



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:24 AM GMT

PDB ID : 3UNH
Title : Mouse 20S immunoproteasome
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 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/ValidationPDFNotes.html>

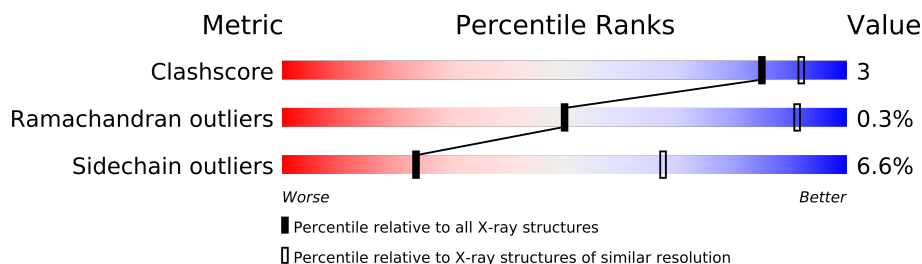
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 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))
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	234	
1	O	234	
2	B	261	
2	P	261	
3	C	248	
3	Q	248	
4	D	241	
4	R	241	
5	E	263	
5	S	263	
6	F	255	
6	T	255	
7	G	246	
7	U	246	
8	H	234	
8	V	234	
9	I	205	

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Mol	Chain	Length	Quality of chain
9	W	205	
10	J	201	
10	X	201	
11	K	204	
11	Y	204	
12	L	213	
12	Z	213	
13	M	219	
13	a	219	
14	N	199	
14	b	199	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 49084 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	0	0
			1801	1150	308	337	6			
1	O	230	Total	C	N	O	S	0	0	0
			1801	1150	308	337	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			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	238	Total	C	N	O	S	0	0	0
			1876	1179	331	361	5			
3	Q	238	Total	C	N	O	S	0	0	0
			1876	1179	331	361	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
			1777	1116	294	356	11			
4	R	233	Total	C	N	O	S	0	0	0
			1777	1116	294	356	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			

- 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			

- 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			

- Molecule 8 is a protein called Proteasome subunit beta type-10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	219	Total	C	N	O	S	0	0	0
			1619	1010	294	307	8			
8	V	219	Total	C	N	O	S	0	0	0
			1619	1010	294	307	8			

- 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
			1591	1013	265	294	19			
9	W	204	Total	C	N	O	S	0	0	0
			1591	1013	265	294	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			

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

- Molecule 11 is a protein called Proteasome subunit beta type-8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	201	Total	C	N	O	S	0	0	0
			1566	981	268	302	15			
11	Y	201	Total	C	N	O	S	0	0	0
			1566	981	268	302	15			

- 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
			1653	1047	284	312	10			
12	Z	213	Total	C	N	O	S	0	0	0
			1653	1047	284	312	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			

- Molecule 14 is a protein called Proteasome subunit beta type-9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	199	Total	C	N	O	S	0	0	0
			1498	947	254	289	8			
14	b	199	Total	C	N	O	S	0	0	0
			1498	947	254	289	8			

- Molecule 15 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	K	1	Total	I	0	0
			1	1		
15	E	1	Total	I	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	H	1	Total I 1 1	0	0
15	b	2	Total I 2 2	0	0
15	I	1	Total I 1 1	0	0
15	C	1	Total I 1 1	0	0
15	V	1	Total I 1 1	0	0
15	W	1	Total I 1 1	0	0
15	A	1	Total I 1 1	0	0
15	N	2	Total I 2 2	0	0
15	O	1	Total I 1 1	0	0
15	Y	1	Total I 1 1	0	0

- Molecule 16 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	P	1	Total Cl 1 1	0	0
16	G	1	Total Cl 1 1	0	0
16	Q	2	Total Cl 2 2	0	0
16	D	1	Total Cl 1 1	0	0
16	K	1	Total Cl 1 1	0	0
16	a	2	Total Cl 2 2	0	0
16	E	1	Total Cl 1 1	0	0
16	H	1	Total Cl 1 1	0	0
16	B	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	b	1	Total 1	Cl 1	0	0
16	V	2	Total 2	Cl 2	0	0
16	Z	1	Total 1	Cl 1	0	0
16	A	1	Total 1	Cl 1	0	0
16	N	2	Total 2	Cl 2	0	0
16	U	1	Total 1	Cl 1	0	0
16	R	1	Total 1	Cl 1	0	0
16	L	1	Total 1	Cl 1	0	0
16	S	1	Total 1	Cl 1	0	0
16	M	1	Total 1	Cl 1	0	0

- Molecule 17 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	D	1	Total 1	K 1	0	0
17	K	1	Total 1	K 1	0	0
17	E	1	Total 1	K 1	0	0
17	H	1	Total 1	K 1	0	0
17	b	1	Total 1	K 1	0	0
17	C	1	Total 1	K 1	0	0
17	T	1	Total 1	K 1	0	0
17	Y	1	Total 1	K 1	0	0
17	S	1	Total 1	K 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	F	1	Total K 1 1	0	0

- Molecule 18 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	20	Total O 20 20	0	0
18	B	18	Total O 18 18	0	0
18	C	24	Total O 24 24	0	0
18	D	16	Total O 16 16	0	0
18	E	22	Total O 22 22	0	0
18	F	17	Total O 17 17	0	0
18	G	23	Total O 23 23	0	0
18	H	18	Total O 18 18	0	0
18	I	18	Total O 18 18	0	0
18	J	14	Total O 14 14	0	0
18	K	14	Total O 14 14	0	0
18	L	22	Total O 22 22	0	0
18	M	24	Total O 24 24	0	0
18	N	18	Total O 18 18	0	0
18	O	10	Total O 10 10	0	0
18	P	20	Total O 20 20	0	0
18	Q	21	Total O 21 21	0	0
18	R	17	Total O 17 17	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	S	23	Total 23	O 23	0	0
18	T	24	Total 24	O 24	0	0
18	U	15	Total 15	O 15	0	0
18	V	14	Total 14	O 14	0	0
18	W	17	Total 17	O 17	0	0
18	X	15	Total 15	O 15	0	0
18	Y	26	Total 26	O 26	0	0
18	Z	25	Total 25	O 25	0	0
18	a	21	Total 21	O 21	0	0
18	b	19	Total 19	O 19	0	0

- Molecule 4: Proteasome subunit alpha type-5

Chain D: 



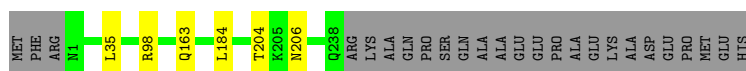
- Molecule 4: Proteasome subunit alpha type-5

Chain R: 



- Molecule 5: Proteasome subunit alpha type-1

Chain E: 



- Molecule 5: Proteasome subunit alpha type-1

Chain S: 



- Molecule 6: Proteasome subunit alpha type-3

Chain F: 



- Molecule 6: Proteasome subunit alpha type-3

Chain T: 



- Molecule 7: Proteasome subunit alpha type-6

Chain G: 



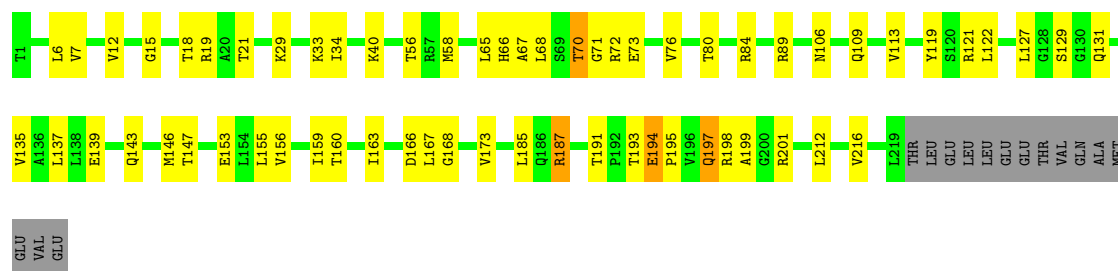
- Molecule 7: Proteasome subunit alpha type-6

Chain U: 



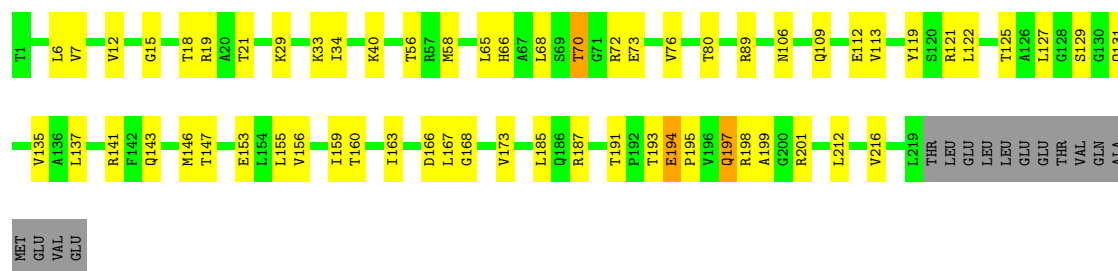
- Molecule 8: Proteasome subunit beta type-10

Chain H: 



- Molecule 8: Proteasome subunit beta type-10

Chain V: 



- Molecule 9: Proteasome subunit beta type-3

Chain I: 



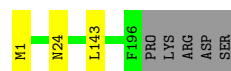
- Molecule 9: Proteasome subunit beta type-3

Chain W: 



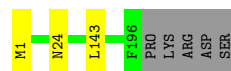
- Molecule 10: Proteasome subunit beta type-2

Chain J: 



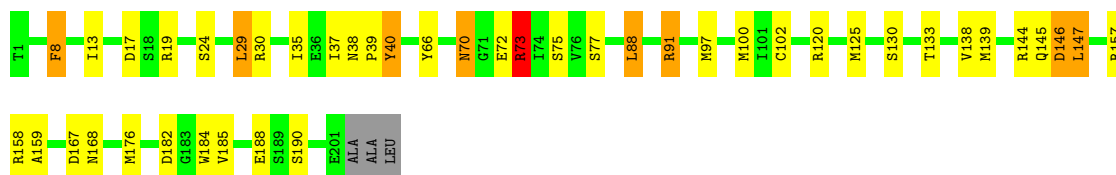
- Molecule 10: Proteasome subunit beta type-2

Chain X: 



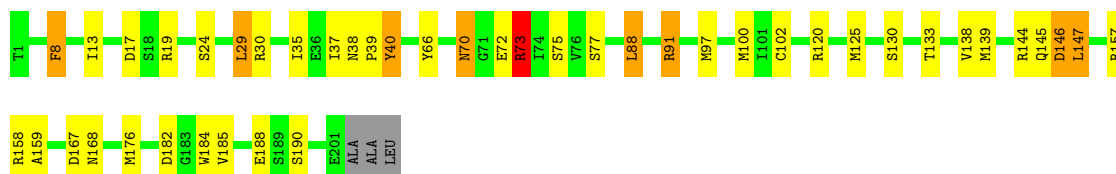
- Molecule 11: Proteasome subunit beta type-8

Chain K: 



- Molecule 11: Proteasome subunit beta type-8

Chain Y:



- Molecule 12: Proteasome subunit beta type-1

Chain L:



- Molecule 12: Proteasome subunit beta type-1

Chain Z:



- Molecule 13: Proteasome subunit beta type-4

Chain M:



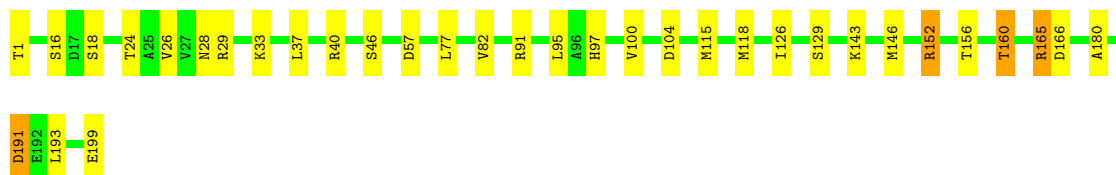
- Molecule 13: Proteasome subunit beta type-4

Chain a:



- Molecule 14: Proteasome subunit beta type-9

Chain N:



- Molecule 14: Proteasome subunit beta type-9

Chain b: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	118.28Å 205.22Å 161.94Å 90.00° 105.70° 90.00°	Depositor
Resolution (Å)	15.00 – 3.20	Depositor
% Data completeness (in resolution range)	99.2 (15.00-3.20)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.6.0119	Depositor
R, R_{free}	0.239 , 0.254	Depositor
Wilson B-factor (Å ²)	62.7	Xtriage
Anisotropy	0.646	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 121329 reflections (0.001%)	Xtriage
Total number of atoms	49084	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: K, IOD, CL

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	0.38	0/1840	0.47	0/2491
1	O	0.38	1/1840 (0.1%)	0.47	0/2491
2	B	0.37	0/1980	0.48	0/2667
2	P	0.37	0/1980	0.48	0/2667
3	C	0.33	0/1903	0.48	0/2569
3	Q	0.33	0/1903	0.48	0/2569
4	D	0.36	0/1804	0.45	0/2437
4	R	0.35	0/1804	0.45	0/2437
5	E	0.37	0/1907	0.48	0/2578
5	S	0.37	0/1907	0.48	0/2578
6	F	0.38	0/1938	0.46	0/2608
6	T	0.38	0/1938	0.46	0/2608
7	G	0.37	1/1924 (0.1%)	0.46	0/2600
7	U	0.37	1/1924 (0.1%)	0.46	0/2600
8	H	0.32	0/1645	0.53	0/2235
8	V	0.32	0/1645	0.53	0/2235
9	I	0.34	0/1620	0.48	0/2185
9	W	0.34	0/1620	0.48	0/2185
10	J	0.33	0/1602	0.47	0/2167
10	X	0.32	0/1602	0.47	0/2167
11	K	0.40	0/1597	0.51	0/2151
11	Y	0.40	0/1597	0.50	0/2151
12	L	0.32	0/1684	0.46	0/2271
12	Z	0.32	0/1684	0.46	0/2271
13	M	0.40	0/1718	0.48	0/2325
13	a	0.40	1/1718 (0.1%)	0.48	0/2325
14	N	0.35	0/1526	0.50	0/2071
14	b	0.35	0/1526	0.50	0/2071
All	All	0.36	4/49376 (0.0%)	0.48	0/66710

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	138	TRP	CD2-CE2	5.08	1.47	1.41
13	a	209	TRP	CD2-CE2	5.06	1.47	1.41
7	G	188	TRP	CD2-CE2	5.05	1.47	1.41
7	U	100	TRP	CD2-CE2	5.02	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1801	0	0	1	0
1	O	1801	0	0	1	0
2	B	1950	0	0	1	0
2	P	1950	0	0	0	0
3	C	1876	0	0	0	0
3	Q	1876	0	0	1	0
4	D	1777	0	0	0	0
4	R	1777	0	0	0	0
5	E	1872	0	0	0	0
5	S	1872	0	0	1	0
6	F	1903	0	0	2	0
6	T	1903	0	0	2	0
7	G	1890	0	0	2	0
7	U	1890	0	0	3	0
8	H	1619	0	0	24	0
8	V	1619	0	0	22	0
9	I	1591	0	0	2	0
9	W	1591	0	0	2	0
10	J	1570	0	0	0	0
10	X	1570	0	0	0	0
11	K	1566	0	0	20	0
11	Y	1566	0	0	21	0
12	L	1653	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	Z	1653	0	0	6	0
13	M	1685	0	0	3	0
13	a	1685	0	0	0	0
14	N	1498	0	0	12	0
14	b	1498	0	0	0	0
15	A	1	0	0	0	0
15	C	1	0	0	0	0
15	E	1	0	0	0	0
15	H	1	0	0	0	0
15	I	1	0	0	0	0
15	K	1	0	0	0	0
15	N	2	0	0	0	0
15	O	1	0	0	0	0
15	V	1	0	0	0	0
15	W	1	0	0	0	0
15	Y	1	0	0	0	0
15	b	2	0	0	0	0
16	A	1	0	0	0	0
16	B	1	0	0	0	0
16	D	1	0	0	0	0
16	E	1	0	0	0	0
16	G	1	0	0	1	0
16	H	1	0	0	0	0
16	K	1	0	0	0	0
16	L	1	0	0	0	0
16	M	1	0	0	0	0
16	N	2	0	0	0	0
16	P	1	0	0	0	0
16	Q	2	0	0	0	0
16	R	1	0	0	0	0
16	S	1	0	0	0	0
16	U	1	0	0	1	0
16	V	2	0	0	0	0
16	Z	1	0	0	0	0
16	a	2	0	0	0	0
16	b	1	0	0	0	0
17	C	1	0	0	0	0
17	D	1	0	0	0	0
17	E	1	0	0	0	0
17	F	1	0	0	0	0
17	H	1	0	0	0	0
17	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	S	1	0	0	0	0
17	T	1	0	0	0	0
17	Y	1	0	0	0	0
17	b	1	0	0	0	0
18	A	20	0	0	0	0
18	B	18	0	0	0	0
18	C	24	0	0	0	0
18	D	16	0	0	0	0
18	E	22	0	0	0	0
18	F	17	0	0	0	0
18	G	23	0	0	0	0
18	H	18	0	0	1	0
18	I	18	0	0	0	0
18	J	14	0	0	0	0
18	K	14	0	0	0	0
18	L	22	0	0	0	0
18	M	24	0	0	1	0
18	N	18	0	0	0	0
18	O	10	0	0	0	0
18	P	20	0	0	0	0
18	Q	21	0	0	1	0
18	R	17	0	0	0	0
18	S	23	0	0	1	0
18	T	24	0	0	0	0
18	U	15	0	0	1	0
18	V	14	0	0	0	0
18	W	17	0	0	0	0
18	X	15	0	0	0	0
18	Y	26	0	0	0	0
18	Z	25	0	0	1	0
18	a	21	0	0	0	0
18	b	19	0	0	0	0
All	All	49084	0	0	112	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (112) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:199:ALA:CB	12:Z:173:ARG:CZ	2.50	0.90
12:L:173:ARG:CZ	8:V:199:ALA:CB	2.52	0.88
11:K:66:TYR:O	11:K:70:ASN:ND2	2.10	0.84

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:Y:66:TYR:O	11:Y:70:ASN:ND2	2.11	0.83
11:Y:144:ARG:O	11:Y:147:LEU:CD1	2.26	0.83
11:K:144:ARG:O	11:K:147:LEU:CD1	2.26	0.83
7:G:152:LYS:NZ	16:G:246:CL:CL	2.51	0.81
13:M:152:GLU:OE1	8:V:141:ARG:NH1	2.14	0.81
8:H:84:ARG:NH1	14:N:57:ASP:OD2	2.14	0.81
8:V:129:SER:OG	8:V:166:ASP:OD2	1.99	0.80
8:H:129:SER:OG	8:H:166:ASP:OD2	2.01	0.78
11:K:125:MET:CE	11:K:139:MET:CE	2.61	0.78
11:Y:125:MET:CE	11:Y:139:MET:CE	2.62	0.77
14:N:18:SER:OG	14:N:29:ARG:O	2.03	0.77
13:M:35:ARG:NH2	18:M:461:HOH:O	2.18	0.76
7:U:152:LYS:NZ	16:U:246:CL:CL	2.57	0.75
8:V:166:ASP:OD1	8:V:168:GLY:N	2.21	0.73
8:H:199:ALA:CB	12:Z:173:ARG:NE	2.52	0.73
8:H:166:ASP:OD1	8:H:168:GLY:N	2.22	0.72
12:L:173:ARG:NE	8:V:199:ALA:CB	2.56	0.69
8:H:139:GLU:OE2	14:N:29:ARG:NH2	2.27	0.68
11:K:130:SER:OG	11:K:167:ASP:OD2	2.14	0.66
11:Y:157:ARG:NH1	11:Y:188:GLU:OE2	2.28	0.66
11:Y:130:SER:OG	11:Y:167:ASP:OD2	2.14	0.66
11:K:157:ARG:NH1	11:K:188:GLU:OE2	2.29	0.66
8:H:66:HIS:O	8:H:70:THR:OG1	2.15	0.64
8:V:66:HIS:O	8:V:70:THR:OG1	2.16	0.64
14:N:40:ARG:NH2	14:N:180:ALA:O	2.34	0.61
8:H:199:ALA:CB	12:Z:173:ARG:CD	2.79	0.61
12:Z:66:LYS:NZ	18:Z:504:HOH:O	2.35	0.60
8:H:187:ARG:NH1	18:H:245:HOH:O	2.34	0.60
12:L:173:ARG:CD	8:V:199:ALA:CB	2.82	0.57
12:L:173:ARG:NH1	8:V:199:ALA:CB	2.67	0.57
8:H:199:ALA:CB	12:Z:173:ARG:NH1	2.67	0.57
11:K:8:PHE:N	11:K:8:PHE:CD1	2.74	0.55
11:Y:8:PHE:CD1	11:Y:8:PHE:N	2.74	0.55
14:N:152:ARG:CG	14:N:152:ARG:NH2	2.69	0.55
11:K:30:ARG:CG	11:K:30:ARG:O	2.54	0.55
11:K:37:ILE:C	11:K:38:ASN:ND2	2.61	0.54
11:Y:30:ARG:CG	11:Y:30:ARG:O	2.56	0.54
8:H:29:LYS:NZ	12:Z:184:GLU:OE1	2.41	0.54
11:K:88:LEU:O	11:K:91:ARG:CG	2.56	0.54
8:H:76:VAL:CG1	8:H:109:GLN:NE2	2.71	0.53
11:Y:88:LEU:O	11:Y:91:ARG:CG	2.57	0.53
8:V:76:VAL:CG1	8:V:109:GLN:NE2	2.71	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:39:ALA:O	1:A:41:ASN:N	2.42	0.53
11:Y:37:ILE:C	11:Y:38:ASN:ND2	2.63	0.52
14:N:156:THR:O	14:N:160:THR:OG1	2.27	0.52
1:O:39:ALA:O	1:O:41:ASN:N	2.43	0.52
11:K:37:ILE:O	11:K:38:ASN:ND2	2.44	0.51
12:L:184:GLU:OE1	8:V:29:LYS:NZ	2.43	0.51
8:H:212:LEU:CD1	9:I:200:LYS:CA	2.90	0.49
11:Y:37:ILE:O	11:Y:38:ASN:ND2	2.45	0.49
5:S:147:SER:N	18:S:506:HOH:O	2.45	0.49
8:V:212:LEU:CD1	9:W:200:LYS:CA	2.91	0.49
11:K:19:ARG:NH1	11:K:168:ASN:O	2.46	0.49
8:H:15:GLY:C	8:H:159:ILE:CD1	2.81	0.48
8:V:15:GLY:C	8:V:159:ILE:CD1	2.82	0.48
11:Y:19:ARG:NH1	11:Y:168:ASN:O	2.46	0.48
14:N:191:ASP:OD1	14:N:191:ASP:N	2.47	0.48
8:H:18:THR:OG1	8:H:29:LYS:O	2.32	0.48
8:V:18:THR:OG1	8:V:29:LYS:O	2.32	0.47
14:N:129:SER:OG	14:N:166:ASP:OD2	2.33	0.47
8:V:19:ARG:O	8:V:33:LYS:NZ	2.48	0.47
14:N:1:THR:OG1	14:N:33:LYS:NZ	2.48	0.47
11:Y:72:GLU:O	11:Y:73:ARG:CB	2.62	0.47
11:K:72:GLU:O	11:K:73:ARG:CB	2.63	0.46
11:K:29:LEU:N	11:K:29:LEU:CD2	2.79	0.46
8:H:19:ARG:O	8:H:33:LYS:NZ	2.48	0.46
8:H:131:GLN:O	8:H:135:VAL:CG2	2.64	0.46
8:V:131:GLN:O	8:V:135:VAL:CG2	2.64	0.46
7:U:171:GLN:NE2	18:U:247:HOH:O	2.48	0.46
11:Y:29:LEU:N	11:Y:29:LEU:CD2	2.79	0.46
13:M:35:ARG:NH2	14:N:126:ILE:O	2.48	0.46
11:K:39:PRO:O	11:K:184:TRP:CD1	2.69	0.45
11:Y:39:PRO:O	11:Y:184:TRP:CD1	2.68	0.45
8:V:143:GLN:O	8:V:146:MET:CG	2.64	0.45
6:T:123:THR:O	7:U:131:ARG:NH1	2.50	0.45
3:Q:4:ARG:NH2	18:Q:277:HOH:O	2.48	0.45
11:K:77:SER:O	11:K:120:ARG:NH2	2.49	0.45
11:Y:77:SER:O	11:Y:120:ARG:NH2	2.50	0.45
8:H:143:GLN:O	8:H:146:MET:CG	2.64	0.45
11:K:138:VAL:CG2	11:K:159:ALA:CA	2.95	0.44
8:V:166:ASP:OD1	8:V:167:LEU:N	2.51	0.44
11:Y:138:VAL:CG2	11:Y:159:ALA:CA	2.95	0.44
8:H:166:ASP:OD1	8:H:167:LEU:N	2.51	0.44
6:T:83:ASP:OD2	6:T:129:ARG:NH2	2.51	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:F:83:ASP:OD2	6:F:129:ARG:NH2	2.51	0.43
9:W:29:ILE:O	9:W:31:ALA:N	2.52	0.43
9:I:29:ILE:O	9:I:31:ALA:N	2.52	0.42
11:Y:144:ARG:NH2	11:Y:146:ASP:O	2.53	0.42
11:Y:40:TYR:CZ	11:Y:73:ARG:CD	3.03	0.42
11:K:40:TYR:CZ	11:K:73:ARG:CD	3.02	0.42
14:N:46:SER:OG	14:N:97:HIS:O	2.37	0.42
6:F:123:THR:O	7:G:131:ARG:NH1	2.52	0.42
11:K:144:ARG:NH2	11:K:146:ASP:O	2.53	0.42
11:Y:8:PHE:C	11:Y:145:GLN:NE2	2.73	0.42
2:B:135:TYR:CD2	14:N:165:ARG:NH1	84.92	0.41
11:K:8:PHE:C	11:K:145:GLN:NE2	2.74	0.41
11:Y:70:ASN:ND2	11:Y:70:ASN:N	2.67	0.41
8:V:19:ARG:NH1	8:V:167:LEU:O	2.54	0.41
8:V:156:VAL:O	8:V:160:THR:OG1	2.38	0.41
11:K:70:ASN:ND2	11:K:70:ASN:N	2.67	0.41
8:H:156:VAL:O	8:H:160:THR:OG1	2.39	0.41
8:H:197:GLN:OE1	8:H:197:GLN:CA	2.68	0.41
11:Y:167:ASP:OD1	11:Y:168:ASN:N	2.54	0.41
8:V:197:GLN:OE1	8:V:197:GLN:CA	2.68	0.41
8:H:19:ARG:NH1	8:H:167:LEU:O	2.54	0.40
8:H:67:ALA:O	8:H:71:GLY:N	2.55	0.40
8:H:194:GLU:C	8:H:194:GLU:CD	2.80	0.40
8:V:112:GLU:OE2	8:V:125:THR:OG1	2.39	0.40
8:V:194:GLU:C	8:V:194:GLU:CD	2.80	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	228/234 (97%)	219 (96%)	8 (4%)	1 (0%)	43	88
1	O	228/234 (97%)	220 (96%)	7 (3%)	1 (0%)	43	88
2	B	246/261 (94%)	241 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P	246/261 (94%)	241 (98%)	5 (2%)	0	100	100
3	C	236/248 (95%)	227 (96%)	9 (4%)	0	100	100
3	Q	236/248 (95%)	227 (96%)	9 (4%)	0	100	100
4	D	231/241 (96%)	221 (96%)	9 (4%)	1 (0%)	43	88
4	R	231/241 (96%)	221 (96%)	9 (4%)	1 (0%)	43	88
5	E	236/263 (90%)	228 (97%)	8 (3%)	0	100	100
5	S	236/263 (90%)	228 (97%)	8 (3%)	0	100	100
6	F	242/255 (95%)	236 (98%)	5 (2%)	1 (0%)	43	88
6	T	242/255 (95%)	236 (98%)	5 (2%)	1 (0%)	43	88
7	G	241/246 (98%)	235 (98%)	6 (2%)	0	100	100
7	U	241/246 (98%)	235 (98%)	6 (2%)	0	100	100
8	H	217/234 (93%)	213 (98%)	3 (1%)	1 (0%)	38	85
8	V	217/234 (93%)	213 (98%)	3 (1%)	1 (0%)	38	85
9	I	202/205 (98%)	192 (95%)	8 (4%)	2 (1%)	22	74
9	W	202/205 (98%)	192 (95%)	8 (4%)	2 (1%)	22	74
10	J	194/201 (96%)	188 (97%)	5 (3%)	1 (0%)	38	85
10	X	194/201 (96%)	188 (97%)	5 (3%)	1 (0%)	38	85
11	K	199/204 (98%)	194 (98%)	4 (2%)	1 (0%)	38	85
11	Y	199/204 (98%)	194 (98%)	4 (2%)	1 (0%)	38	85
12	L	211/213 (99%)	206 (98%)	4 (2%)	1 (0%)	38	85
12	Z	211/213 (99%)	206 (98%)	4 (2%)	1 (0%)	38	85
13	M	214/219 (98%)	205 (96%)	9 (4%)	0	100	100
13	a	214/219 (98%)	205 (96%)	9 (4%)	0	100	100
14	N	197/199 (99%)	194 (98%)	3 (2%)	0	100	100
14	b	197/199 (99%)	194 (98%)	3 (2%)	0	100	100
All	All	6188/6446 (96%)	5999 (97%)	171 (3%)	18 (0%)	50	91

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	216	VAL
8	H	195	PRO
9	I	30	GLN

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Mol	Chain	Res	Type
10	J	24	ASN
6	T	216	VAL
8	V	195	PRO
9	W	30	GLN
10	X	24	ASN
1	A	40	ALA
9	I	116	PHE
1	O	40	ALA
9	W	116	PHE
4	D	112	ALA
11	K	73	ARG
11	Y	73	ARG
12	L	191	ASP
4	R	112	ALA
12	Z	191	ASP

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%)	182 (96%)	7 (4%)	45	85
1	O	189/191 (99%)	182 (96%)	7 (4%)	45	85
2	B	208/221 (94%)	194 (93%)	14 (7%)	23	66
2	P	208/221 (94%)	193 (93%)	15 (7%)	21	63
3	C	202/211 (96%)	188 (93%)	14 (7%)	22	65
3	Q	202/211 (96%)	188 (93%)	14 (7%)	22	65
4	D	195/203 (96%)	191 (98%)	4 (2%)	66	92
4	R	195/203 (96%)	190 (97%)	5 (3%)	59	90
5	E	204/224 (91%)	198 (97%)	6 (3%)	55	88
5	S	204/224 (91%)	198 (97%)	6 (3%)	55	88
6	F	200/211 (95%)	192 (96%)	8 (4%)	42	83
6	T	200/211 (95%)	192 (96%)	8 (4%)	42	83
7	G	207/210 (99%)	200 (97%)	7 (3%)	49	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	U	207/210 (99%)	200 (97%)	7 (3%)	49	86
8	H	169/183 (92%)	133 (79%)	36 (21%)	1	7
8	V	169/183 (92%)	133 (79%)	36 (21%)	1	7
9	I	174/175 (99%)	162 (93%)	12 (7%)	22	65
9	W	174/175 (99%)	162 (93%)	12 (7%)	22	65
10	J	166/171 (97%)	164 (99%)	2 (1%)	82	96
10	X	166/171 (97%)	164 (99%)	2 (1%)	82	96
11	K	165/166 (99%)	142 (86%)	23 (14%)	5	24
11	Y	165/166 (99%)	142 (86%)	23 (14%)	5	24
12	L	178/178 (100%)	173 (97%)	5 (3%)	56	89
12	Z	178/178 (100%)	173 (97%)	5 (3%)	56	89
13	M	178/180 (99%)	167 (94%)	11 (6%)	26	70
13	a	178/180 (99%)	167 (94%)	11 (6%)	26	70
14	N	155/155 (100%)	134 (86%)	21 (14%)	6	26
14	b	155/155 (100%)	134 (86%)	21 (14%)	6	26
All	All	5180/5358 (97%)	4838 (93%)	342 (7%)	24	67

All (342) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	3	ARG
1	A	19	VAL
1	A	28	VAL
1	A	67	ILE
1	A	83	ARG
1	A	201	GLN
2	B	43	LEU
2	B	49	ARG
2	B	51	ILE
2	B	75	VAL
2	B	97	LEU
2	B	163	ILE
2	B	177	ASP
2	B	179	LYS
2	B	184	THR
2	B	191	LEU

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Mol	Chain	Res	Type
2	B	217	ARG
2	B	234	GLN
2	B	240	GLU
2	B	243	GLU
3	C	4	ARG
3	C	39	ILE
3	C	46	LYS
3	C	56	ARG
3	C	76	THR
3	C	124	ARG
3	C	138	ASP
3	C	145	GLN
3	C	162	ARG
3	C	177	ASP
3	C	195	LEU
3	C	220	ASN
3	C	223	GLU
3	C	236	GLU
4	D	140	GLU
4	D	162	ILE
4	D	201	LYS
4	D	228	GLU
5	E	35	LEU
5	E	98	ARG
5	E	163	GLN
5	E	184	LEU
5	E	204	THR
5	E	206	ASN
6	F	30	VAL
6	F	39	ILE
6	F	66	LEU
6	F	129	ARG
6	F	181	MET
6	F	205	LYS
6	F	214	SER
6	F	230	ASP
7	G	80	THR
7	G	113	LEU
7	G	140	ILE
7	G	178	LEU
7	G	209	PHE
7	G	220	THR

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Mol	Chain	Res	Type
7	G	222	GLU
8	H	6	LEU
8	H	7	VAL
8	H	12	VAL
8	H	21	THR
8	H	34	ILE
8	H	40	LYS
8	H	56	THR
8	H	58	MET
8	H	65	LEU
8	H	68	LEU
8	H	70	THR
8	H	72	ARG
8	H	73	GLU
8	H	80	THR
8	H	89	ARG
8	H	106	ASN
8	H	113	VAL
8	H	119	TYR
8	H	121	ARG
8	H	122	LEU
8	H	127	LEU
8	H	137	LEU
8	H	147	THR
8	H	153	GLU
8	H	155	LEU
8	H	163	ILE
8	H	173	VAL
8	H	185	LEU
8	H	187	ARG
8	H	191	THR
8	H	193	THR
8	H	194	GLU
8	H	197	GLN
8	H	198	ARG
8	H	201	ARG
8	H	216	VAL
9	I	21	ILE
9	I	33	MET
9	I	84	TYR
9	I	108	ILE
9	I	115	THR

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Mol	Chain	Res	Type
9	I	116	PHE
9	I	120	ILE
9	I	131	VAL
9	I	144	GLN
9	I	166	ILE
9	I	171	LEU
9	I	192	ASP
10	J	1	MET
10	J	143	LEU
11	K	8	PHE
11	K	13	ILE
11	K	17	ASP
11	K	24	SER
11	K	29	LEU
11	K	35	ILE
11	K	40	TYR
11	K	70	ASN
11	K	73	ARG
11	K	75	SER
11	K	88	LEU
11	K	91	ARG
11	K	97	MET
11	K	100	MET
11	K	102	CYS
11	K	133	THR
11	K	146	ASP
11	K	147	LEU
11	K	158	ARG
11	K	176	MET
11	K	182	ASP
11	K	185	VAL
11	K	190	SER
12	L	31	GLU
12	L	133	ASP
12	L	162	GLU
12	L	166	LEU
12	L	173	ARG
13	M	3	ASN
13	M	35	ARG
13	M	39	ILE
13	M	44	ARG
13	M	46	ASN

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Mol	Chain	Res	Type
13	M	49	THR
13	M	94	ARG
13	M	100	ARG
13	M	109	THR
13	M	152	GLU
13	M	168	LEU
14	N	16	SER
14	N	24	THR
14	N	26	VAL
14	N	28	ASN
14	N	37	LEU
14	N	77	LEU
14	N	82	VAL
14	N	91	ARG
14	N	95	LEU
14	N	100	VAL
14	N	104	ASP
14	N	115	MET
14	N	118	MET
14	N	143	LYS
14	N	146	MET
14	N	152	ARG
14	N	160	THR
14	N	165	ARG
14	N	191	ASP
14	N	193	LEU
14	N	199	GLU
1	O	2	LYS
1	O	3	ARG
1	O	19	VAL
1	O	28	VAL
1	O	67	ILE
1	O	83	ARG
1	O	201	GLN
2	P	43	LEU
2	P	49	ARG
2	P	51	ILE
2	P	75	VAL
2	P	97	LEU
2	P	116	ILE
2	P	163	ILE
2	P	177	ASP

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Mol	Chain	Res	Type
2	P	179	LYS
2	P	184	THR
2	P	191	LEU
2	P	217	ARG
2	P	234	GLN
2	P	240	GLU
2	P	243	GLU
3	Q	4	ARG
3	Q	39	ILE
3	Q	46	LYS
3	Q	56	ARG
3	Q	76	THR
3	Q	124	ARG
3	Q	138	ASP
3	Q	145	GLN
3	Q	162	ARG
3	Q	177	ASP
3	Q	195	LEU
3	Q	220	ASN
3	Q	223	GLU
3	Q	236	GLU
4	R	140	GLU
4	R	162	ILE
4	R	201	LYS
4	R	207	ILE
4	R	228	GLU
5	S	35	LEU
5	S	98	ARG
5	S	163	GLN
5	S	184	LEU
5	S	204	THR
5	S	206	ASN
6	T	30	VAL
6	T	39	ILE
6	T	66	LEU
6	T	129	ARG
6	T	181	MET
6	T	205	LYS
6	T	214	SER
6	T	230	ASP
7	U	80	THR
7	U	113	LEU

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Mol	Chain	Res	Type
7	U	140	ILE
7	U	178	LEU
7	U	209	PHE
7	U	220	THR
7	U	222	GLU
8	V	6	LEU
8	V	7	VAL
8	V	12	VAL
8	V	21	THR
8	V	34	ILE
8	V	40	LYS
8	V	56	THR
8	V	58	MET
8	V	65	LEU
8	V	68	LEU
8	V	70	THR
8	V	72	ARG
8	V	73	GLU
8	V	80	THR
8	V	89	ARG
8	V	106	ASN
8	V	113	VAL
8	V	119	TYR
8	V	121	ARG
8	V	122	LEU
8	V	127	LEU
8	V	137	LEU
8	V	147	THR
8	V	153	GLU
8	V	155	LEU
8	V	163	ILE
8	V	173	VAL
8	V	185	LEU
8	V	187	ARG
8	V	191	THR
8	V	193	THR
8	V	194	GLU
8	V	197	GLN
8	V	198	ARG
8	V	201	ARG
8	V	216	VAL
9	W	21	ILE

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Mol	Chain	Res	Type
9	W	33	MET
9	W	84	TYR
9	W	108	ILE
9	W	115	THR
9	W	116	PHE
9	W	120	ILE
9	W	131	VAL
9	W	144	GLN
9	W	166	ILE
9	W	171	LEU
9	W	192	ASP
10	X	1	MET
10	X	143	LEU
11	Y	8	PHE
11	Y	13	ILE
11	Y	17	ASP
11	Y	24	SER
11	Y	29	LEU
11	Y	35	ILE
11	Y	40	TYR
11	Y	70	ASN
11	Y	73	ARG
11	Y	75	SER
11	Y	88	LEU
11	Y	91	ARG
11	Y	97	MET
11	Y	100	MET
11	Y	102	CYS
11	Y	133	THR
11	Y	146	ASP
11	Y	147	LEU
11	Y	158	ARG
11	Y	176	MET
11	Y	182	ASP
11	Y	185	VAL
11	Y	190	SER
12	Z	31	GLU
12	Z	133	ASP
12	Z	162	GLU
12	Z	166	LEU
12	Z	173	ARG
13	a	3	ASN

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Mol	Chain	Res	Type
13	a	35	ARG
13	a	39	ILE
13	a	44	ARG
13	a	46	ASN
13	a	49	THR
13	a	94	ARG
13	a	100	ARG
13	a	109	THR
13	a	152	GLU
13	a	168	LEU
14	b	16	SER
14	b	24	THR
14	b	26	VAL
14	b	28	ASN
14	b	37	LEU
14	b	77	LEU
14	b	82	VAL
14	b	91	ARG
14	b	95	LEU
14	b	100	VAL
14	b	104	ASP
14	b	115	MET
14	b	118	MET
14	b	143	LYS
14	b	146	MET
14	b	152	ARG
14	b	160	THR
14	b	165	ARG
14	b	191	ASP
14	b	193	LEU
14	b	199	GLU

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

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 47 ligands modelled in this entry, 47 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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