/1980	0.72	0/2667
2	d	0.49	0/1980	0.72	0/2667
2	r	0.49	0/1980	0.72	0/2667
3	C	0.46	0/1908	0.73	0/2576
3	Q	0.46	0/1908	0.75	0/2576
3	e	0.47	0/1908	0.74	0/2576
3	s	0.47	0/1908	0.73	0/2576
4	D	0.51	0/1805	0.73	0/2437
4	R	0.52	0/1805	0.74	0/2437
4	f	0.52	0/1805	0.73	0/2437
4	t	0.52	0/1805	0.72	0/2437
5	E	0.57	0/1907	0.74	0/2578
5	S	0.57	0/1907	0.74	0/2578
5	g	0.57	0/1907	0.71	0/2578
5	u	0.57	0/1907	0.74	0/2578
6	F	0.51	0/1938	0.71	0/2608
6	T	0.51	0/1938	0.72	0/2608
6	h	0.52	0/1938	0.71	0/2608
6	v	0.51	0/1938	0.72	0/2608
7	G	0.49	0/1929	0.73	0/2607
7	U	0.48	0/1929	0.73	0/2607
7	i	0.48	0/1929	0.73	0/2607
7	w	0.48	0/1929	0.74	0/2607
8	H	0.49	0/1683	0.72	0/2276
8	V	0.49	0/1683	0.74	0/2276
8	j	0.49	0/1683	0.73	0/2276
8	x	0.49	0/1683	0.72	0/2276
9	I	0.46	0/1621	0.73	0/2185
9	W	0.45	0/1621	0.73	0/2185

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	k	0.46	0/1621	0.72	0/2185
9	y	0.46	0/1621	0.71	0/2185
10	J	0.51	0/1602	0.69	0/2167
10	X	0.51	0/1602	0.69	0/2167
10	l	0.51	0/1602	0.70	0/2167
10	z	0.51	0/1602	0.70	0/2167
11	l	0.50	0/1588	0.68	0/2145
11	K	0.50	0/1588	0.69	0/2145
11	Y	0.50	0/1588	0.68	0/2145
11	m	0.50	0/1588	0.69	0/2145
12	2	0.48	0/1685	0.69	0/2271
12	L	0.48	0/1685	0.69	0/2271
12	Z	0.48	0/1685	0.70	0/2271
12	n	0.48	0/1685	0.69	0/2271
13	3	0.50	0/1718	0.69	0/2325
13	M	0.50	0/1718	0.71	0/2325
13	a	0.50	0/1718	0.70	0/2325
13	o	0.50	0/1718	0.70	0/2325
14	4	0.51	0/1546	0.73	1/2094 (0.0%)
14	N	0.51	0/1546	0.71	0/2094
14	b	0.51	0/1546	0.70	0/2094
14	p	0.52	0/1546	0.72	0/2094
All	All	0.50	0/99064	0.72	1/133792 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	4	190	LEU	N-CA-C	5.50	113.29	108.78

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1817	0	1812	21	0
1	O	1817	0	1812	18	0
1	c	1817	0	1812	18	0
1	q	1817	0	1812	15	0
2	B	1950	0	1970	7	0
2	P	1950	0	1970	5	0
2	d	1950	0	1970	11	0
2	r	1950	0	1970	4	0
3	C	1881	0	1901	10	0
3	Q	1881	0	1901	12	0
3	e	1881	0	1901	14	0
3	s	1881	0	1901	14	0
4	D	1778	0	1764	12	0
4	R	1778	0	1764	14	0
4	f	1778	0	1764	12	0
4	t	1778	0	1764	8	0
5	E	1872	0	1856	11	0
5	S	1872	0	1856	18	0
5	g	1872	0	1856	15	0
5	u	1872	0	1856	16	0
6	F	1903	0	1894	11	0
6	T	1903	0	1894	14	0
6	h	1903	0	1894	8	0
6	v	1903	0	1894	15	0
7	G	1895	0	1899	12	0
7	U	1895	0	1899	9	0
7	i	1895	0	1899	7	0
7	w	1895	0	1899	13	0
8	H	1656	0	1685	17	0
8	V	1656	0	1685	13	0
8	j	1656	0	1685	12	0
8	x	1656	0	1685	12	0
9	I	1592	0	1612	15	0
9	W	1592	0	1612	6	0
9	k	1592	0	1612	10	0
9	y	1592	0	1612	12	0
10	J	1570	0	1573	7	0
10	X	1570	0	1573	5	0
10	l	1570	0	1573	5	0
10	z	1570	0	1573	8	0
11	1	1557	0	1526	5	0
11	K	1557	0	1526	6	0
11	Y	1557	0	1526	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	m	1557	0	1526	7	0
12	2	1654	0	1652	9	0
12	L	1654	0	1652	11	0
12	Z	1654	0	1652	8	0
12	n	1654	0	1652	12	0
13	3	1685	0	1664	11	0
13	M	1685	0	1664	11	0
13	a	1685	0	1664	12	0
13	o	1685	0	1664	11	0
14	4	1519	0	1488	8	0
14	N	1519	0	1488	8	0
14	b	1519	0	1488	6	0
14	p	1519	0	1488	5	0
15	1	12	0	0	0	0
15	2	17	0	0	0	0
15	3	10	0	0	0	0
15	4	7	0	0	0	0
15	A	12	0	0	0	0
15	B	11	0	0	0	0
15	C	7	0	0	0	0
15	D	5	0	0	0	0
15	E	8	0	0	0	0
15	F	11	0	0	0	0
15	G	11	0	0	0	0
15	H	17	0	0	0	0
15	I	12	0	0	0	0
15	J	13	0	0	0	0
15	K	11	0	0	0	0
15	L	18	0	0	0	0
15	M	15	0	0	0	0
15	N	13	0	0	0	0
15	O	18	0	0	0	0
15	P	24	0	0	0	0
15	Q	12	0	0	0	0
15	R	12	0	0	0	0
15	S	19	0	0	0	0
15	T	13	0	0	0	0
15	U	21	0	0	0	0
15	V	19	0	0	0	0
15	W	21	0	0	0	0
15	X	8	0	0	0	0
15	Y	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	Z	16	0	0	0	0
15	a	16	0	0	0	0
15	b	20	0	0	0	0
15	c	15	0	0	0	0
15	d	9	0	0	0	0
15	e	3	0	0	0	0
15	f	3	0	0	0	0
15	g	7	0	0	0	0
15	h	7	0	0	0	0
15	i	10	0	0	0	0
15	j	13	0	0	0	0
15	k	11	0	0	0	0
15	l	8	0	0	0	0
15	m	11	0	0	0	0
15	n	13	0	0	0	0
15	o	11	0	0	0	0
15	p	6	0	0	0	0
15	q	3	0	0	0	0
15	r	10	0	0	0	0
15	s	7	0	0	0	0
15	t	6	0	0	0	0
15	u	7	0	0	0	0
15	v	11	0	0	0	0
15	w	10	0	0	0	0
15	x	6	0	0	0	0
15	y	10	0	0	0	0
15	z	6	0	0	0	0
All	All	97956	0	97184	525	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 3.

All (525) 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)
1:q:4:GLY:HA2	7:w:130:GLU:HG2	1.63	0.81
8:x:187:ARG:HB3	8:x:188:PRO:HD3	1.64	0.80
1:A:4:GLY:HA2	7:G:130:GLU:HG2	1.64	0.78
8:j:187:ARG:HB3	8:j:188:PRO:HD3	1.65	0.77
8:H:187:ARG:HB3	8:H:188:PRO:HD3	1.67	0.77
8:V:187:ARG:HB3	8:V:188:PRO:HD3	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:x:35:HIS:HB3	8:x:56:THR:HG21	1.69	0.73
1:q:67:ILE:HD11	1:q:73:LEU:HD12	1.72	0.71
5:g:121:GLN:HG3	6:h:129:ARG:HG2	1.74	0.70
13:3:46:ASN:HD22	13:3:48:SER:H	1.39	0.70
5:E:50:LYS:HE3	5:E:211:SER:HB2	1.76	0.68
1:c:4:GLY:HA2	7:i:130:GLU:HG2	1.76	0.67
10:z:35:MET:HG2	10:z:45:LEU:HD22	1.75	0.67
10:J:35:MET:HG2	10:J:45:LEU:HD22	1.77	0.66
12:2:8:ASN:HD22	12:2:58:HIS:H	1.43	0.66
1:c:58:GLU:HG2	1:c:205:ASP:HB3	1.78	0.65
5:g:50:LYS:HE3	5:g:211:SER:HB2	1.77	0.65
1:O:4:GLY:HA2	7:U:130:GLU:HG2	1.79	0.65
5:u:50:LYS:HE3	5:u:211:SER:HB2	1.79	0.65
12:L:8:ASN:HD22	12:L:58:HIS:H	1.45	0.64
13:o:46:ASN:HD22	13:o:48:SER:H	1.46	0.63
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.82	0.62
1:A:174:GLU:HB3	2:B:55:LEU:HD11	1.82	0.62
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.81	0.62
5:u:50:LYS:HB3	5:u:59:HIS:HB3	1.82	0.61
8:x:59:ILE:HD12	8:x:82:MET:HB3	1.82	0.61
1:O:198:PHE:HZ	1:O:206:ASN:HB3	1.64	0.61
13:3:27:LEU:HD11	13:3:34:ALA:HB1	1.83	0.61
9:y:33:MET:HE3	9:y:36:THR:HG23	1.82	0.61
1:c:159:ALA:HB1	1:c:173:LEU:HD23	1.82	0.60
1:q:159:ALA:HB1	1:q:173:LEU:HD23	1.84	0.60
13:M:122:LEU:HG	13:M:137:LEU:HD12	1.83	0.60
12:L:13:LEU:HD11	12:L:149:LEU:HD11	1.83	0.60
13:a:27:LEU:HD11	13:a:34:ALA:HB1	1.84	0.60
2:P:45:LEU:HD13	2:P:75:SER:HB2	1.84	0.59
5:u:206:THR:H	5:u:209:ASN:HD21	1.50	0.59
13:M:46:ASN:HD22	13:M:48:SER:H	1.47	0.59
13:o:122:LEU:HG	13:o:137:LEU:HD12	1.82	0.59
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.83	0.59
3:s:212:ARG:HB2	3:s:215:GLN:HB2	1.83	0.59
14:p:1:THR:HG23	14:p:33:LYS:HE2	1.85	0.59
8:H:59:ILE:HD12	8:H:82:MET:HB3	1.85	0.58
13:a:122:LEU:HG	13:a:137:LEU:HD12	1.85	0.58
8:V:59:ILE:HD12	8:V:82:MET:HB3	1.84	0.58
8:j:59:ILE:HD12	8:j:82:MET:HB3	1.86	0.58
7:i:141:ILE:HG22	7:i:151:VAL:HG22	1.86	0.58
13:o:192:VAL:HG12	13:o:197:VAL:HG22	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:3:122:LEU:HG	13:3:137:LEU:HD12	1.85	0.58
2:r:45:LEU:HD13	2:r:75:SER:HB2	1.85	0.58
5:S:50:LYS:HB3	5:S:59:HIS:HB3	1.86	0.57
12:n:8:ASN:HD22	12:n:58:HIS:H	1.51	0.57
8:j:163:ILE:HG23	8:j:170:GLY:HA2	1.86	0.57
13:3:192:VAL:HG12	13:3:197:VAL:HG22	1.87	0.57
14:N:30:VAL:HG12	14:N:30:VAL:O	2.03	0.57
5:E:7:ASP:HB2	5:E:24:TYR:HE1	1.70	0.57
2:B:8:ARG:HB3	2:B:11:ILE:HD12	1.86	0.56
2:B:45:LEU:HD13	2:B:75:SER:HB2	1.86	0.56
5:u:81:ALA:HB2	5:u:130:VAL:HG21	1.87	0.56
2:B:123:GLN:HG3	3:C:125:ARG:HG2	1.87	0.56
9:I:44:MET:HE3	9:I:70:LEU:HD22	1.87	0.56
2:d:45:LEU:HD13	2:d:75:SER:HB2	1.86	0.56
8:x:163:ILE:HG23	8:x:170:GLY:HA2	1.87	0.56
13:o:212:ALA:HA	14:4:30:VAL:HG21	1.88	0.56
9:y:106:PRO:HG2	9:y:123:LEU:HB2	1.87	0.56
12:Z:8:ASN:HD22	12:Z:58:HIS:H	1.52	0.56
13:M:96:MET:HE3	13:M:127:MET:HA	1.88	0.56
13:a:46:ASN:HD22	13:a:48:SER:H	1.53	0.55
4:R:234:LEU:O	4:R:238:ILE:HG12	2.06	0.55
4:f:234:LEU:O	4:f:238:ILE:HG12	2.06	0.55
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.88	0.55
9:k:157:MET:HE2	9:k:161:HIS:HB3	1.87	0.55
13:o:96:MET:HE3	13:o:127:MET:HA	1.89	0.55
6:v:65:ARG:HH21	6:v:78:ALA:HA	1.72	0.55
8:x:97:ALA:HB1	8:x:127:MET:HE3	1.89	0.55
5:E:38:LEU:HD13	5:E:187:LEU:HD22	1.88	0.55
11:m:87:VAL:HG21	11:m:97:MET:HE2	1.88	0.54
1:O:55:LEU:HD22	7:U:165:ALA:HB3	1.90	0.54
8:V:50:ALA:HB2	9:W:128:CYS:HB2	1.90	0.54
4:D:234:LEU:O	4:D:238:ILE:HG12	2.07	0.54
13:M:15:LYS:HE2	13:M:135:PRO:HA	1.88	0.54
13:a:192:VAL:HG12	13:a:197:VAL:HG22	1.89	0.54
5:E:215:VAL:HB	5:E:221:PHE:HD1	1.72	0.54
12:L:12:VAL:HG13	12:L:109:ILE:HD12	1.90	0.54
13:M:212:ALA:HA	14:b:30:VAL:HG21	1.90	0.54
13:a:27:LEU:HD22	13:a:184:TYR:HB2	1.90	0.54
8:H:97:ALA:HB1	8:H:127:MET:HE3	1.90	0.53
1:q:202:MET:HB3	1:q:229:LEU:HD11	1.90	0.53
5:g:215:VAL:HB	5:g:221:PHE:HD1	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:30:VAL:O	14:N:30:VAL:CG1	2.56	0.53
10:z:108:ASP:HB3	10:z:112:GLY:H	1.74	0.53
9:W:157:MET:HE2	9:W:161:HIS:HB3	1.91	0.53
4:t:168:ARG:HH22	5:u:53:GLN:HB3	1.74	0.53
3:e:51:ALA:C	3:e:53:LEU:H	2.16	0.53
3:s:208:LEU:HG	3:s:225:ILE:HD11	1.90	0.53
10:X:85:ARG:HH12	10:X:86:ARG:HH21	1.55	0.53
9:y:36:THR:HG22	9:y:182:MET:HB3	1.92	0.52
8:V:43:CYS:SG	8:V:98:LEU:HB3	2.49	0.52
4:t:180:SER:HB3	4:t:201:ILE:HD12	1.90	0.52
6:v:35:THR:HA	6:v:166:GLY:HA3	1.91	0.52
3:C:51:ALA:C	3:C:53:LEU:H	2.18	0.52
13:a:43:MET:HE3	13:a:45:VAL:HG22	1.91	0.52
5:u:224:TYR:HD2	5:u:228:ASP:HB3	1.75	0.52
6:T:168:ALA:HB3	6:T:200:VAL:HG13	1.91	0.52
1:q:58:GLU:HG2	1:q:205:ASP:HB3	1.92	0.52
7:w:141:ILE:HG22	7:w:151:VAL:HG22	1.92	0.52
1:c:159:ALA:HB3	2:d:55:LEU:HD22	1.92	0.52
9:I:87:MET:HE3	9:I:129:PRO:HB2	1.92	0.51
2:d:37:ILE:HD11	2:d:189:ALA:HB1	1.91	0.51
1:A:58:GLU:HG2	1:A:205:ASP:HB3	1.91	0.51
1:q:39:ALA:C	1:q:41:ASN:H	2.18	0.51
9:I:157:MET:HE2	9:I:161:HIS:HB3	1.92	0.51
13:3:27:LEU:HD22	13:3:184:TYR:HB2	1.93	0.51
4:t:234:LEU:O	4:t:238:ILE:HG12	2.10	0.51
11:1:115:ASP:HB2	11:1:119:ASN:HB2	1.93	0.51
3:Q:40:ILE:HG22	3:Q:212:ARG:HA	1.92	0.51
6:h:3:ILE:HD13	6:h:3:ILE:H	1.75	0.51
3:s:98:VAL:HG12	3:s:100:ASP:H	1.76	0.51
8:H:50:ALA:HB2	9:I:128:CYS:HB2	1.93	0.51
7:U:143:ILE:HG12	7:U:220:VAL:HG12	1.93	0.51
7:G:141:ILE:HG22	7:G:151:VAL:HG22	1.93	0.51
5:g:206:THR:H	5:g:209:ASN:HD21	1.59	0.51
9:y:157:MET:HE2	9:y:161:HIS:HB3	1.93	0.51
4:D:202:LEU:HG	4:D:206:MET:HE3	1.92	0.50
5:S:121:GLN:HG3	6:T:129:ARG:HG3	1.93	0.50
6:T:35:THR:HA	6:T:166:GLY:HA3	1.93	0.50
7:U:141:ILE:HG22	7:U:151:VAL:HG22	1.93	0.50
3:C:108:THR:HG23	3:C:133:ILE:HD13	1.93	0.50
11:K:38:ASN:HD22	11:K:41:LEU:HD12	1.76	0.50
6:F:1:SER:HB2	6:F:19:ARG:HH22	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:e:108:THR:HG23	3:e:133:ILE:HD13	1.92	0.50
1:A:55:LEU:HD22	7:G:165:ALA:HB3	1.93	0.50
13:a:96:MET:HE3	13:a:127:MET:HA	1.94	0.49
6:h:35:THR:HA	6:h:166:GLY:HA3	1.94	0.49
13:3:96:MET:HE3	13:3:127:MET:HA	1.94	0.49
9:I:46:ASP:O	9:I:47:ARG:CB	2.59	0.49
8:V:106:THR:HB	8:V:109:HIS:HE2	1.76	0.49
11:K:115:ASP:HB2	11:K:119:ASN:HB2	1.94	0.49
11:m:38:ASN:HD22	11:m:41:LEU:HD12	1.78	0.49
13:o:27:LEU:HD11	13:o:34:ALA:HB1	1.94	0.49
3:C:158:ALA:HB3	4:D:58:LEU:HD22	1.94	0.49
3:s:108:THR:HG23	3:s:133:ILE:HD13	1.94	0.49
2:B:123:GLN:HA	3:C:125:ARG:HD3	1.95	0.49
8:H:35:HIS:CB	8:H:56:THR:HG21	2.43	0.49
5:u:121:GLN:HG3	6:v:129:ARG:HG3	1.94	0.49
5:E:50:LYS:HB3	5:E:59:HIS:HB3	1.94	0.49
13:a:15:LYS:HE2	13:a:135:PRO:HA	1.94	0.49
1:c:55:LEU:HD22	7:i:165:ALA:HB3	1.95	0.49
2:r:123:GLN:HA	3:s:125:ARG:HD3	1.95	0.49
1:q:51:GLN:HG3	1:q:56:TYR:HB2	1.94	0.49
3:s:91:CYS:HA	3:s:102:VAL:HG21	1.94	0.49
1:A:198:PHE:O	1:A:199:GLU:HG2	2.13	0.49
1:c:149:ASP:HB2	1:c:150:PRO:HD2	1.95	0.49
8:x:27:ALA:HB1	9:y:130:MET:HE1	1.96	0.48
11:m:115:ASP:HB2	11:m:119:ASN:HB2	1.95	0.48
13:o:15:LYS:HE2	13:o:135:PRO:HA	1.93	0.48
1:A:42:GLY:HA3	1:A:183:LEU:HD13	1.96	0.48
6:h:168:ALA:HB3	6:h:200:VAL:HG13	1.93	0.48
4:D:182:GLN:HG2	5:E:56:LEU:HD23	1.95	0.48
6:T:39:ILE:HD11	6:T:189:VAL:HG13	1.96	0.48
3:s:158:ALA:HB3	4:t:58:LEU:HD22	1.95	0.48
4:D:44:GLU:HG3	4:D:191:LEU:HB2	1.95	0.48
6:F:65:ARG:HH21	6:F:78:ALA:HA	1.79	0.48
5:g:50:LYS:HB3	5:g:59:HIS:HB3	1.95	0.48
9:y:13:MET:HB2	9:y:166:ILE:HD12	1.95	0.48
1:A:106:THR:H	1:A:139:ASN:HD21	1.60	0.48
5:S:109:VAL:HA	5:S:112:ILE:HD12	1.96	0.48
1:A:198:PHE:HZ	1:A:206:ASN:HB3	1.79	0.48
1:O:198:PHE:O	1:O:199:GLU:HG2	2.14	0.48
4:D:51:GLU:HB3	4:D:206:MET:HE2	1.96	0.47
5:E:196:ARG:HD3	5:E:239:ARG:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:14:LEU:HD21	14:N:101:ALA:HB3	1.95	0.47
3:e:40:ILE:HG22	3:e:212:ARG:HA	1.96	0.47
6:F:168:ALA:HB3	6:F:200:VAL:HG13	1.96	0.47
7:G:52:THR:OG1	7:G:79:VAL:HG21	2.14	0.47
13:M:27:LEU:HD11	13:M:34:ALA:HB1	1.95	0.47
14:N:164:MET:HB3	14:N:171:GLY:HA2	1.96	0.47
2:B:21:VAL:HG11	2:B:153:SER:HB3	1.96	0.47
1:c:106:THR:O	1:c:110:VAL:HG23	2.14	0.47
1:c:198:PHE:HZ	1:c:206:ASN:HB3	1.79	0.47
2:d:52:ILE:HG21	2:d:210:LYS:HG2	1.97	0.47
13:o:32:SER:HA	13:o:182:ARG:HE	1.79	0.47
5:u:83:LEU:HD23	5:u:128:TYR:HE2	1.80	0.47
13:M:211:ILE:HG22	13:M:214:MET:HE3	1.97	0.47
12:n:146:GLN:HA	12:n:149:LEU:HD12	1.97	0.47
13:o:27:LEU:HD22	13:o:184:TYR:HB2	1.96	0.47
1:q:203:THR:H	1:q:206:ASN:HB2	1.78	0.47
14:4:30:VAL:HG22	14:4:175:ARG:HH21	1.79	0.47
3:Q:83:VAL:HG21	3:Q:129:ILE:HD11	1.97	0.47
12:Z:12:VAL:HG13	12:Z:109:ILE:HD12	1.95	0.47
3:s:20:GLU:HA	3:s:23:GLN:HE21	1.78	0.47
11:m:14:VAL:HB	11:m:177:TYR:HB2	1.96	0.47
6:F:35:THR:HA	6:F:166:GLY:HA3	1.96	0.47
7:G:165:ALA:HB1	7:G:179:LEU:HG	1.97	0.47
4:R:180:SER:HB3	4:R:201:ILE:HD12	1.95	0.47
3:e:158:ALA:HB3	4:f:58:LEU:HD22	1.96	0.47
6:h:213:LEU:HD12	6:h:232:ARG:HG3	1.96	0.47
4:t:197:SER:O	4:t:201:ILE:HG12	2.14	0.47
5:u:109:VAL:HA	5:u:112:ILE:HD12	1.97	0.47
1:A:67:ILE:HD11	1:A:73:LEU:HD12	1.97	0.47
12:L:161:VAL:HG12	12:L:163:HIS:H	1.80	0.47
3:Q:69:VAL:HG11	3:Q:107:ILE:HG21	1.95	0.47
3:Q:108:THR:HG23	3:Q:133:ILE:HD13	1.97	0.47
4:f:97:GLN:HB3	11:m:61:ARG:HG3	1.96	0.47
13:3:20:VAL:HG11	13:3:122:LEU:HD13	1.96	0.47
1:A:45:LEU:HB3	1:A:74:VAL:HG21	1.96	0.47
7:G:137:CYS:SG	7:G:153:LYS:HE2	2.55	0.47
3:Q:91:CYS:HA	3:Q:102:VAL:HG21	1.97	0.47
5:S:40:SER:HB3	5:S:187:LEU:HG	1.97	0.47
1:q:198:PHE:HZ	1:q:206:ASN:HB3	1.80	0.47
10:z:101:ASN:HB3	10:z:132:HIS:CE1	2.49	0.47
3:Q:120:GLN:HG3	4:R:135:ARG:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:3:46:ASN:HD21	13:3:49:THR:HG22	1.79	0.46
1:A:149:ASP:HB2	1:A:150:PRO:HD2	1.98	0.46
11:Y:115:ASP:HB2	11:Y:119:ASN:HB2	1.97	0.46
14:b:30:VAL:HG22	14:b:175:ARG:HH21	1.79	0.46
10:J:4:LEU:HB2	10:J:132:HIS:HB2	1.97	0.46
1:c:53:SER:C	1:c:55:LEU:H	2.24	0.46
8:j:42:TYR:HB2	8:j:178:ILE:HD11	1.98	0.46
8:H:22:GLU:HG2	8:H:27:ALA:HB2	1.97	0.46
14:N:194:ILE:HG13	14:N:195:PRO:HD2	1.97	0.46
14:4:14:LEU:HD21	14:4:101:ALA:HB3	1.97	0.46
3:e:95:ARG:HB3	10:l:62:LYS:HE2	1.97	0.46
4:f:209:LYS:H	4:f:209:LYS:HD3	1.80	0.46
8:x:219:LEU:HD22	9:y:47:ARG:HD3	1.97	0.46
12:2:62:LEU:HD22	13:3:94:ARG:HH12	1.80	0.46
7:i:113:MET:HE1	8:j:69:THR:HG22	1.98	0.46
4:R:36:THR:HA	4:R:171:GLY:HA3	1.98	0.46
3:e:98:VAL:HG12	3:e:100:ASP:H	1.80	0.46
1:A:194:LEU:HB3	1:A:202:MET:HE1	1.98	0.46
3:Q:51:ALA:C	3:Q:53:LEU:H	2.24	0.46
9:k:45:GLY:C	9:k:47:ARG:H	2.24	0.46
12:n:83:MET:HE3	12:n:88:ILE:HG12	1.98	0.46
13:o:85:PRO:HB3	13:o:114:GLY:HA3	1.97	0.46
6:v:83:ASP:HB3	6:v:131:PHE:HD2	1.81	0.46
4:D:36:THR:HA	4:D:171:GLY:HA3	1.97	0.46
5:S:215:VAL:HB	5:S:221:PHE:HD1	1.79	0.46
8:j:219:LEU:HD13	9:k:47:ARG:HD3	1.97	0.46
3:C:120:GLN:HG3	4:D:135:ARG:HG3	1.98	0.46
1:O:53:SER:C	1:O:55:LEU:H	2.24	0.46
1:O:67:ILE:HD11	1:O:73:LEU:HD12	1.97	0.46
2:P:115:CYS:HB3	3:Q:81:ARG:HH22	1.81	0.46
9:I:115:THR:O	9:I:117:LYS:N	2.45	0.45
1:O:127:ARG:HH21	7:U:126:THR:HG22	1.81	0.45
9:k:125:LEU:HD12	9:k:126:ILE:HG23	1.98	0.45
4:R:157:ASP:HB2	4:R:158:PRO:HD2	1.98	0.45
5:S:74:ILE:HG22	5:S:132:LEU:HD22	1.98	0.45
6:T:187:ARG:HA	6:T:215:TRP:HH2	1.81	0.45
6:F:136:MET:HE3	6:F:163:CYS:HB3	1.98	0.45
11:Y:38:ASN:HD22	11:Y:41:LEU:HD12	1.82	0.45
8:j:50:ALA:HB2	9:k:128:CYS:HB2	1.98	0.45
1:q:49:LYS:HD2	1:q:208:GLU:HB2	1.97	0.45
14:4:142:THR:HB	14:4:155:PHE:HE1	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:61:THR:HG23	10:J:86:ARG:HH22	1.82	0.45
3:Q:20:GLU:HA	3:Q:23:GLN:HE21	1.80	0.45
4:R:35:SER:HB2	4:R:51:GLU:HG3	1.99	0.45
4:f:50:VAL:HG11	4:f:66:LYS:HB2	1.98	0.45
11:l:6:PHE:HE2	11:l:156:ALA:HB2	1.81	0.45
10:z:103:LEU:HD13	10:z:132:HIS:CD2	2.52	0.45
1:A:39:ALA:C	1:A:41:ASN:H	2.24	0.45
1:A:64:VAL:HG22	1:A:74:VAL:HG22	1.99	0.45
12:L:123:SER:HB3	12:L:136:LYS:HG2	1.99	0.45
14:b:18:SER:HB2	14:b:30:VAL:HA	1.99	0.45
9:k:13:MET:HB2	9:k:166:ILE:HD12	1.98	0.45
4:R:210:LEU:HD21	4:R:238:ILE:HD12	1.99	0.45
7:G:211:LYS:HB3	7:G:212:PRO:HD2	1.99	0.45
5:g:109:VAL:HA	5:g:112:ILE:HD12	1.99	0.45
5:g:33:SER:HB3	5:g:51:ARG:HG3	1.98	0.45
1:q:55:LEU:HD22	7:w:165:ALA:HB3	1.99	0.45
5:E:121:GLN:HG3	6:F:129:ARG:HG3	1.98	0.44
7:G:25:VAL:HG21	7:G:126:THR:HG23	1.98	0.44
8:V:22:GLU:HG2	8:V:27:ALA:HB2	1.99	0.44
4:f:182:GLN:HG2	5:g:56:LEU:HD23	1.99	0.44
13:o:20:VAL:HG11	13:o:122:LEU:HD13	1.99	0.44
8:x:50:ALA:HB2	9:y:128:CYS:HB2	1.99	0.44
5:E:47:VAL:HG12	5:E:195:LEU:HD22	1.98	0.44
1:O:149:ASP:HB2	1:O:150:PRO:HD2	1.98	0.44
4:R:182:GLN:HG2	5:S:56:LEU:HD23	2.00	0.44
3:e:120:GLN:HG3	4:f:135:ARG:HG3	1.99	0.44
8:j:219:LEU:HD11	9:k:194:ILE:HG13	1.99	0.44
5:u:33:SER:HB3	5:u:62:LYS:HE3	1.98	0.44
5:u:47:VAL:HG12	5:u:195:LEU:HD22	1.98	0.44
2:B:48:GLU:HG3	2:B:201:MET:HE3	2.00	0.44
6:F:213:LEU:HD12	6:F:232:ARG:HG3	1.99	0.44
9:I:70:LEU:HD11	9:I:81:ILE:HG21	2.00	0.44
2:P:21:VAL:HG11	2:P:153:SER:HB3	2.00	0.44
5:S:45:VAL:HG22	5:S:214:ILE:HG12	1.99	0.44
9:W:13:MET:HB2	9:W:166:ILE:HD12	1.98	0.44
5:u:33:SER:HB2	5:u:51:ARG:HG3	2.00	0.44
10:z:171:PHE:CE2	10:z:173:LEU:HB2	2.52	0.44
1:A:203:THR:H	1:A:206:ASN:HB2	1.82	0.44
5:E:7:ASP:HB2	5:E:24:TYR:CE1	2.52	0.44
5:g:38:LEU:HD13	5:g:187:LEU:HD13	1.99	0.44
1:O:159:ALA:HB3	2:P:55:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:136:TYR:HE1	2:P:150:SER:HB2	1.82	0.44
5:S:33:SER:HB3	5:S:51:ARG:HG3	1.99	0.44
3:e:91:CYS:HA	3:e:102:VAL:HG21	2.00	0.44
8:H:219:LEU:HD11	9:I:194:ILE:HG13	2.00	0.44
4:R:66:LYS:HA	4:R:78:MET:HE2	2.00	0.44
4:R:197:SER:O	4:R:201:ILE:HG12	2.18	0.44
12:n:27:THR:HB	12:n:40:SER:H	1.83	0.44
12:n:69:GLU:HA	12:n:72:LEU:HD12	1.98	0.44
1:A:212:CYS:HB2	1:A:217:PHE:HD1	1.83	0.44
6:F:156:VAL:HG13	7:G:88:ARG:HH12	1.83	0.44
5:S:63:ILE:HD12	5:S:211:SER:HB3	2.00	0.44
9:W:61:THR:HG23	10:X:86:ARG:HH22	1.83	0.44
1:q:10:THR:HG23	1:q:20:GLN:HB2	2.00	0.44
10:l:35:MET:HG2	10:l:45:LEU:HD22	2.00	0.44
7:w:25:VAL:HG21	7:w:126:THR:HG23	1.99	0.44
7:w:239:LEU:HA	7:w:242:LEU:HD12	1.99	0.44
12:2:16:ALA:HB2	12:2:121:VAL:HG23	2.00	0.44
1:O:58:GLU:HG2	1:O:205:ASP:HB3	2.00	0.43
5:S:47:VAL:HG12	5:S:195:LEU:HD22	2.00	0.43
4:f:180:SER:HB3	4:f:201:ILE:HD12	2.00	0.43
5:g:74:ILE:HG21	5:g:81:ALA:HB1	2.00	0.43
6:v:228:PRO:HD2	6:v:231:ILE:HD12	1.99	0.43
8:H:219:LEU:HD13	9:I:47:ARG:HD3	2.00	0.43
2:d:21:VAL:HG11	2:d:153:SER:HB3	1.99	0.43
10:z:117:TYR:HD1	10:z:130:ALA:HB1	1.83	0.43
5:u:26:MET:HA	5:u:149:PRO:HG2	1.99	0.43
9:y:137:VAL:HG11	9:y:145:MET:HB3	2.00	0.43
3:e:48:LYS:HB3	3:e:50:VAL:HG23	2.01	0.43
12:n:136:LYS:HD3	12:n:146:GLN:HE22	1.83	0.43
3:s:33:VAL:HG23	3:s:160:ALA:HB2	2.00	0.43
12:2:72:LEU:HD23	12:2:83:MET:HE2	2.01	0.43
6:F:83:ASP:HB3	6:F:131:PHE:HD2	1.84	0.43
7:U:25:VAL:HG21	7:U:126:THR:HG23	1.99	0.43
7:G:13:ILE:HG13	7:G:15:ILE:HG12	2.00	0.43
4:R:50:VAL:HG11	4:R:66:LYS:HB2	2.00	0.43
12:Z:137:ALA:H	12:Z:146:GLN:HE21	1.66	0.43
3:e:80:ALA:HA	3:e:129:ILE:HD13	2.00	0.43
9:W:47:ARG:HG2	9:W:111:LEU:HB2	2.00	0.43
10:X:4:LEU:HD22	10:X:45:LEU:HD12	1.99	0.43
1:c:64:VAL:HG22	1:c:74:VAL:HG22	2.00	0.43
2:r:171:ALA:HB2	2:r:200:THR:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:s:40:ILE:HG22	3:s:212:ARG:HG3	2.01	0.43
6:v:152:ASP:HB2	6:v:153:PRO:HD2	2.01	0.43
6:v:215:TRP:CD1	6:v:227:VAL:HG22	2.53	0.43
12:2:83:MET:HE3	12:2:88:ILE:HG12	2.01	0.43
1:A:49:LYS:HD2	1:A:208:GLU:HB2	2.00	0.43
1:A:230:ALA:O	1:A:232:ILE:N	2.51	0.43
3:C:20:GLU:HA	3:C:23:GLN:HE21	1.84	0.43
8:V:219:LEU:HD13	9:W:47:ARG:HD3	2.00	0.43
13:a:46:ASN:HD22	13:a:47:ASP:H	1.66	0.43
4:f:36:THR:HA	4:f:171:GLY:HA3	1.99	0.43
10:l:8:GLN:HE21	10:l:8:GLN:HB3	1.65	0.43
7:w:92:GLN:HE22	14:4:69:GLU:HG3	1.82	0.43
8:H:43:CYS:SG	8:H:98:LEU:HB3	2.59	0.43
2:d:197:LEU:O	2:d:201:MET:HB2	2.19	0.43
3:e:200:GLN:O	3:e:201:SER:C	2.61	0.43
6:h:141:SER:HB3	6:h:144:ASP:HB2	2.01	0.43
6:v:186:CYS:HA	6:v:189:VAL:HB	2.01	0.43
8:x:18:THR:HB	8:x:30:ASN:HA	1.99	0.43
9:I:137:VAL:HG11	9:I:145:MET:HB3	2.01	0.43
10:J:101:ASN:HB3	10:J:132:HIS:CE1	2.54	0.43
13:M:22:ILE:HB	13:M:50:MET:HE3	2.00	0.43
1:c:45:LEU:HB3	1:c:74:VAL:HG21	2.00	0.43
4:f:157:ASP:HB2	4:f:158:PRO:HD2	2.01	0.43
7:w:49:VAL:HG11	7:w:195:VAL:HA	2.01	0.43
9:y:35:THR:HG22	9:y:37:ASP:H	1.84	0.43
11:1:144:SER:HB3	11:1:147:LEU:HG	2.01	0.43
11:Y:14:VAL:HB	11:Y:177:TYR:HB2	2.01	0.42
14:p:201:THR:HG21	13:3:38:ASN:CB	2.49	0.42
3:s:98:VAL:HG13	11:1:78:ALA:HB2	2.00	0.42
7:w:78:CYS:HB3	7:w:140:LEU:HD23	2.01	0.42
8:x:177:VAL:HB	8:x:184:ASP:HB2	2.01	0.42
4:D:97:GLN:HB3	11:K:61:ARG:HG3	2.01	0.42
14:N:142:THR:HB	14:N:155:PHE:HE1	1.84	0.42
5:g:209:ASN:HD22	5:g:209:ASN:H	1.67	0.42
3:s:69:VAL:HG11	3:s:107:ILE:HG21	2.01	0.42
11:1:38:ASN:HD22	11:1:41:LEU:HD12	1.84	0.42
12:2:14:ALA:HA	12:2:22:ILE:O	2.18	0.42
8:H:106:THR:HB	8:H:109:HIS:HE2	1.84	0.42
14:b:30:VAL:O	14:b:30:VAL:HG13	2.19	0.42
1:c:44:VAL:HG21	1:c:187:ILE:HA	2.01	0.42
1:q:127:ARG:HH21	7:w:126:THR:HG22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:27:LEU:HD22	13:M:184:TYR:HB2	2.00	0.42
13:M:43:MET:HE2	13:M:45:VAL:HG22	2.01	0.42
8:V:113:ILE:HG12	8:V:119:THR:HG22	2.01	0.42
3:C:98:VAL:HG13	11:K:78:ALA:HB2	2.01	0.42
4:D:157:ASP:HB2	4:D:158:PRO:HD2	2.00	0.42
5:S:39:LYS:HB3	5:S:144:ILE:HG12	2.02	0.42
4:t:60:GLU:HA	4:t:61:PRO:HD3	1.86	0.42
6:v:39:ILE:HD11	6:v:189:VAL:HG13	2.01	0.42
8:x:42:TYR:HB2	8:x:178:ILE:HD11	2.01	0.42
10:z:19:ARG:HD3	10:z:179:SER:OG	2.19	0.42
4:D:186:HIS:CD2	4:D:188:SER:H	2.38	0.42
1:O:73:LEU:HD21	1:O:135:ILE:HG13	2.02	0.42
1:O:230:ALA:O	1:O:232:ILE:N	2.51	0.42
6:T:136:MET:HE3	6:T:163:CYS:HB3	2.02	0.42
8:V:45:GLY:HA3	8:V:52:THR:HG21	2.02	0.42
10:X:4:LEU:HB2	10:X:132:HIS:HB2	2.02	0.42
14:N:166:ARG:HG3	14:b:136:TYR:HB3	2.00	0.42
5:S:26:MET:HA	5:S:149:PRO:HG2	2.02	0.42
2:d:67:LYS:HE2	2:d:225:ILE:HD12	2.01	0.42
2:d:123:GLN:HG3	3:e:125:ARG:HD3	2.00	0.42
1:q:106:THR:O	1:q:110:VAL:HG23	2.20	0.42
5:u:215:VAL:HB	5:u:221:PHE:HD1	1.84	0.42
7:w:10:ASP:HA	7:w:15:ILE:HG13	2.02	0.42
14:N:179:ILE:HG12	14:N:184:VAL:HG22	2.02	0.42
6:T:207:LYS:HG2	6:T:208:ALA:H	1.83	0.42
7:U:13:ILE:HG13	7:U:15:ILE:HG12	2.02	0.42
7:i:25:VAL:HG21	7:i:126:THR:HG23	2.02	0.42
6:v:37:ILE:HD11	6:v:176:ILE:HD11	2.01	0.42
12:2:69:GLU:HA	12:2:72:LEU:HD12	2.02	0.42
4:D:107:MET:HE3	4:D:112:VAL:HG22	2.02	0.42
8:H:209:THR:HG22	9:I:168:GLN:HE21	1.83	0.42
9:I:10:VAL:HG23	9:I:53:ALA:HB2	2.02	0.42
12:L:125:ASP:HB2	12:L:126:PRO:HD2	2.02	0.42
12:L:137:ALA:HB3	12:L:146:GLN:HG2	2.01	0.42
6:T:156:VAL:HG13	7:U:88:ARG:HH12	1.85	0.42
1:c:67:ILE:HD11	1:c:73:LEU:HD12	2.01	0.42
6:h:123:THR:HG22	6:h:130:PRO:HB3	2.01	0.42
6:v:173:LYS:HA	6:v:176:ILE:HD12	2.01	0.42
12:2:12:VAL:HG21	12:2:53:GLY:HA3	2.02	0.42
1:A:10:THR:HG23	1:A:20:GLN:HB2	2.02	0.42
3:C:80:ALA:HA	3:C:129:ILE:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:152:ASP:HB2	6:F:153:PRO:HD2	2.02	0.42
7:G:10:ASP:HA	7:G:15:ILE:HG13	2.02	0.42
10:J:21:ALA:HB3	10:J:29:LYS:HB2	2.01	0.42
11:K:138:VAL:HG11	11:K:162:GLN:HG3	2.01	0.42
6:T:144:ASP:HB3	6:T:147:GLN:HE21	1.84	0.42
1:c:212:CYS:HB2	1:c:217:PHE:HD1	1.85	0.42
12:L:83:MET:HE3	12:L:88:ILE:HG12	2.02	0.41
4:R:97:GLN:HB3	11:Y:61:ARG:HG3	2.02	0.41
12:Z:83:MET:HE3	12:Z:88:ILE:HG12	2.02	0.41
12:n:123:SER:HB3	12:n:136:LYS:HG2	2.02	0.41
12:n:161:VAL:HG12	12:n:163:HIS:H	1.85	0.41
2:r:115:CYS:HB3	3:s:81:ARG:HH22	1.85	0.41
3:Q:98:VAL:HG13	11:Y:78:ALA:HB2	2.02	0.41
9:y:10:VAL:HG23	9:y:53:ALA:HB2	2.02	0.41
14:4:30:VAL:HG13	14:4:30:VAL:O	2.20	0.41
1:O:45:LEU:HB3	1:O:74:VAL:HG21	2.02	0.41
3:Q:80:ALA:HA	3:Q:129:ILE:HD13	2.02	0.41
5:S:34:ALA:HA	5:S:162:GLY:HA3	2.03	0.41
8:V:48:THR:HB	8:V:51:ASP:HB2	2.02	0.41
2:d:95:GLN:HE22	9:k:71:ASN:HD22	1.68	0.41
4:f:202:LEU:HG	4:f:206:MET:HE2	2.03	0.41
3:C:230:ALA:O	3:C:234:LYS:HB2	2.21	0.41
8:H:48:THR:HB	8:H:51:ASP:HB2	2.02	0.41
12:n:16:ALA:HB2	12:n:121:VAL:HG23	2.02	0.41
4:t:35:SER:HB2	4:t:51:GLU:HG3	2.02	0.41
8:H:162:GLY:O	8:H:166:ASP:HB3	2.20	0.41
12:L:145:LEU:HD22	12:L:178:VAL:HB	2.02	0.41
4:R:163:VAL:HB	5:S:60:GLN:HE21	1.84	0.41
12:Z:14:ALA:HA	12:Z:22:ILE:O	2.20	0.41
12:Z:16:ALA:HB2	12:Z:121:VAL:HG23	2.01	0.41
13:a:49:THR:HG22	13:a:85:PRO:HG3	2.02	0.41
7:i:13:ILE:HG13	7:i:15:ILE:HG12	2.02	0.41
9:k:61:THR:HG23	10:l:86:ARG:HH22	1.86	0.41
12:n:72:LEU:HD23	12:n:83:MET:HE2	2.01	0.41
3:s:120:GLN:HG3	4:t:135:ARG:HG3	2.03	0.41
6:v:207:LYS:HG2	6:v:208:ALA:H	1.84	0.41
12:2:161:VAL:HG12	12:2:163:HIS:H	1.85	0.41
1:A:106:THR:O	1:A:110:VAL:HG23	2.20	0.41
7:U:10:ASP:HA	7:U:15:ILE:HG13	2.01	0.41
5:g:34:ALA:HA	5:g:162:GLY:HA3	2.02	0.41
14:p:3:ILE:HB	14:p:44:CYS:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:u:176:MET:HE1	6:v:56:LYS:HG2	2.03	0.41
9:y:14:LYS:HG3	9:y:120:ILE:HG12	2.02	0.41
1:A:159:ALA:HB1	1:A:173:LEU:HD22	2.03	0.41
3:e:69:VAL:HG11	3:e:107:ILE:HG21	2.02	0.41
4:f:13:ASN:HB3	5:g:126:ARG:HB3	2.02	0.41
8:j:22:GLU:HG2	8:j:27:ALA:HB2	2.02	0.41
8:j:43:CYS:SG	8:j:98:LEU:HB3	2.60	0.41
10:l:108:ASP:HB3	10:l:112:GLY:H	1.85	0.41
7:w:93:ARG:HE	7:w:121:ILE:HD13	1.86	0.41
7:w:143:ILE:HG12	7:w:149:PRO:HA	2.03	0.41
10:z:43:LEU:HD12	10:z:183:ILE:HD11	2.03	0.41
14:4:21:THR:HG22	14:4:26:ILE:HG13	2.01	0.41
6:T:6:GLY:C	6:T:8:ASP:H	2.29	0.41
8:V:38:SER:C	8:V:40:ASN:H	2.29	0.41
10:X:43:LEU:HD12	10:X:183:ILE:HD11	2.03	0.41
8:j:177:VAL:HB	8:j:184:ASP:HB2	2.03	0.41
9:k:94:LEU:HD11	9:k:106:PRO:HG2	2.03	0.41
11:m:97:MET:HG3	11:m:116:SER:HB3	2.01	0.41
1:O:68:THR:HG22	1:O:71:ILE:HB	2.02	0.41
4:R:167:ALA:HB3	5:S:56:LEU:HD12	2.03	0.41
6:T:141:SER:HB3	6:T:144:ASP:HB2	2.03	0.41
6:T:173:LYS:HA	6:T:176:ILE:HD12	2.02	0.41
13:a:20:VAL:HG11	13:a:122:LEU:HD13	2.03	0.41
14:b:142:THR:HB	14:b:155:PHE:HE1	1.86	0.41
1:c:127:ARG:HH21	7:i:126:THR:HG22	1.86	0.41
1:c:194:LEU:HB3	1:c:202:MET:HE1	2.03	0.41
5:g:39:LYS:HB3	5:g:144:ILE:HG12	2.03	0.41
8:j:8:TYR:CE1	8:j:10:ASP:HB2	2.55	0.41
11:m:188:SER:HB3	11:m:190:ASP:OD1	2.21	0.41
12:n:187:VAL:HG12	8:x:167:LEU:HD22	2.03	0.41
5:E:72:ILE:HG22	5:E:134:ILE:HG12	2.03	0.41
7:G:72:ILE:HD11	7:G:78:CYS:SG	2.61	0.41
10:J:8:GLN:HE21	10:J:8:GLN:HB3	1.59	0.41
11:K:180:ARG:HH21	11:K:185:ILE:HD13	1.86	0.41
1:O:212:CYS:HB2	1:O:217:PHE:HD1	1.86	0.41
2:d:14:PRO:HA	3:e:21:TYR:CE2	2.56	0.41
10:J:85:ARG:HA	10:J:118:MET:HE1	2.03	0.40
12:L:69:GLU:HA	12:L:72:LEU:HD12	2.03	0.40
1:O:106:THR:O	1:O:110:VAL:HG23	2.21	0.40
5:S:176:MET:HE1	6:T:56:LYS:HB3	2.02	0.40
5:S:224:TYR:HD2	5:S:228:ASP:HB3	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:10:THR:HG23	1:c:20:GLN:HB2	2.03	0.40
5:g:47:VAL:HG12	5:g:195:LEU:HD22	2.02	0.40
6:h:168:ALA:HB1	6:h:171:ALA:HB3	2.03	0.40
14:p:30:VAL:O	14:p:30:VAL:CG1	2.68	0.40
6:v:67:PHE:HB2	6:v:75:MET:HB3	2.03	0.40
13:3:184:TYR:HE2	13:3:186:ARG:HD3	1.86	0.40
6:F:136:MET:HE2	6:F:148:LEU:HD11	2.04	0.40
1:O:75:TYR:HB3	1:O:82:TYR:CD1	2.56	0.40
1:O:202:MET:HB3	1:O:229:LEU:HD11	2.02	0.40
12:Z:72:LEU:HD23	12:Z:83:MET:HE2	2.04	0.40
14:p:166:ARG:HG3	14:4:136:TYR:HB3	2.04	0.40
1:q:149:ASP:HB2	1:q:150:PRO:HD2	2.03	0.40
7:w:92:GLN:HE21	7:w:92:GLN:HA	1.84	0.40
9:I:141:CYS:HB2	9:I:144:GLN:HB2	2.01	0.40
12:L:83:MET:HG2	12:L:88:ILE:HG13	2.03	0.40
2:d:87:THR:HA	2:d:90:LEU:HD12	2.04	0.40
5:u:236:LEU:HD23	5:u:236:LEU:H	1.85	0.40
13:M:72:ILE:O	13:M:76:LEU:HG	2.22	0.40
3:Q:131:ALA:O	3:Q:146:GLN:HA	2.20	0.40
6:T:152:ASP:HB2	6:T:153:PRO:HD2	2.03	0.40
13:a:46:ASN:HD22	13:a:47:ASP:N	2.18	0.40
1:c:73:LEU:HD21	1:c:133:LEU:HB3	2.04	0.40
12:n:146:GLN:N	12:n:147:PRO:HD2	2.36	0.40
6:v:227:VAL:HA	6:v:228:PRO:HD3	1.94	0.40
8:H:27:ALA:HB1	9:I:130:MET:HE1	2.03	0.40
8:H:42:TYR:HB2	8:H:178:ILE:HD11	2.04	0.40
12:Z:69:GLU:HA	12:Z:72:LEU:HD12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	231/234 (99%)	213 (92%)	14 (6%)	4 (2%)	7	35
1	O	231/234 (99%)	217 (94%)	11 (5%)	3 (1%)	9	40
1	c	231/234 (99%)	213 (92%)	14 (6%)	4 (2%)	7	35
1	q	231/234 (99%)	213 (92%)	12 (5%)	6 (3%)	4	26
2	B	246/261 (94%)	240 (98%)	5 (2%)	1 (0%)	30	62
2	P	246/261 (94%)	240 (98%)	5 (2%)	1 (0%)	30	62
2	d	246/261 (94%)	240 (98%)	5 (2%)	1 (0%)	30	62
2	r	246/261 (94%)	239 (97%)	6 (2%)	1 (0%)	30	62
3	C	237/248 (96%)	226 (95%)	10 (4%)	1 (0%)	30	62
3	Q	237/248 (96%)	229 (97%)	7 (3%)	1 (0%)	30	62
3	e	237/248 (96%)	227 (96%)	8 (3%)	2 (1%)	16	50
3	s	237/248 (96%)	230 (97%)	6 (2%)	1 (0%)	30	62
4	D	231/241 (96%)	219 (95%)	12 (5%)	0	100	100
4	R	231/241 (96%)	219 (95%)	12 (5%)	0	100	100
4	f	231/241 (96%)	218 (94%)	13 (6%)	0	100	100
4	t	231/241 (96%)	217 (94%)	14 (6%)	0	100	100
5	E	236/263 (90%)	228 (97%)	7 (3%)	1 (0%)	30	62
5	S	236/263 (90%)	228 (97%)	8 (3%)	0	100	100
5	g	236/263 (90%)	227 (96%)	8 (3%)	1 (0%)	30	62
5	u	236/263 (90%)	224 (95%)	11 (5%)	1 (0%)	30	62
6	F	242/255 (95%)	229 (95%)	11 (4%)	2 (1%)	16	50
6	T	242/255 (95%)	228 (94%)	12 (5%)	2 (1%)	16	50
6	h	242/255 (95%)	230 (95%)	10 (4%)	2 (1%)	16	50
6	v	242/255 (95%)	229 (95%)	12 (5%)	1 (0%)	30	62
7	G	242/246 (98%)	232 (96%)	10 (4%)	0	100	100
7	U	242/246 (98%)	232 (96%)	10 (4%)	0	100	100
7	i	242/246 (98%)	230 (95%)	11 (4%)	1 (0%)	30	62
7	w	242/246 (98%)	232 (96%)	9 (4%)	1 (0%)	30	62
8	H	218/234 (93%)	204 (94%)	13 (6%)	1 (0%)	24	59
8	V	218/234 (93%)	208 (95%)	9 (4%)	1 (0%)	24	59
8	j	218/234 (93%)	208 (95%)	9 (4%)	1 (0%)	24	59
8	x	218/234 (93%)	204 (94%)	13 (6%)	1 (0%)	24	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	202/205 (98%)	187 (93%)	8 (4%)	7 (4%)	3	20
9	W	202/205 (98%)	189 (94%)	9 (4%)	4 (2%)	6	31
9	k	202/205 (98%)	187 (93%)	12 (6%)	3 (2%)	8	37
9	y	202/205 (98%)	186 (92%)	13 (6%)	3 (2%)	8	37
10	J	194/201 (96%)	186 (96%)	7 (4%)	1 (0%)	24	59
10	X	194/201 (96%)	185 (95%)	8 (4%)	1 (0%)	24	59
10	l	194/201 (96%)	182 (94%)	11 (6%)	1 (0%)	24	59
10	z	194/201 (96%)	185 (95%)	8 (4%)	1 (0%)	24	59
11	1	199/205 (97%)	188 (94%)	11 (6%)	0	100	100
11	K	199/205 (97%)	188 (94%)	11 (6%)	0	100	100
11	Y	199/205 (97%)	190 (96%)	9 (4%)	0	100	100
11	m	199/205 (97%)	190 (96%)	9 (4%)	0	100	100
12	2	211/213 (99%)	202 (96%)	8 (4%)	1 (0%)	24	59
12	L	211/213 (99%)	202 (96%)	8 (4%)	1 (0%)	24	59
12	Z	211/213 (99%)	203 (96%)	7 (3%)	1 (0%)	24	59
12	n	211/213 (99%)	201 (95%)	9 (4%)	1 (0%)	24	59
13	3	214/219 (98%)	203 (95%)	11 (5%)	0	100	100
13	M	214/219 (98%)	204 (95%)	10 (5%)	0	100	100
13	a	214/219 (98%)	204 (95%)	10 (5%)	0	100	100
13	o	214/219 (98%)	202 (94%)	12 (6%)	0	100	100
14	4	200/205 (98%)	187 (94%)	13 (6%)	0	100	100
14	N	200/205 (98%)	192 (96%)	8 (4%)	0	100	100
14	b	200/205 (98%)	191 (96%)	9 (4%)	0	100	100
14	p	200/205 (98%)	188 (94%)	11 (6%)	1 (0%)	24	59
All	All	12412/12920 (96%)	11795 (95%)	549 (4%)	68 (0%)	24	59

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	201	GLN
9	I	116	PHE
10	J	24	ASN
1	O	201	GLN
10	X	24	ASN

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Mol	Chain	Res	Type
1	c	201	GLN
10	z	24	ASN
1	A	199	GLU
6	F	216	VAL
9	I	47	ARG
1	O	54	ILE
1	O	231	ALA
6	T	216	VAL
1	c	54	ILE
6	h	216	VAL
10	l	24	ASN
1	q	230	ALA
1	q	231	ALA
6	v	216	VAL
9	y	100	GLY
9	I	30	GLN
9	I	46	ASP
3	Q	201	SER
9	W	30	GLN
1	c	199	GLU
3	e	201	SER
6	h	207	LYS
7	i	3	ARG
9	k	30	GLN
12	n	191	ASP
1	q	201	GLN
3	s	201	SER
7	w	3	ARG
9	y	30	GLN
9	y	155	PRO
12	2	191	ASP
1	A	231	ALA
8	H	188	PRO
9	I	16	LYS
12	L	191	ASP
2	P	206	LEU
9	W	45	GLY
12	Z	191	ASP
1	c	229	LEU
3	e	52	LYS
14	p	190	LEU
1	q	199	GLU

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Mol	Chain	Res	Type
2	r	206	LEU
2	B	206	LEU
6	F	207	LYS
9	I	155	PRO
8	V	188	PRO
2	d	206	LEU
8	j	188	PRO
1	q	52	LYS
5	u	240	PRO
3	C	201	SER
6	T	3	ILE
1	q	54	ILE
8	x	188	PRO
9	W	100	GLY
5	g	240	PRO
5	E	240	PRO
9	W	155	PRO
9	k	155	PRO
1	A	54	ILE
9	I	100	GLY
9	k	100	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	189/191 (99%)	183 (97%)	6 (3%)	34	65
1	O	189/191 (99%)	181 (96%)	8 (4%)	26	60
1	c	189/191 (99%)	182 (96%)	7 (4%)	30	63
1	q	189/191 (99%)	184 (97%)	5 (3%)	40	69
2	B	208/221 (94%)	202 (97%)	6 (3%)	37	67
2	P	208/221 (94%)	200 (96%)	8 (4%)	29	62
2	d	208/221 (94%)	201 (97%)	7 (3%)	32	64
2	r	208/221 (94%)	198 (95%)	10 (5%)	23	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	202/211 (96%)	193 (96%)	9 (4%)	24	58
3	Q	202/211 (96%)	193 (96%)	9 (4%)	24	58
3	e	202/211 (96%)	192 (95%)	10 (5%)	22	55
3	s	202/211 (96%)	195 (96%)	7 (4%)	32	64
4	D	195/203 (96%)	188 (96%)	7 (4%)	31	63
4	R	195/203 (96%)	190 (97%)	5 (3%)	40	69
4	f	195/203 (96%)	190 (97%)	5 (3%)	40	69
4	t	195/203 (96%)	191 (98%)	4 (2%)	47	71
5	E	204/224 (91%)	197 (97%)	7 (3%)	32	64
5	S	204/224 (91%)	195 (96%)	9 (4%)	25	59
5	g	204/224 (91%)	196 (96%)	8 (4%)	28	62
5	u	204/224 (91%)	198 (97%)	6 (3%)	37	67
6	F	200/211 (95%)	193 (96%)	7 (4%)	32	64
6	T	200/211 (95%)	192 (96%)	8 (4%)	28	61
6	h	200/211 (95%)	192 (96%)	8 (4%)	28	61
6	v	200/211 (95%)	194 (97%)	6 (3%)	36	66
7	G	207/210 (99%)	203 (98%)	4 (2%)	50	73
7	U	207/210 (99%)	201 (97%)	6 (3%)	37	67
7	i	207/210 (99%)	202 (98%)	5 (2%)	43	70
7	w	207/210 (99%)	200 (97%)	7 (3%)	32	64
8	H	181/195 (93%)	175 (97%)	6 (3%)	33	65
8	V	181/195 (93%)	178 (98%)	3 (2%)	53	75
8	j	181/195 (93%)	176 (97%)	5 (3%)	38	68
8	x	181/195 (93%)	175 (97%)	6 (3%)	33	65
9	I	174/175 (99%)	171 (98%)	3 (2%)	53	75
9	W	174/175 (99%)	170 (98%)	4 (2%)	44	70
9	k	174/175 (99%)	171 (98%)	3 (2%)	53	75
9	y	174/175 (99%)	168 (97%)	6 (3%)	32	64
10	J	166/171 (97%)	162 (98%)	4 (2%)	43	70
10	X	166/171 (97%)	162 (98%)	4 (2%)	43	70
10	l	166/171 (97%)	165 (99%)	1 (1%)	78	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	z	166/171 (97%)	158 (95%)	8 (5%)	23	56
11	1	157/161 (98%)	152 (97%)	5 (3%)	34	65
11	K	157/161 (98%)	153 (98%)	4 (2%)	42	69
11	Y	157/161 (98%)	152 (97%)	5 (3%)	34	65
11	m	157/161 (98%)	152 (97%)	5 (3%)	34	65
12	2	178/178 (100%)	171 (96%)	7 (4%)	28	62
12	L	178/178 (100%)	170 (96%)	8 (4%)	24	58
12	Z	178/178 (100%)	175 (98%)	3 (2%)	53	75
12	n	178/178 (100%)	172 (97%)	6 (3%)	32	64
13	3	178/180 (99%)	174 (98%)	4 (2%)	45	71
13	M	178/180 (99%)	175 (98%)	3 (2%)	53	75
13	a	178/180 (99%)	175 (98%)	3 (2%)	53	75
13	o	178/180 (99%)	172 (97%)	6 (3%)	32	64
14	4	159/162 (98%)	159 (100%)	0	100	100
14	N	159/162 (98%)	157 (99%)	2 (1%)	61	78
14	b	159/162 (98%)	158 (99%)	1 (1%)	78	84
14	p	159/162 (98%)	157 (99%)	2 (1%)	61	78
All	All	10392/10772 (96%)	10081 (97%)	311 (3%)	36	66

All (311) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	17	LYS
1	A	43	VAL
1	A	194	LEU
1	A	207	ILE
1	A	214	GLU
2	B	25	MET
2	B	44	LEU
2	B	98	LEU
2	B	192	LEU
2	B	199	LYS
2	B	229	LYS
3	C	43	LEU
3	C	47	LYS

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Mol	Chain	Res	Type
3	C	57	ARG
3	C	59	VAL
3	C	107	ILE
3	C	172	LEU
3	C	206	ILE
3	C	221	ASN
3	C	225	ILE
4	D	89	ILE
4	D	148	GLU
4	D	203	LYS
4	D	208	GLU
4	D	209	LYS
4	D	217	LEU
4	D	231	LYS
5	E	5	GLN
5	E	38	LEU
5	E	62	LYS
5	E	74	ILE
5	E	101	ARG
5	E	187	LEU
5	E	209	ASN
6	F	56	LYS
6	F	90	ILE
6	F	181	MET
6	F	197	ILE
6	F	203	GLU
6	F	205	LYS
6	F	219	LEU
7	G	84	THR
7	G	166	THR
7	G	179	LEU
7	G	221	THR
8	H	6	VAL
8	H	40	ASN
8	H	121	LYS
8	H	180	LYS
8	H	194	LYS
8	H	201	ARG
9	I	19	VAL
9	I	136	VAL
9	I	144	GLN
10	J	8	GLN

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Mol	Chain	Res	Type
10	J	45	LEU
10	J	143	LEU
10	J	191	LEU
11	K	58	LEU
11	K	71	LYS
11	K	128	VAL
11	K	176	LEU
12	L	62	LEU
12	L	67	ILE
12	L	118	LYS
12	L	148	LEU
12	L	160	ASN
12	L	173	ARG
12	L	174	LEU
12	L	203	ILE
13	M	44	ARG
13	M	94	ARG
13	M	192	VAL
14	N	116	MET
14	N	194	ILE
1	O	2	LYS
1	O	19	VAL
1	O	43	VAL
1	O	54	ILE
1	O	192	LEU
1	O	194	LEU
1	O	195	LYS
1	O	207	ILE
2	P	25	MET
2	P	28	ILE
2	P	37	ILE
2	P	44	LEU
2	P	52	ILE
2	P	56	LEU
2	P	98	LEU
2	P	192	LEU
3	Q	5	ARG
3	Q	42	VAL
3	Q	43	LEU
3	Q	59	VAL
3	Q	107	ILE
3	Q	172	LEU

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Mol	Chain	Res	Type
3	Q	221	ASN
3	Q	225	ILE
3	Q	236	LYS
4	R	89	ILE
4	R	170	ILE
4	R	203	LYS
4	R	224	GLN
4	R	231	LYS
5	S	38	LEU
5	S	62	LYS
5	S	74	ILE
5	S	84	LEU
5	S	187	LEU
5	S	202	GLU
5	S	206	THR
5	S	209	ASN
5	S	211	SER
6	T	56	LYS
6	T	90	ILE
6	T	108	LEU
6	T	165	ILE
6	T	181	MET
6	T	187	ARG
6	T	219	LEU
6	T	233	GLU
7	U	52	THR
7	U	166	THR
7	U	179	LEU
7	U	186	LYS
7	U	221	THR
7	U	226	LYS
8	V	40	ASN
8	V	121	LYS
8	V	180	LYS
9	W	13	MET
9	W	136	VAL
9	W	144	GLN
9	W	195	THR
10	X	47	VAL
10	X	143	LEU
10	X	154	GLU
10	X	191	LEU

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Mol	Chain	Res	Type
11	Y	58	LEU
11	Y	71	LYS
11	Y	124	THR
11	Y	128	VAL
11	Y	176	LEU
12	Z	148	LEU
12	Z	160	ASN
12	Z	174	LEU
13	a	44	ARG
13	a	46	ASN
13	a	94	ARG
14	b	173	VAL
1	c	54	ILE
1	c	83	ARG
1	c	173	LEU
1	c	181	LEU
1	c	194	LEU
1	c	207	ILE
1	c	229	LEU
2	d	25	MET
2	d	37	ILE
2	d	44	LEU
2	d	52	ILE
2	d	98	LEU
2	d	164	ILE
2	d	199	LYS
3	e	5	ARG
3	e	42	VAL
3	e	47	LYS
3	e	59	VAL
3	e	96	LEU
3	e	107	ILE
3	e	125	ARG
3	e	134	VAL
3	e	172	LEU
3	e	225	ILE
4	f	89	ILE
4	f	126	GLU
4	f	170	ILE
4	f	209	LYS
4	f	217	LEU
5	g	38	LEU

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Mol	Chain	Res	Type
5	g	56	LEU
5	g	62	LYS
5	g	74	ILE
5	g	83	LEU
5	g	187	LEU
5	g	209	ASN
5	g	241	GLN
6	h	3	ILE
6	h	37	ILE
6	h	56	LYS
6	h	64	LYS
6	h	90	ILE
6	h	106	ILE
6	h	181	MET
6	h	207	LYS
7	i	73	THR
7	i	166	THR
7	i	170	VAL
7	i	179	LEU
7	i	221	THR
8	j	6	VAL
8	j	12	ILE
8	j	40	ASN
8	j	65	LEU
8	j	121	LYS
9	k	16	LYS
9	k	136	VAL
9	k	144	GLN
10	l	8	GLN
11	m	32	LYS
11	m	58	LEU
11	m	121	ILE
11	m	128	VAL
11	m	176	LEU
12	n	67	ILE
12	n	148	LEU
12	n	160	ASN
12	n	166	LEU
12	n	173	ARG
12	n	174	LEU
13	o	44	ARG
13	o	46	ASN

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Mol	Chain	Res	Type
13	o	69	GLN
13	o	94	ARG
13	o	159	VAL
13	o	192	VAL
14	p	95	MET
14	p	173	VAL
1	q	2	LYS
1	q	43	VAL
1	q	51	GLN
1	q	207	ILE
1	q	214	GLU
2	r	25	MET
2	r	44	LEU
2	r	52	ILE
2	r	164	ILE
2	r	192	LEU
2	r	201	MET
2	r	222	LYS
2	r	236	LEU
2	r	242	GLU
2	r	243	GLU
3	s	59	VAL
3	s	96	LEU
3	s	107	ILE
3	s	134	VAL
3	s	161	ILE
3	s	213	ARG
3	s	225	ILE
4	t	64	ILE
4	t	89	ILE
4	t	203	LYS
4	t	217	LEU
5	u	38	LEU
5	u	56	LEU
5	u	74	ILE
5	u	132	LEU
5	u	205	LEU
5	u	241	GLN
6	v	56	LYS
6	v	90	ILE
6	v	181	MET
6	v	203	GLU

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Mol	Chain	Res	Type
6	v	219	LEU
6	v	232	ARG
7	w	56	VAL
7	w	60	LEU
7	w	92	GLN
7	w	114	LEU
7	w	166	THR
7	w	179	LEU
7	w	221	THR
8	x	58	LEU
8	x	65	LEU
8	x	83	LEU
8	x	121	LYS
8	x	180	LYS
8	x	201	ARG
9	y	13	MET
9	y	36	THR
9	y	50	ILE
9	y	136	VAL
9	y	144	GLN
9	y	171	LEU
10	z	8	GLN
10	z	45	LEU
10	z	103	LEU
10	z	143	LEU
10	z	154	GLU
10	z	155	ARG
10	z	185	LYS
10	z	191	LEU
11	1	58	LEU
11	1	71	LYS
11	1	82	LEU
11	1	124	THR
11	1	128	VAL
12	2	62	LEU
12	2	67	ILE
12	2	127	VAL
12	2	148	LEU
12	2	160	ASN
12	2	166	LEU
12	2	173	ARG
13	3	35	ARG

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Mol	Chain	Res	Type
13	3	46	ASN
13	3	69	GLN
13	3	94	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (218) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	101	GLN
1	A	139	ASN
2	B	88	ASN
2	B	100	GLN
2	B	155	ASN
3	C	23	GLN
3	C	154	HIS
4	D	41	GLN
4	D	97	GLN
4	D	99	HIS
4	D	186	HIS
4	D	211	ASN
5	E	5	GLN
5	E	146	GLN
5	E	183	ASN
5	E	190	HIS
6	F	147	GLN
7	G	53	GLN
7	G	92	GLN
7	G	100	ASN
7	G	127	GLN
7	G	147	GLN
8	H	40	ASN
8	H	80	ASN
9	I	6	ASN
9	I	32	GLN
9	I	39	GLN
9	I	64	GLN
9	I	144	GLN
10	J	8	GLN
10	J	27	GLN
10	J	55	GLN
10	J	82	ASN
10	J	174	ASN

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Mol	Chain	Res	Type
11	K	38	ASN
12	L	8	ASN
12	L	58	HIS
12	L	79	ASN
12	L	131	GLN
12	L	146	GLN
12	L	151	ASN
12	L	157	ASN
13	M	2	GLN
13	M	38	ASN
13	M	46	ASN
13	M	89	HIS
14	N	66	HIS
14	N	77	HIS
14	N	187	GLN
14	N	193	GLN
1	O	41	ASN
1	O	101	GLN
1	O	139	ASN
1	O	168	ASN
2	P	95	GLN
2	P	100	GLN
2	P	123	GLN
3	Q	23	GLN
3	Q	159	ASN
4	R	41	GLN
4	R	97	GLN
4	R	99	HIS
4	R	152	GLN
4	R	186	HIS
4	R	204	GLN
4	R	221	GLN
4	R	224	GLN
5	S	60	GLN
5	S	146	GLN
6	T	147	GLN
7	U	92	GLN
7	U	127	GLN
7	U	150	GLN
8	V	30	ASN
8	V	40	ASN
8	V	80	ASN

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Mol	Chain	Res	Type
9	W	6	ASN
9	W	39	GLN
9	W	64	GLN
9	W	80	GLN
9	W	144	GLN
9	W	156	ASN
10	X	8	GLN
10	X	27	GLN
10	X	55	GLN
10	X	61	GLN
10	X	71	ASN
10	X	82	ASN
10	X	174	ASN
11	Y	38	ASN
12	Z	8	ASN
12	Z	77	HIS
12	Z	79	ASN
12	Z	131	GLN
12	Z	146	GLN
12	Z	152	GLN
13	a	38	ASN
13	a	46	ASN
13	a	157	GLN
13	a	208	ASN
14	b	66	HIS
14	b	77	HIS
14	b	110	GLN
14	b	158	ASN
14	b	187	GLN
14	b	193	GLN
1	c	41	ASN
1	c	87	HIS
1	c	108	GLN
1	c	111	GLN
1	c	139	ASN
1	c	147	GLN
1	c	178	ASN
2	d	95	GLN
2	d	100	GLN
2	d	155	ASN
2	d	198	ASN
3	e	122	ASN

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Mol	Chain	Res	Type
3	e	205	ASN
3	e	215	GLN
3	e	221	ASN
4	f	99	HIS
4	f	152	GLN
4	f	204	GLN
5	g	146	GLN
5	g	209	ASN
6	h	201	HIS
7	i	92	GLN
7	i	100	ASN
7	i	127	GLN
7	i	150	GLN
7	i	193	GLN
8	j	40	ASN
8	j	80	ASN
9	k	6	ASN
9	k	32	GLN
9	k	39	GLN
9	k	64	GLN
9	k	144	GLN
9	k	161	HIS
10	l	8	GLN
10	l	27	GLN
10	l	61	GLN
10	l	71	ASN
11	m	38	ASN
12	n	8	ASN
12	n	131	GLN
12	n	146	GLN
12	n	151	ASN
12	n	152	GLN
13	o	38	ASN
13	o	46	ASN
13	o	81	HIS
13	o	89	HIS
13	o	147	GLN
13	o	157	GLN
14	p	7	GLN
14	p	77	HIS
14	p	106	GLN
14	p	110	GLN

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Mol	Chain	Res	Type
14	p	187	GLN
1	q	41	ASN
1	q	62	HIS
1	q	101	GLN
1	q	108	GLN
1	q	139	ASN
2	r	88	ASN
2	r	95	GLN
2	r	100	GLN
2	r	123	GLN
2	r	166	ASN
2	r	198	ASN
3	s	23	GLN
3	s	159	ASN
3	s	221	ASN
4	t	114	GLN
4	t	152	GLN
4	t	155	HIS
4	t	204	GLN
4	t	211	ASN
5	u	146	GLN
5	u	209	ASN
6	v	147	GLN
7	w	92	GLN
7	w	100	ASN
8	x	80	ASN
8	x	116	HIS
9	y	6	ASN
9	y	32	GLN
9	y	39	GLN
9	y	144	GLN
10	z	8	GLN
10	z	27	GLN
10	z	55	GLN
10	z	71	ASN
10	z	82	ASN
10	z	132	HIS
11	1	29	GLN
11	1	38	ASN
11	1	175	ASN
12	2	8	ASN
12	2	146	GLN

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Mol	Chain	Res	Type
12	2	151	ASN
12	2	152	GLN
12	2	157	ASN
12	2	160	ASN
13	3	2	GLN
13	3	46	ASN
13	3	69	GLN
13	3	147	GLN
13	3	208	ASN
14	4	40	HIS
14	4	77	HIS
14	4	110	GLN
14	4	154	GLN
14	4	158	ASN
14	4	187	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	233/234 (99%)	-0.10	2 (0%) 81 64	68, 101, 151, 178	0
1	O	233/234 (99%)	-0.27	3 (1%) 75 55	56, 79, 133, 166	0
1	c	233/234 (99%)	-0.26	0 100 100	75, 107, 157, 181	0
1	q	233/234 (99%)	-0.22	1 (0%) 88 79	80, 107, 155, 173	0
2	B	248/261 (95%)	-0.33	0 100 100	65, 95, 143, 169	0
2	P	248/261 (95%)	-0.38	0 100 100	51, 78, 117, 157	0
2	d	248/261 (95%)	-0.31	1 (0%) 88 79	65, 110, 164, 202	0
2	r	248/261 (95%)	-0.31	0 100 100	78, 110, 148, 167	0
3	C	239/248 (96%)	-0.23	2 (0%) 82 67	73, 109, 169, 202	0
3	Q	239/248 (96%)	-0.28	0 100 100	61, 98, 156, 197	0
3	e	239/248 (96%)	-0.22	0 100 100	80, 125, 178, 204	0
3	s	239/248 (96%)	-0.20	0 100 100	91, 125, 174, 196	0
4	D	233/241 (96%)	-0.29	0 100 100	59, 96, 130, 154	0
4	R	233/241 (96%)	-0.35	0 100 100	67, 101, 139, 176	0
4	f	233/241 (96%)	-0.27	0 100 100	77, 124, 155, 185	0
4	t	233/241 (96%)	-0.28	1 (0%) 88 79	71, 120, 157, 190	0
5	E	238/263 (90%)	-0.34	0 100 100	57, 93, 148, 178	0
5	S	238/263 (90%)	-0.25	1 (0%) 88 79	66, 98, 154, 184	0
5	g	238/263 (90%)	-0.14	0 100 100	81, 117, 163, 192	0
5	u	238/263 (90%)	-0.26	1 (0%) 88 79	66, 108, 162, 182	0
6	F	244/255 (95%)	-0.28	0 100 100	63, 97, 146, 162	0
6	T	244/255 (95%)	-0.29	0 100 100	58, 89, 143, 168	0
6	h	244/255 (95%)	-0.19	1 (0%) 88 79	87, 121, 165, 179	0
6	v	244/255 (95%)	-0.27	0 100 100	81, 109, 149, 169	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
7	G	244/246 (99%)	-0.28	0 100 100	66, 101, 149, 170	0
7	U	244/246 (99%)	-0.35	0 100 100	57, 81, 114, 144	0
7	i	244/246 (99%)	-0.24	0 100 100	81, 121, 159, 180	0
7	w	244/246 (99%)	-0.22	0 100 100	78, 107, 150, 169	0
8	H	220/234 (94%)	-0.24	0 100 100	62, 81, 130, 169	0
8	V	220/234 (94%)	-0.38	0 100 100	49, 65, 103, 153	0
8	j	220/234 (94%)	-0.32	0 100 100	71, 87, 125, 151	0
8	x	220/234 (94%)	-0.23	0 100 100	69, 93, 142, 175	0
9	I	204/205 (99%)	-0.29	0 100 100	64, 79, 118, 146	0
9	W	204/205 (99%)	-0.44	1 (0%) 87 76	52, 66, 96, 129	0
9	k	204/205 (99%)	-0.35	0 100 100	69, 84, 120, 141	0
9	y	204/205 (99%)	-0.19	0 100 100	75, 100, 146, 156	0
10	J	196/201 (97%)	-0.41	0 100 100	58, 75, 104, 124	0
10	X	196/201 (97%)	-0.42	0 100 100	53, 70, 99, 132	0
10	l	196/201 (97%)	-0.35	0 100 100	66, 92, 122, 146	0
10	z	196/201 (97%)	-0.35	0 100 100	70, 95, 130, 158	0
11	1	201/205 (98%)	-0.38	0 100 100	60, 86, 119, 147	0
11	K	201/205 (98%)	-0.39	0 100 100	53, 70, 102, 123	0
11	Y	201/205 (98%)	-0.37	1 (0%) 87 76	59, 77, 106, 137	0
11	m	201/205 (98%)	-0.27	0 100 100	69, 95, 130, 159	0
12	2	213/213 (100%)	-0.36	0 100 100	66, 84, 110, 157	0
12	L	213/213 (100%)	-0.41	0 100 100	53, 68, 98, 146	0
12	Z	213/213 (100%)	-0.28	0 100 100	56, 84, 125, 172	0
12	n	213/213 (100%)	-0.26	0 100 100	75, 102, 138, 166	0
13	3	216/219 (98%)	-0.40	0 100 100	65, 82, 112, 153	0
13	M	216/219 (98%)	-0.39	0 100 100	54, 70, 99, 119	0
13	a	216/219 (98%)	-0.33	0 100 100	53, 75, 106, 129	0
13	o	216/219 (98%)	-0.34	0 100 100	64, 91, 122, 132	0
14	4	202/205 (98%)	-0.38	0 100 100	61, 86, 125, 159	0
14	N	202/205 (98%)	-0.39	0 100 100	47, 74, 112, 157	0
14	b	202/205 (98%)	-0.40	0 100 100	55, 69, 113, 160	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
14	p	202/205 (98%)	-0.30	0 100 100	68, 89, 139, 164	0
All	All	12524/12920 (96%)	-0.30	15 (0%) 92 89	47, 93, 150, 204	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	40	ALA	2.9
5	u	151	ALA	2.8
1	O	233	ALA	2.7
5	S	158	ALA	2.6
3	C	46	GLU	2.5
1	q	1	ALA	2.3
1	A	233	ALA	2.3
2	d	245	ALA	2.2
1	O	1	ALA	2.2
6	h	216	VAL	2.2
3	C	47	LYS	2.1
1	O	232	ILE	2.1
9	W	124	ASP	2.0
11	Y	115	ASP	2.0
4	t	241	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.