



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:04 AM UTC

PDB ID : 5NYW / pdb_00005nyw
Title : Anbu (ancestral beta-subunit) from Yersinia bercovieri
Authors : Piasecka, A.; Czapinska, H.; Vielberg, M.; Szczepanowski, R.H.; Reed, S.; Groll, M.; Bochtler, M.
Deposited on : 2017-05-12
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

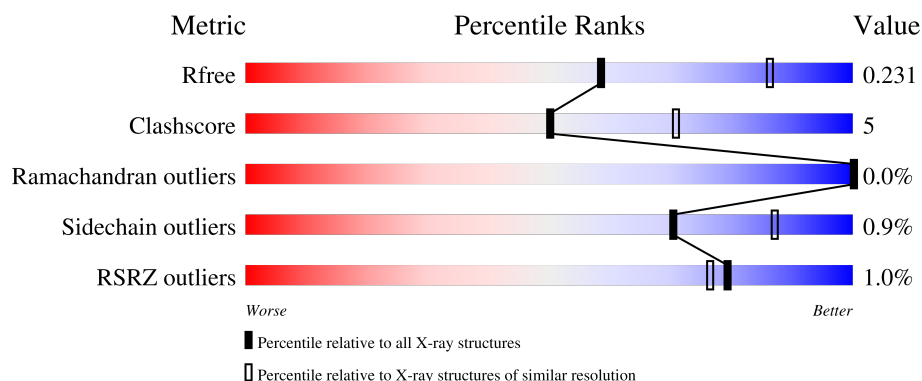
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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.



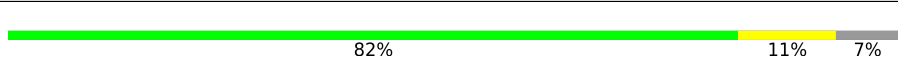
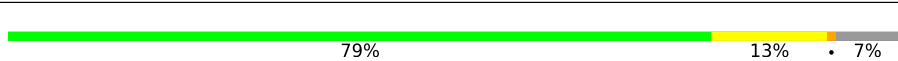
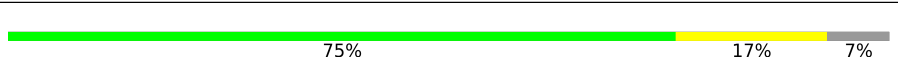
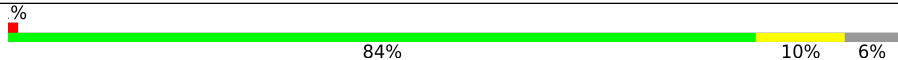
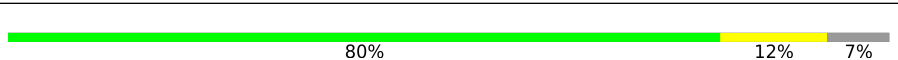
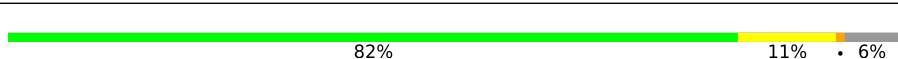
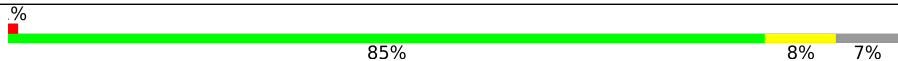
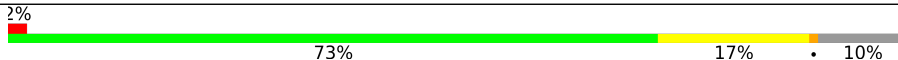
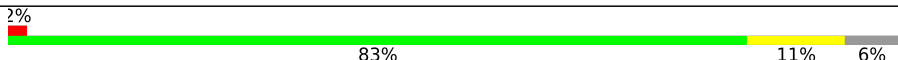
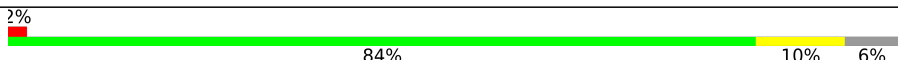
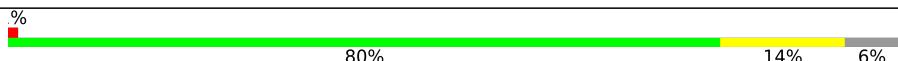
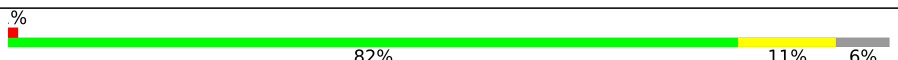
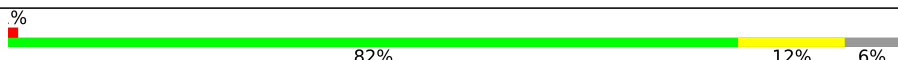
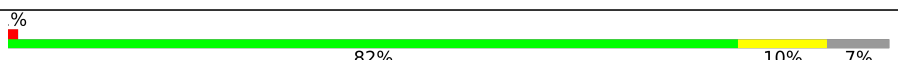
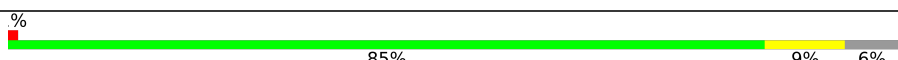
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	1	251	
1	2	251	
1	A	251	
1	B	251	
1	C	251	

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Mol	Chain	Length	Quality of chain
1	D	251	
1	E	251	
1	F	251	
1	G	251	
1	H	251	
1	I	251	
1	J	251	
1	K	251	
1	L	251	
1	M	251	
1	N	251	
1	O	251	
1	P	251	
1	Q	251	
1	R	251	
1	S	251	
1	T	251	
1	U	251	
1	V	251	
1	W	251	
1	X	251	
1	Y	251	
1	Z	251	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	2	301	-	-	X	-
2	SO4	X	302	-	-	X	-
3	EDO	F	301	-	-	X	-
4	CL	T	301	-	-	X	-
5	UNX	Q	302	-	-	-	X
5	UNX	Q	303	-	-	-	X
6	AZI	J	301	-	X	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 52945 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 Peptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	2	0
			1781	1125	304	339	13			
1	B	233	Total	C	N	O	S	0	0	0
			1821	1150	311	348	12			
1	C	236	Total	C	N	O	S	0	0	0
			1836	1158	314	352	12			
1	D	234	Total	C	N	O	S	0	0	0
			1828	1154	312	350	12			
1	E	233	Total	C	N	O	S	0	0	0
			1824	1152	311	349	12			
1	F	234	Total	C	N	O	S	0	0	0
			1828	1154	312	350	12			
1	G	234	Total	C	N	O	S	0	0	0
			1828	1154	312	350	12			
1	H	234	Total	C	N	O	S	0	0	0
			1828	1154	312	350	12			
1	I	233	Total	C	N	O	S	0	0	0
			1821	1150	311	348	12			
1	J	235	Total	C	N	O	S	0	0	0
			1832	1156	313	351	12			
1	K	233	Total	C	N	O	S	0	0	0
			1824	1152	311	349	12			
1	L	237	Total	C	N	O	S	0	0	0
			1847	1164	318	353	12			
1	M	233	Total	C	N	O	S	0	0	0
			1821	1150	311	348	12			
1	N	226	Total	C	N	O	S	0	0	0
			1774	1122	302	338	12			
1	O	225	Total	C	N	O	S	0	0	0
			1764	1117	300	335	12			
1	P	234	Total	C	N	O	S	0	1	0
			1839	1160	316	351	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	237	Total	C	N	O	S	0	0	0
			1853	1168	320	353	12			
1	R	236	Total	C	N	O	S	0	1	0
			1854	1168	321	353	12			
1	S	235	Total	C	N	O	S	0	0	0
			1832	1156	313	351	12			
1	T	235	Total	C	N	O	S	0	0	0
			1832	1156	313	351	12			
1	U	235	Total	C	N	O	S	0	0	0
			1832	1156	313	351	12			
1	V	234	Total	C	N	O	S	0	0	0
			1828	1154	312	350	12			
1	W	233	Total	C	N	O	S	0	0	0
			1824	1152	311	349	12			
1	X	236	Total	C	N	O	S	0	0	0
			1836	1158	314	352	12			
1	Y	233	Total	C	N	O	S	0	1	0
			1830	1155	313	350	12			
1	Z	236	Total	C	N	O	S	0	0	0
			1836	1158	314	352	12			
1	1	234	Total	C	N	O	S	0	0	0
			1825	1152	312	349	12			
1	2	220	Total	C	N	O	S	0	0	0
			1730	1095	295	328	12			

There are 308 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	ALA	VAL	conflict	UNP A0A2G4U6U6
A	106	HIS	GLY	conflict	UNP A0A2G4U6U6
A	112	CYS	GLY	conflict	UNP A0A2G4U6U6
A	244	LEU	-	expression tag	UNP A0A2G4U6U6
A	245	GLU	-	expression tag	UNP A0A2G4U6U6
A	246	HIS	-	expression tag	UNP A0A2G4U6U6
A	247	HIS	-	expression tag	UNP A0A2G4U6U6
A	248	HIS	-	expression tag	UNP A0A2G4U6U6
A	249	HIS	-	expression tag	UNP A0A2G4U6U6
A	250	HIS	-	expression tag	UNP A0A2G4U6U6
A	251	HIS	-	expression tag	UNP A0A2G4U6U6
B	13	ALA	VAL	conflict	UNP A0A2G4U6U6
B	106	HIS	GLY	conflict	UNP A0A2G4U6U6
B	112	CYS	GLY	conflict	UNP A0A2G4U6U6
B	244	LEU	-	expression tag	UNP A0A2G4U6U6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	245	GLU	-	expression tag	UNP A0A2G4U6U6
B	246	HIS	-	expression tag	UNP A0A2G4U6U6
B	247	HIS	-	expression tag	UNP A0A2G4U6U6
B	248	HIS	-	expression tag	UNP A0A2G4U6U6
B	249	HIS	-	expression tag	UNP A0A2G4U6U6
B	250	HIS	-	expression tag	UNP A0A2G4U6U6
B	251	HIS	-	expression tag	UNP A0A2G4U6U6
C	13	ALA	VAL	conflict	UNP A0A2G4U6U6
C	106	HIS	GLY	conflict	UNP A0A2G4U6U6
C	112	CYS	GLY	conflict	UNP A0A2G4U6U6
C	244	LEU	-	expression tag	UNP A0A2G4U6U6
C	245	GLU	-	expression tag	UNP A0A2G4U6U6
C	246	HIS	-	expression tag	UNP A0A2G4U6U6
C	247	HIS	-	expression tag	UNP A0A2G4U6U6
C	248	HIS	-	expression tag	UNP A0A2G4U6U6
C	249	HIS	-	expression tag	UNP A0A2G4U6U6
C	250	HIS	-	expression tag	UNP A0A2G4U6U6
C	251	HIS	-	expression tag	UNP A0A2G4U6U6
D	13	ALA	VAL	conflict	UNP A0A2G4U6U6
D	106	HIS	GLY	conflict	UNP A0A2G4U6U6
D	112	CYS	GLY	conflict	UNP A0A2G4U6U6
D	244	LEU	-	expression tag	UNP A0A2G4U6U6
D	245	GLU	-	expression tag	UNP A0A2G4U6U6
D	246	HIS	-	expression tag	UNP A0A2G4U6U6
D	247	HIS	-	expression tag	UNP A0A2G4U6U6
D	248	HIS	-	expression tag	UNP A0A2G4U6U6
D	249	HIS	-	expression tag	UNP A0A2G4U6U6
D	250	HIS	-	expression tag	UNP A0A2G4U6U6
D	251	HIS	-	expression tag	UNP A0A2G4U6U6
E	13	ALA	VAL	conflict	UNP A0A2G4U6U6
E	106	HIS	GLY	conflict	UNP A0A2G4U6U6
E	112	CYS	GLY	conflict	UNP A0A2G4U6U6
E	244	LEU	-	expression tag	UNP A0A2G4U6U6
E	245	GLU	-	expression tag	UNP A0A2G4U6U6
E	246	HIS	-	expression tag	UNP A0A2G4U6U6
E	247	HIS	-	expression tag	UNP A0A2G4U6U6
E	248	HIS	-	expression tag	UNP A0A2G4U6U6
E	249	HIS	-	expression tag	UNP A0A2G4U6U6
E	250	HIS	-	expression tag	UNP A0A2G4U6U6
E	251	HIS	-	expression tag	UNP A0A2G4U6U6
F	13	ALA	VAL	conflict	UNP A0A2G4U6U6
F	106	HIS	GLY	conflict	UNP A0A2G4U6U6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	112	CYS	GLY	conflict	UNP A0A2G4U6U6
F	244	LEU	-	expression tag	UNP A0A2G4U6U6
F	245	GLU	-	expression tag	UNP A0A2G4U6U6
F	246	HIS	-	expression tag	UNP A0A2G4U6U6
F	247	HIS	-	expression tag	UNP A0A2G4U6U6
F	248	HIS	-	expression tag	UNP A0A2G4U6U6
F	249	HIS	-	expression tag	UNP A0A2G4U6U6
F	250	HIS	-	expression tag	UNP A0A2G4U6U6
F	251	HIS	-	expression tag	UNP A0A2G4U6U6
G	13	ALA	VAL	conflict	UNP A0A2G4U6U6
G	106	HIS	GLY	conflict	UNP A0A2G4U6U6
G	112	CYS	GLY	conflict	UNP A0A2G4U6U6
G	244	LEU	-	expression tag	UNP A0A2G4U6U6
G	245	GLU	-	expression tag	UNP A0A2G4U6U6
G	246	HIS	-	expression tag	UNP A0A2G4U6U6
G	247	HIS	-	expression tag	UNP A0A2G4U6U6
G	248	HIS	-	expression tag	UNP A0A2G4U6U6
G	249	HIS	-	expression tag	UNP A0A2G4U6U6
G	250	HIS	-	expression tag	UNP A0A2G4U6U6
G	251	HIS	-	expression tag	UNP A0A2G4U6U6
H	13	ALA	VAL	conflict	UNP A0A2G4U6U6
H	106	HIS	GLY	conflict	UNP A0A2G4U6U6
H	112	CYS	GLY	conflict	UNP A0A2G4U6U6
H	244	LEU	-	expression tag	UNP A0A2G4U6U6
H	245	GLU	-	expression tag	UNP A0A2G4U6U6
H	246	HIS	-	expression tag	UNP A0A2G4U6U6
H	247	HIS	-	expression tag	UNP A0A2G4U6U6
H	248	HIS	-	expression tag	UNP A0A2G4U6U6
H	249	HIS	-	expression tag	UNP A0A2G4U6U6
H	250	HIS	-	expression tag	UNP A0A2G4U6U6
H	251	HIS	-	expression tag	UNP A0A2G4U6U6
I	13	ALA	VAL	conflict	UNP A0A2G4U6U6
I	106	HIS	GLY	conflict	UNP A0A2G4U6U6
I	112	CYS	GLY	conflict	UNP A0A2G4U6U6
I	244	LEU	-	expression tag	UNP A0A2G4U6U6
I	245	GLU	-	expression tag	UNP A0A2G4U6U6
I	246	HIS	-	expression tag	UNP A0A2G4U6U6
I	247	HIS	-	expression tag	UNP A0A2G4U6U6
I	248	HIS	-	expression tag	UNP A0A2G4U6U6
I	249	HIS	-	expression tag	UNP A0A2G4U6U6
I	250	HIS	-	expression tag	UNP A0A2G4U6U6
I	251	HIS	-	expression tag	UNP A0A2G4U6U6

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Chain	Residue	Modelled	Actual	Comment	Reference
J	13	ALA	VAL	conflict	UNP A0A2G4U6U6
J	106	HIS	GLY	conflict	UNP A0A2G4U6U6
J	112	CYS	GLY	conflict	UNP A0A2G4U6U6
J	244	LEU	-	expression tag	UNP A0A2G4U6U6
J	245	GLU	-	expression tag	UNP A0A2G4U6U6
J	246	HIS	-	expression tag	UNP A0A2G4U6U6
J	247	HIS	-	expression tag	UNP A0A2G4U6U6
J	248	HIS	-	expression tag	UNP A0A2G4U6U6
J	249	HIS	-	expression tag	UNP A0A2G4U6U6
J	250	HIS	-	expression tag	UNP A0A2G4U6U6
J	251	HIS	-	expression tag	UNP A0A2G4U6U6
K	13	ALA	VAL	conflict	UNP A0A2G4U6U6
K	106	HIS	GLY	conflict	UNP A0A2G4U6U6
K	112	CYS	GLY	conflict	UNP A0A2G4U6U6
K	244	LEU	-	expression tag	UNP A0A2G4U6U6
K	245	GLU	-	expression tag	UNP A0A2G4U6U6
K	246	HIS	-	expression tag	UNP A0A2G4U6U6
K	247	HIS	-	expression tag	UNP A0A2G4U6U6
K	248	HIS	-	expression tag	UNP A0A2G4U6U6
K	249	HIS	-	expression tag	UNP A0A2G4U6U6
K	250	HIS	-	expression tag	UNP A0A2G4U6U6
K	251	HIS	-	expression tag	UNP A0A2G4U6U6
L	13	ALA	VAL	conflict	UNP A0A2G4U6U6
L	106	HIS	GLY	conflict	UNP A0A2G4U6U6
L	112	CYS	GLY	conflict	UNP A0A2G4U6U6
L	244	LEU	-	expression tag	UNP A0A2G4U6U6
L	245	GLU	-	expression tag	UNP A0A2G4U6U6
L	246	HIS	-	expression tag	UNP A0A2G4U6U6
L	247	HIS	-	expression tag	UNP A0A2G4U6U6
L	248	HIS	-	expression tag	UNP A0A2G4U6U6
L	249	HIS	-	expression tag	UNP A0A2G4U6U6
L	250	HIS	-	expression tag	UNP A0A2G4U6U6
L	251	HIS	-	expression tag	UNP A0A2G4U6U6
M	13	ALA	VAL	conflict	UNP A0A2G4U6U6
M	106	HIS	GLY	conflict	UNP A0A2G4U6U6
M	112	CYS	GLY	conflict	UNP A0A2G4U6U6
M	244	LEU	-	expression tag	UNP A0A2G4U6U6
M	245	GLU	-	expression tag	UNP A0A2G4U6U6
M	246	HIS	-	expression tag	UNP A0A2G4U6U6
M	247	HIS	-	expression tag	UNP A0A2G4U6U6
M	248	HIS	-	expression tag	UNP A0A2G4U6U6
M	249	HIS	-	expression tag	UNP A0A2G4U6U6

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Chain	Residue	Modelled	Actual	Comment	Reference
M	250	HIS	-	expression tag	UNP A0A2G4U6U6
M	251	HIS	-	expression tag	UNP A0A2G4U6U6
N	13	ALA	VAL	conflict	UNP A0A2G4U6U6
N	106	HIS	GLY	conflict	UNP A0A2G4U6U6
N	112	CYS	GLY	conflict	UNP A0A2G4U6U6
N	244	LEU	-	expression tag	UNP A0A2G4U6U6
N	245	GLU	-	expression tag	UNP A0A2G4U6U6
N	246	HIS	-	expression tag	UNP A0A2G4U6U6
N	247	HIS	-	expression tag	UNP A0A2G4U6U6
N	248	HIS	-	expression tag	UNP A0A2G4U6U6
N	249	HIS	-	expression tag	UNP A0A2G4U6U6
N	250	HIS	-	expression tag	UNP A0A2G4U6U6
N	251	HIS	-	expression tag	UNP A0A2G4U6U6
O	13	ALA	VAL	conflict	UNP A0A2G4U6U6
O	106	HIS	GLY	conflict	UNP A0A2G4U6U6
O	112	CYS	GLY	conflict	UNP A0A2G4U6U6
O	244	LEU	-	expression tag	UNP A0A2G4U6U6
O	245	GLU	-	expression tag	UNP A0A2G4U6U6
O	246	HIS	-	expression tag	UNP A0A2G4U6U6
O	247	HIS	-	expression tag	UNP A0A2G4U6U6
O	248	HIS	-	expression tag	UNP A0A2G4U6U6
O	249	HIS	-	expression tag	UNP A0A2G4U6U6
O	250	HIS	-	expression tag	UNP A0A2G4U6U6
O	251	HIS	-	expression tag	UNP A0A2G4U6U6
P	13	ALA	VAL	conflict	UNP A0A2G4U6U6
P	106	HIS	GLY	conflict	UNP A0A2G4U6U6
P	112	CYS	GLY	conflict	UNP A0A2G4U6U6
P	244	LEU	-	expression tag	UNP A0A2G4U6U6
P	245	GLU	-	expression tag	UNP A0A2G4U6U6
P	246	HIS	-	expression tag	UNP A0A2G4U6U6
P	247	HIS	-	expression tag	UNP A0A2G4U6U6
P	248	HIS	-	expression tag	UNP A0A2G4U6U6
P	249	HIS	-	expression tag	UNP A0A2G4U6U6
P	250	HIS	-	expression tag	UNP A0A2G4U6U6
P	251	HIS	-	expression tag	UNP A0A2G4U6U6
Q	13	ALA	VAL	conflict	UNP A0A2G4U6U6
Q	106	HIS	GLY	conflict	UNP A0A2G4U6U6
Q	112	CYS	GLY	conflict	UNP A0A2G4U6U6
Q	244	LEU	-	expression tag	UNP A0A2G4U6U6
Q	245	GLU	-	expression tag	UNP A0A2G4U6U6
Q	246	HIS	-	expression tag	UNP A0A2G4U6U6
Q	247	HIS	-	expression tag	UNP A0A2G4U6U6

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	248	HIS	-	expression tag	UNP A0A2G4U6U6
Q	249	HIS	-	expression tag	UNP A0A2G4U6U6
Q	250	HIS	-	expression tag	UNP A0A2G4U6U6
Q	251	HIS	-	expression tag	UNP A0A2G4U6U6
R	13	ALA	VAL	conflict	UNP A0A2G4U6U6
R	106	HIS	GLY	conflict	UNP A0A2G4U6U6
R	112	CYS	GLY	conflict	UNP A0A2G4U6U6
R	244	LEU	-	expression tag	UNP A0A2G4U6U6
R	245	GLU	-	expression tag	UNP A0A2G4U6U6
R	246	HIS	-	expression tag	UNP A0A2G4U6U6
R	247	HIS	-	expression tag	UNP A0A2G4U6U6
R	248	HIS	-	expression tag	UNP A0A2G4U6U6
R	249	HIS	-	expression tag	UNP A0A2G4U6U6
R	250	HIS	-	expression tag	UNP A0A2G4U6U6
R	251	HIS	-	expression tag	UNP A0A2G4U6U6
S	13	ALA	VAL	conflict	UNP A0A2G4U6U6
S	106	HIS	GLY	conflict	UNP A0A2G4U6U6
S	112	CYS	GLY	conflict	UNP A0A2G4U6U6
S	244	LEU	-	expression tag	UNP A0A2G4U6U6
S	245	GLU	-	expression tag	UNP A0A2G4U6U6
S	246	HIS	-	expression tag	UNP A0A2G4U6U6
S	247	HIS	-	expression tag	UNP A0A2G4U6U6
S	248	HIS	-	expression tag	UNP A0A2G4U6U6
S	249	HIS	-	expression tag	UNP A0A2G4U6U6
S	250	HIS	-	expression tag	UNP A0A2G4U6U6
S	251	HIS	-	expression tag	UNP A0A2G4U6U6
T	13	ALA	VAL	conflict	UNP A0A2G4U6U6
T	106	HIS	GLY	conflict	UNP A0A2G4U6U6
T	112	CYS	GLY	conflict	UNP A0A2G4U6U6
T	244	LEU	-	expression tag	UNP A0A2G4U6U6
T	245	GLU	-	expression tag	UNP A0A2G4U6U6
T	246	HIS	-	expression tag	UNP A0A2G4U6U6
T	247	HIS	-	expression tag	UNP A0A2G4U6U6
T	248	HIS	-	expression tag	UNP A0A2G4U6U6
T	249	HIS	-	expression tag	UNP A0A2G4U6U6
T	250	HIS	-	expression tag	UNP A0A2G4U6U6
T	251	HIS	-	expression tag	UNP A0A2G4U6U6
U	13	ALA	VAL	conflict	UNP A0A2G4U6U6
U	106	HIS	GLY	conflict	UNP A0A2G4U6U6
U	112	CYS	GLY	conflict	UNP A0A2G4U6U6
U	244	LEU	-	expression tag	UNP A0A2G4U6U6
U	245	GLU	-	expression tag	UNP A0A2G4U6U6

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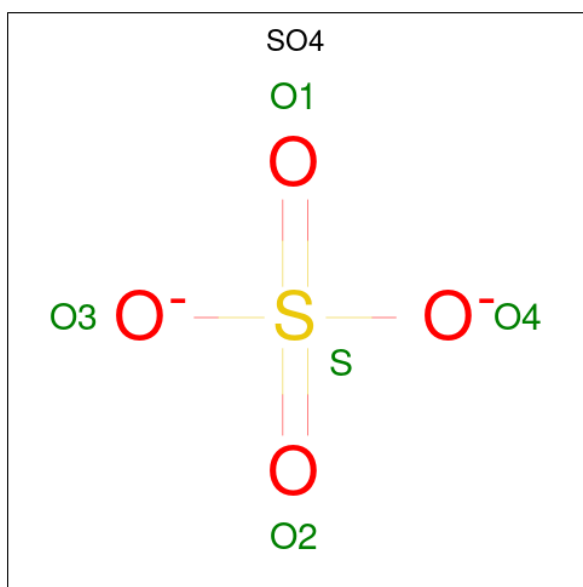
Chain	Residue	Modelled	Actual	Comment	Reference
U	246	HIS	-	expression tag	UNP A0A2G4U6U6
U	247	HIS	-	expression tag	UNP A0A2G4U6U6
U	248	HIS	-	expression tag	UNP A0A2G4U6U6
U	249	HIS	-	expression tag	UNP A0A2G4U6U6
U	250	HIS	-	expression tag	UNP A0A2G4U6U6
U	251	HIS	-	expression tag	UNP A0A2G4U6U6
V	13	ALA	VAL	conflict	UNP A0A2G4U6U6
V	106	HIS	GLY	conflict	UNP A0A2G4U6U6
V	112	CYS	GLY	conflict	UNP A0A2G4U6U6
V	244	LEU	-	expression tag	UNP A0A2G4U6U6
V	245	GLU	-	expression tag	UNP A0A2G4U6U6
V	246	HIS	-	expression tag	UNP A0A2G4U6U6
V	247	HIS	-	expression tag	UNP A0A2G4U6U6
V	248	HIS	-	expression tag	UNP A0A2G4U6U6
V	249	HIS	-	expression tag	UNP A0A2G4U6U6
V	250	HIS	-	expression tag	UNP A0A2G4U6U6
V	251	HIS	-	expression tag	UNP A0A2G4U6U6
W	13	ALA	VAL	conflict	UNP A0A2G4U6U6
W	106	HIS	GLY	conflict	UNP A0A2G4U6U6
W	112	CYS	GLY	conflict	UNP A0A2G4U6U6
W	244	LEU	-	expression tag	UNP A0A2G4U6U6
W	245	GLU	-	expression tag	UNP A0A2G4U6U6
W	246	HIS	-	expression tag	UNP A0A2G4U6U6
W	247	HIS	-	expression tag	UNP A0A2G4U6U6
W	248	HIS	-	expression tag	UNP A0A2G4U6U6
W	249	HIS	-	expression tag	UNP A0A2G4U6U6
W	250	HIS	-	expression tag	UNP A0A2G4U6U6
W	251	HIS	-	expression tag	UNP A0A2G4U6U6
X	13	ALA	VAL	conflict	UNP A0A2G4U6U6
X	106	HIS	GLY	conflict	UNP A0A2G4U6U6
X	112	CYS	GLY	conflict	UNP A0A2G4U6U6
X	244	LEU	-	expression tag	UNP A0A2G4U6U6
X	245	GLU	-	expression tag	UNP A0A2G4U6U6
X	246	HIS	-	expression tag	UNP A0A2G4U6U6
X	247	HIS	-	expression tag	UNP A0A2G4U6U6
X	248	HIS	-	expression tag	UNP A0A2G4U6U6
X	249	HIS	-	expression tag	UNP A0A2G4U6U6
X	250	HIS	-	expression tag	UNP A0A2G4U6U6
X	251	HIS	-	expression tag	UNP A0A2G4U6U6
Y	13	ALA	VAL	conflict	UNP A0A2G4U6U6
Y	106	HIS	GLY	conflict	UNP A0A2G4U6U6
Y	112	CYS	GLY	conflict	UNP A0A2G4U6U6

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	244	LEU	-	expression tag	UNP A0A2G4U6U6
Y	245	GLU	-	expression tag	UNP A0A2G4U6U6
Y	246	HIS	-	expression tag	UNP A0A2G4U6U6
Y	247	HIS	-	expression tag	UNP A0A2G4U6U6
Y	248	HIS	-	expression tag	UNP A0A2G4U6U6
Y	249	HIS	-	expression tag	UNP A0A2G4U6U6
Y	250	HIS	-	expression tag	UNP A0A2G4U6U6
Y	251	HIS	-	expression tag	UNP A0A2G4U6U6
Z	13	ALA	VAL	conflict	UNP A0A2G4U6U6
Z	106	HIS	GLY	conflict	UNP A0A2G4U6U6
Z	112	CYS	GLY	conflict	UNP A0A2G4U6U6
Z	244	LEU	-	expression tag	UNP A0A2G4U6U6
Z	245	GLU	-	expression tag	UNP A0A2G4U6U6
Z	246	HIS	-	expression tag	UNP A0A2G4U6U6
Z	247	HIS	-	expression tag	UNP A0A2G4U6U6
Z	248	HIS	-	expression tag	UNP A0A2G4U6U6
Z	249	HIS	-	expression tag	UNP A0A2G4U6U6
Z	250	HIS	-	expression tag	UNP A0A2G4U6U6
Z	251	HIS	-	expression tag	UNP A0A2G4U6U6
1	13	ALA	VAL	conflict	UNP A0A2G4U6U6
1	106	HIS	GLY	conflict	UNP A0A2G4U6U6
1	112	CYS	GLY	conflict	UNP A0A2G4U6U6
1	244	LEU	-	expression tag	UNP A0A2G4U6U6
1	245	GLU	-	expression tag	UNP A0A2G4U6U6
1	246	HIS	-	expression tag	UNP A0A2G4U6U6
1	247	HIS	-	expression tag	UNP A0A2G4U6U6
1	248	HIS	-	expression tag	UNP A0A2G4U6U6
1	249	HIS	-	expression tag	UNP A0A2G4U6U6
1	250	HIS	-	expression tag	UNP A0A2G4U6U6
1	251	HIS	-	expression tag	UNP A0A2G4U6U6
2	13	ALA	VAL	conflict	UNP A0A2G4U6U6
2	106	HIS	GLY	conflict	UNP A0A2G4U6U6
2	112	CYS	GLY	conflict	UNP A0A2G4U6U6
2	244	LEU	-	expression tag	UNP A0A2G4U6U6
2	245	GLU	-	expression tag	UNP A0A2G4U6U6
2	246	HIS	-	expression tag	UNP A0A2G4U6U6
2	247	HIS	-	expression tag	UNP A0A2G4U6U6
2	248	HIS	-	expression tag	UNP A0A2G4U6U6
2	249	HIS	-	expression tag	UNP A0A2G4U6U6
2	250	HIS	-	expression tag	UNP A0A2G4U6U6
2	251	HIS	-	expression tag	UNP A0A2G4U6U6

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



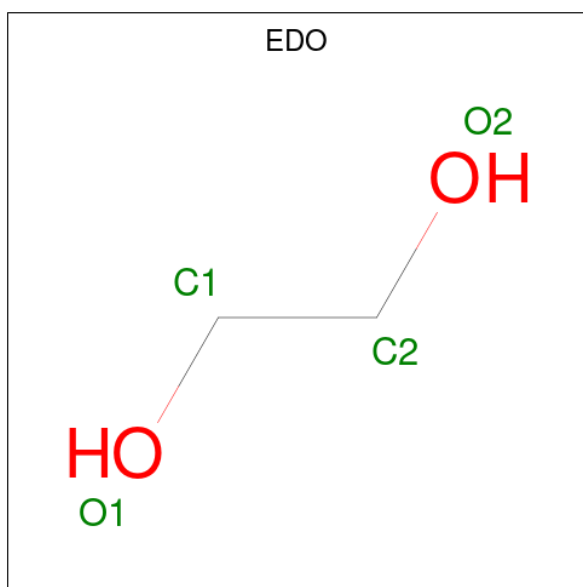
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		
2	V	1	Total	O	S	0	0
			5	4	1		
2	W	1	Total	O	S	0	0
			5	4	1		
2	X	1	Total	O	S	0	0
			5	4	1		
2	X	1	Total	O	S	0	0
			5	4	1		
2	X	1	Total	O	S	0	0
			5	4	1		
2	Z	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	1	1	Total	O	S	0	0
			5	4	1		
2	2	1	Total	O	S	0	0
			5	4	1		
2	2	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	K	1	Total	C	O	0	0
			4	2	2		
3	L	1	Total	C	O	0	0
			4	2	2		
3	O	1	Total	C	O	0	0
			4	2	2		

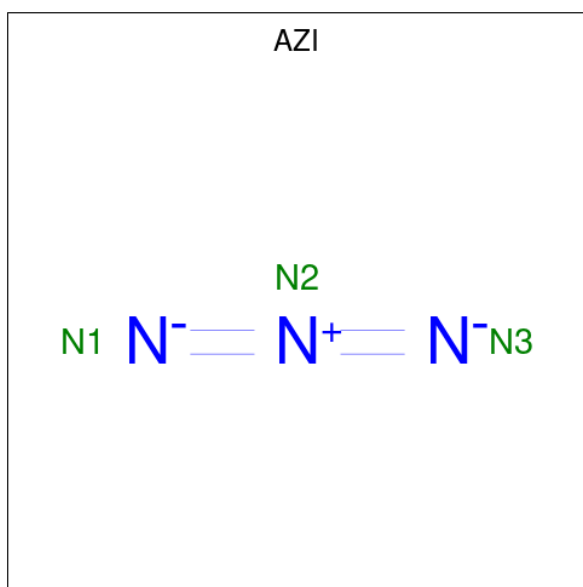
- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total Cl 1 1	0	0
4	D	2	Total Cl 2 2	0	0
4	G	1	Total Cl 1 1	0	0
4	K	2	Total Cl 2 2	0	0
4	L	1	Total Cl 1 1	0	0
4	M	1	Total Cl 1 1	0	0
4	P	1	Total Cl 1 1	0	0
4	Q	1	Total Cl 1 1	0	0
4	R	1	Total Cl 1 1	0	0
4	S	1	Total Cl 1 1	0	0
4	T	1	Total Cl 1 1	0	0
4	U	1	Total Cl 1 1	0	0
4	W	1	Total Cl 1 1	0	0
4	Z	1	Total Cl 1 1	0	0
4	1	1	Total Cl 1 1	0	0

- Molecule 5 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

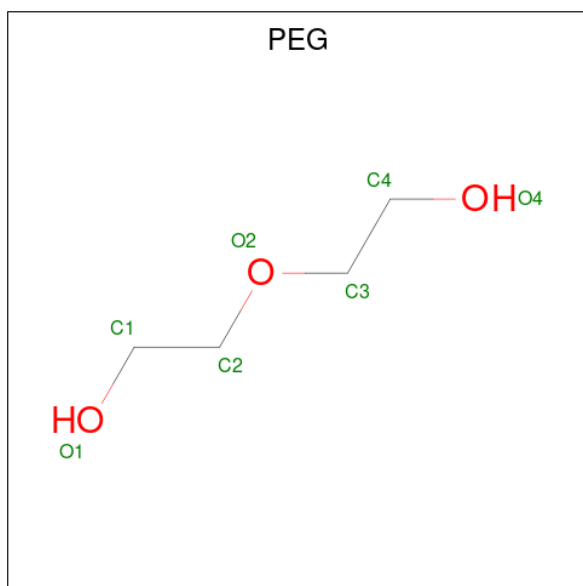
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	I	1	Total X 1 1	0	0
5	Q	2	Total X 2 2	0	0
5	U	1	Total X 1 1	0	0

- Molecule 6 is AZIDE ION (CCD ID: AZI) (formula: N₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	J	1	Total	N		0	0
			3	3			

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	N	1	Total	C	O	0	0
			7	4	3		
7	T	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	52	Total O 52 52	0	0
8	B	95	Total O 95 95	0	0
8	C	83	Total O 83 83	0	0
8	D	85	Total O 85 85	0	0
8	E	81	Total O 81 81	0	0
8	F	59	Total O 59 59	0	0
8	G	55	Total O 55 55	0	0
8	H	33	Total O 33 33	0	0
8	I	51	Total O 51 51	0	0
8	J	50	Total O 50 50	0	0
8	K	57	Total O 57 57	0	0
8	L	71	Total O 71 71	0	0
8	M	63	Total O 63 63	0	0
8	N	54	Total O 54 54	0	0
8	O	44	Total O 44 44	0	0
8	P	86	Total O 86 86	0	0
8	Q	52	Total O 52 52	0	0
8	R	63	Total O 63 63	0	0
8	S	40	Total O 40 40	0	0
8	T	56	Total O 56 56	0	0
8	U	46	Total O 46 46	0	0
8	V	57	Total O 57 57	0	0

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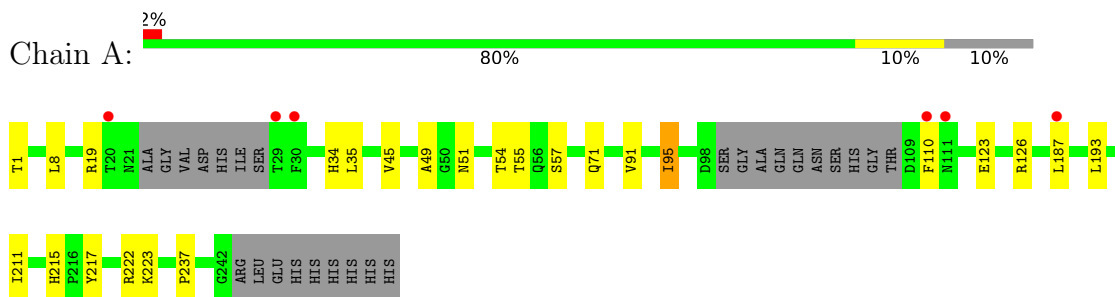
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	W	74	Total 74	O 74	0	0
8	X	83	Total 83	O 83	0	0
8	Y	102	Total 102	O 102	0	0
8	Z	81	Total 81	O 81	0	0
8	1	76	Total 76	O 76	0	0
8	2	41	Total 41	O 41	0	0

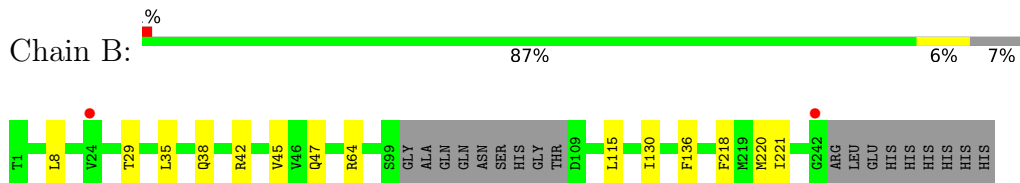
3 Residue-property plots [i](#)

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.

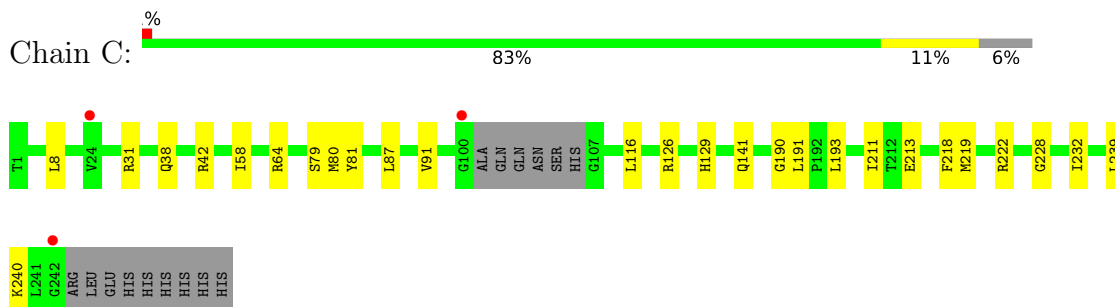
- Molecule 1: Peptidase



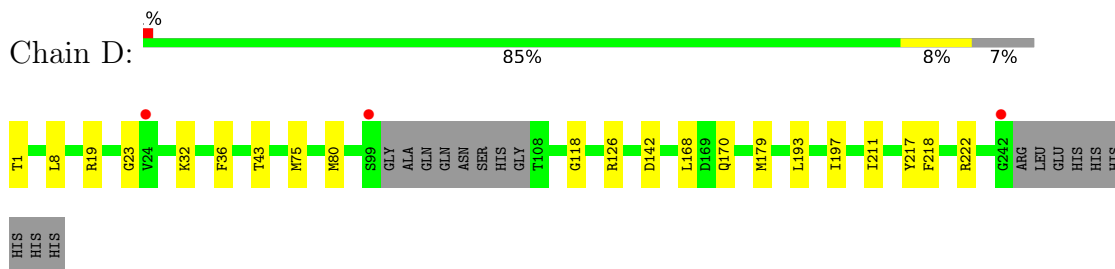
- Molecule 1: Peptidase



- Molecule 1: Peptidase

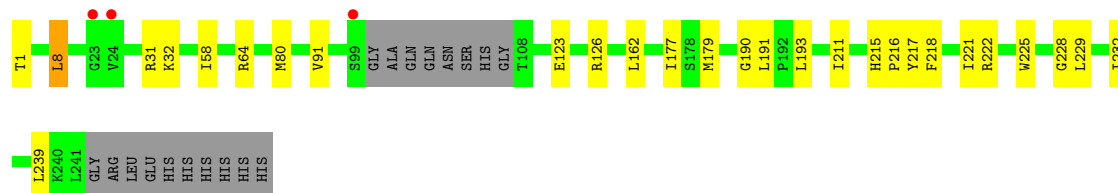


- Molecule 1: Peptidase



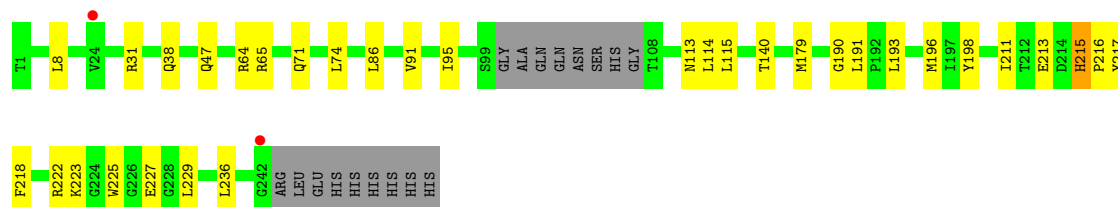
- Molecule 1: Peptidase

Chain E: 



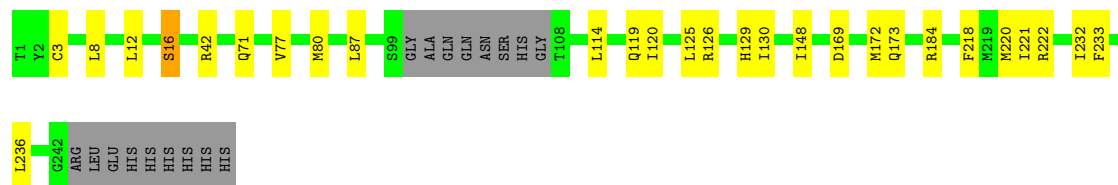
- Molecule 1: Peptidase

Chain F: 



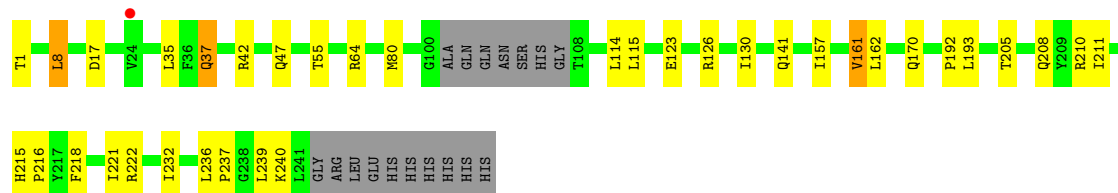
- Molecule 1: Peptidase

Chain G: 



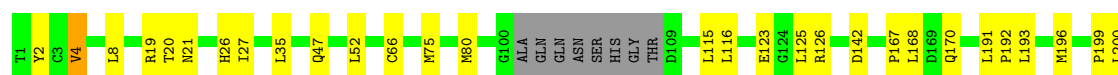
- Molecule 1: Peptidase

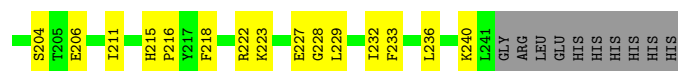
Chain H: 



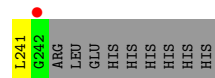
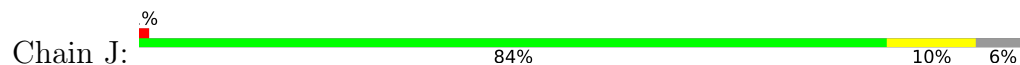
- Molecule 1: Peptidase

Chain I: 

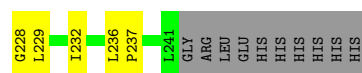
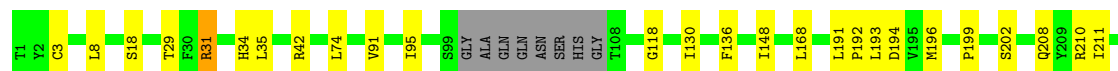
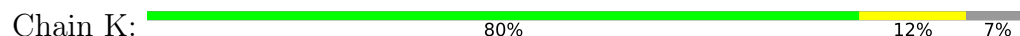




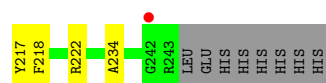
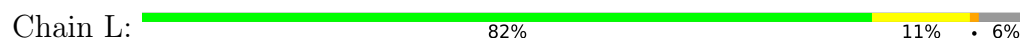
● Molecule 1: Peptidase



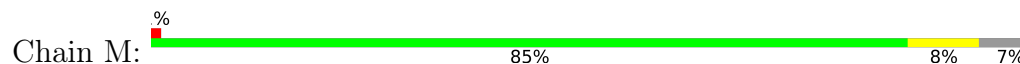
● Molecule 1: Peptidase



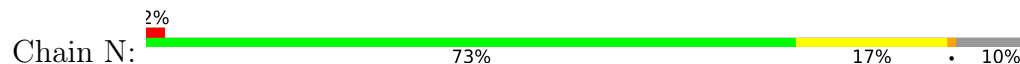
● Molecule 1: Peptidase



● Molecule 1: Peptidase

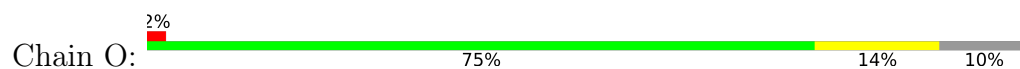


● Molecule 1: Peptidase

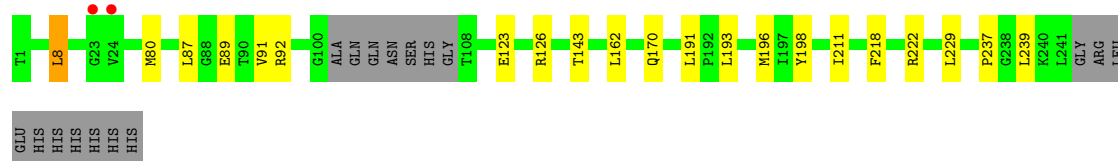
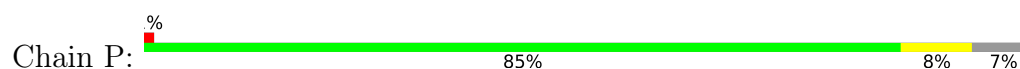




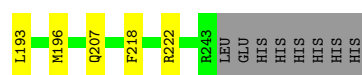
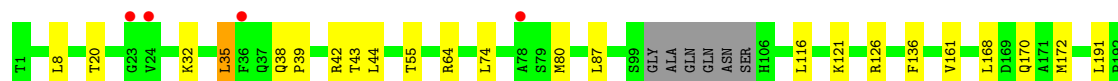
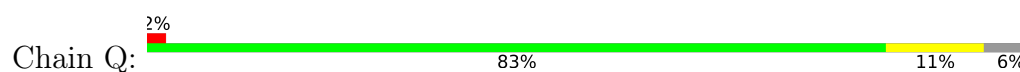
● Molecule 1: Peptidase



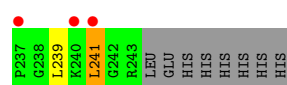
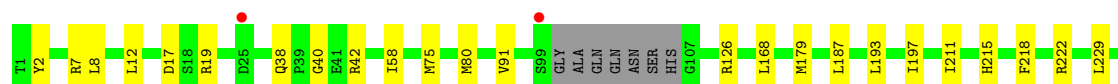
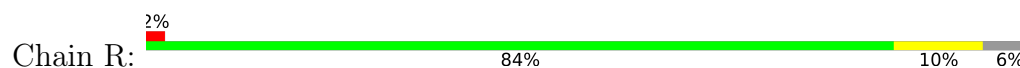
● Molecule 1: Peptidase



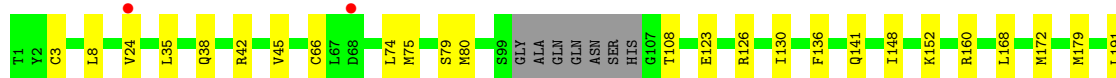
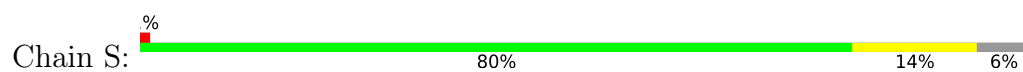
● Molecule 1: Peptidase



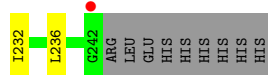
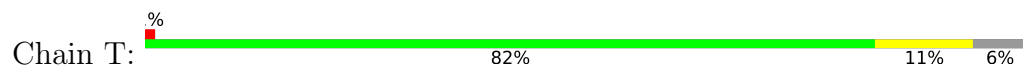
● Molecule 1: Peptidase



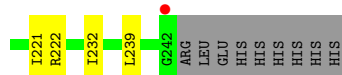
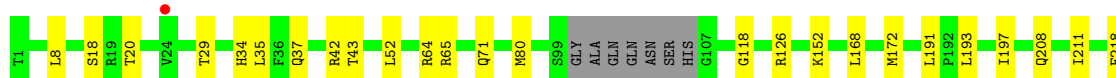
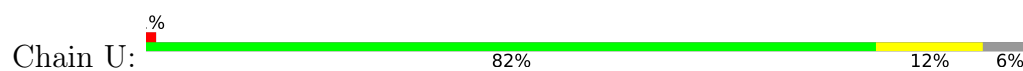
● Molecule 1: Peptidase



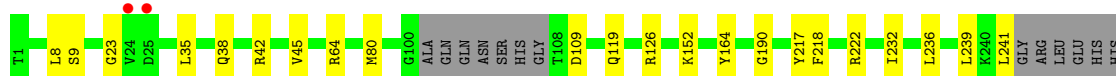
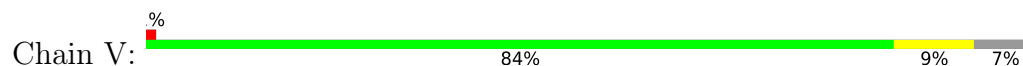
• Molecule 1: Peptidase



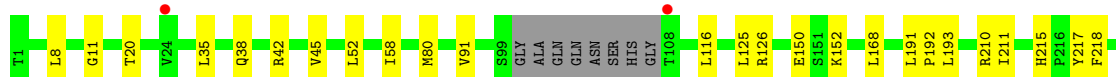
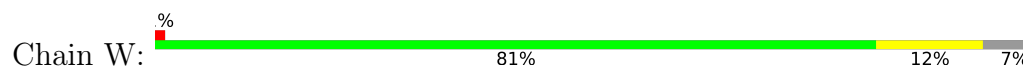
• Molecule 1: Peptidase

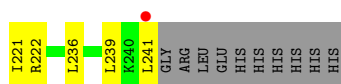


• Molecule 1: Peptidase



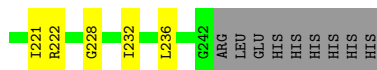
• Molecule 1: Peptidase





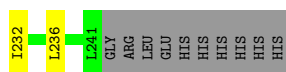
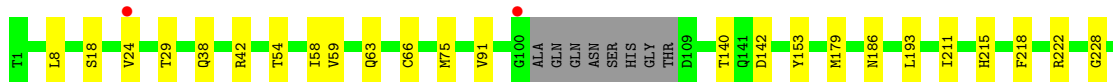
● Molecule 1: Peptidase

Chain X: 81% 13% 6%



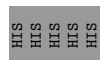
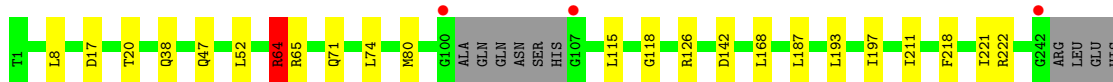
● Molecule 1: Peptidase

Chain Y: 82% 10% 7%



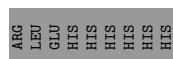
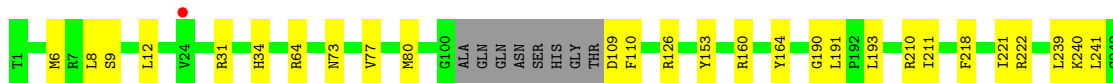
● Molecule 1: Peptidase

Chain Z: 85% 9% 6%



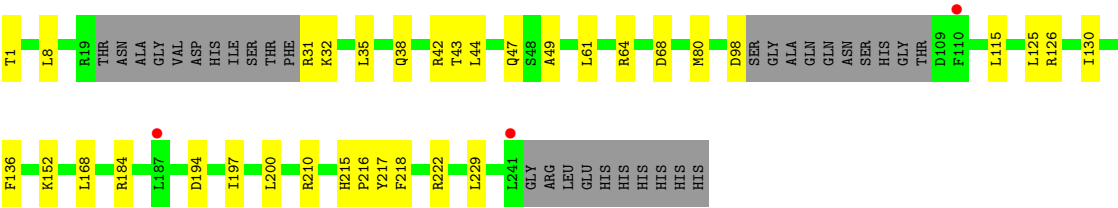
● Molecule 1: Peptidase

Chain 1: 82% 11% 7%



● Molecule 1: Peptidase

Chain 2: 74% 14% 12%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.53Å 285.37Å 179.21Å 90.00° 91.78° 90.00°	Depositor
Resolution (Å)	49.19 – 2.50 49.19 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.19-2.50) 99.0 (49.19-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.183 , 0.230 0.189 , 0.231	Depositor DCC
R_{free} test set	1983 reflections (0.60%)	wwPDB-VP
Wilson B-factor (Å ²)	55.1	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 64.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.085 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	52945	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AZI, EDO, UNX, PEG, SO4, 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	1	0.60	0/1858	0.90	1/2514 (0.0%)
1	2	0.56	0/1760	0.87	2/2379 (0.1%)
1	A	0.56	0/1812	0.88	1/2450 (0.0%)
1	B	0.57	0/1854	0.87	0/2509
1	C	0.59	0/1869	0.90	1/2529 (0.0%)
1	D	0.60	0/1861	0.91	1/2519 (0.0%)
1	E	0.59	0/1857	0.88	1/2514 (0.0%)
1	F	0.56	0/1861	0.89	5/2519 (0.2%)
1	G	0.53	0/1861	0.86	0/2519
1	H	0.54	0/1861	0.85	0/2519
1	I	0.50	0/1854	0.88	2/2509 (0.1%)
1	J	0.54	0/1865	0.85	0/2524
1	K	0.57	0/1857	0.87	1/2514 (0.0%)
1	L	0.56	0/1880	0.91	2/2543 (0.1%)
1	M	0.50	0/1854	0.89	2/2509 (0.1%)
1	N	0.54	0/1805	0.90	3/2441 (0.1%)
1	O	0.56	0/1795	0.88	2/2427 (0.1%)
1	P	0.58	0/1872	0.90	2/2533 (0.1%)
1	Q	0.53	0/1887	0.88	2/2553 (0.1%)
1	R	0.56	0/1887	0.89	3/2552 (0.1%)
1	S	0.51	0/1865	0.83	2/2524 (0.1%)
1	T	0.53	0/1865	0.86	4/2524 (0.2%)
1	U	0.52	0/1865	0.85	0/2524
1	V	0.51	0/1861	0.85	2/2519 (0.1%)
1	W	0.56	0/1857	0.83	0/2514
1	X	0.58	0/1869	0.85	0/2529
1	Y	0.62	0/1863	0.92	3/2521 (0.1%)
1	Z	0.58	0/1869	0.90	3/2529 (0.1%)
All	All	0.56	0/51924	0.88	45/70260 (0.1%)

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	215	HIS	CA-C-N	7.58	127.46	119.05
1	L	215	HIS	C-N-CA	7.58	127.46	119.05
1	D	23	GLY	N-CA-C	-6.86	99.17	110.56
1	I	215	HIS	CA-C-N	6.38	125.60	118.97
1	I	215	HIS	C-N-CA	6.38	125.60	118.97
1	N	215	HIS	CA-C-N	6.07	125.28	118.97
1	N	215	HIS	C-N-CA	6.07	125.28	118.97
1	T	236	LEU	CA-C-N	5.82	125.72	119.85
1	T	236	LEU	C-N-CA	5.82	125.72	119.85
1	P	143	THR	CA-C-N	5.81	127.10	119.84
1	P	143	THR	C-N-CA	5.81	127.10	119.84
1	Z	64	ARG	CG-CD-NE	5.63	124.38	112.00
1	F	38	GLN	CA-C-N	5.62	125.94	119.93
1	F	38	GLN	C-N-CA	5.62	125.94	119.93
1	E	190	GLY	N-CA-C	5.53	119.38	110.87
1	Y	215	HIS	CA-C-N	5.49	124.68	118.97
1	Y	215	HIS	C-N-CA	5.49	124.68	118.97
1	Q	136	PHE	N-CA-C	5.47	117.17	108.79
1	Z	38	GLN	CA-C-N	5.39	125.69	119.93
1	Z	38	GLN	C-N-CA	5.39	125.69	119.93
1	R	241	LEU	N-CA-C	-5.38	106.71	113.28
1	T	38	GLN	CA-C-N	5.34	125.65	119.93
1	T	38	GLN	C-N-CA	5.34	125.65	119.93
1	2	215	HIS	CA-C-N	5.29	124.47	118.97
1	2	215	HIS	C-N-CA	5.29	124.47	118.97
1	1	190	GLY	N-CA-C	5.26	118.98	110.87
1	V	190	GLY	N-CA-C	5.26	118.97	110.87
1	F	190	GLY	N-CA-C	5.24	118.94	110.87
1	C	190	GLY	N-CA-C	5.20	118.87	110.87
1	O	96	ASN	N-CA-C	5.20	117.02	111.36
1	Q	168	LEU	N-CA-C	5.19	117.34	111.11
1	R	215	HIS	CA-C-N	5.18	124.36	118.97
1	R	215	HIS	C-N-CA	5.18	124.36	118.97
1	V	23	GLY	N-CA-C	-5.17	101.97	110.56
1	F	215	HIS	CA-C-N	5.15	124.33	118.97
1	F	215	HIS	C-N-CA	5.15	124.33	118.97
1	N	21	ASN	N-CA-C	5.12	117.73	110.10
1	K	118	GLY	N-CA-C	5.10	116.81	110.29
1	M	143	THR	CA-C-N	5.08	126.19	119.84
1	M	143	THR	C-N-CA	5.08	126.19	119.84
1	A	95	ILE	CB-CA-C	-5.07	105.49	111.97
1	O	190	GLY	N-CA-C	5.06	118.66	110.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	108	THR	N-CA-C	-5.06	106.02	113.61
1	S	24	VAL	N-CA-C	5.05	115.27	110.42
1	Y	24	VAL	N-CA-C	5.05	115.27	110.42

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	1	1825	0	1814	20	0
1	2	1730	0	1729	24	0
1	A	1781	0	1771	18	0
1	B	1821	0	1811	9	0
1	C	1836	0	1824	18	1
1	D	1828	0	1818	14	0
1	E	1824	0	1815	24	0
1	F	1828	0	1818	27	0
1	G	1828	0	1818	25	0
1	H	1828	0	1818	28	0
1	I	1821	0	1811	29	0
1	J	1832	0	1821	17	0
1	K	1824	0	1815	18	0
1	L	1847	0	1837	22	1
1	M	1821	0	1811	15	0
1	N	1774	0	1768	31	0
1	O	1764	0	1763	29	0
1	P	1839	0	1830	14	0
1	Q	1853	0	1841	18	0
1	R	1854	0	1846	19	0
1	S	1832	0	1821	26	0
1	T	1832	0	1821	23	0
1	U	1832	0	1820	23	0
1	V	1828	0	1818	14	0
1	W	1824	0	1815	26	0
1	X	1836	0	1824	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Y	1830	0	1818	16	0
1	Z	1836	0	1824	18	0
2	1	5	0	0	1	0
2	2	10	0	0	4	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0
2	E	10	0	0	0	0
2	L	5	0	0	0	0
2	P	10	0	0	0	0
2	V	5	0	0	1	0
2	W	5	0	0	0	0
2	X	15	0	0	2	0
2	Z	5	0	0	1	0
3	C	4	0	6	1	0
3	D	4	0	6	1	0
3	F	4	0	6	5	0
3	K	4	0	6	0	0
3	L	4	0	6	2	0
3	O	4	0	6	1	0
4	1	1	0	0	1	0
4	C	1	0	0	1	0
4	D	2	0	0	0	0
4	G	1	0	0	0	0
4	K	2	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	P	1	0	0	0	0
4	Q	1	0	0	1	0
4	R	1	0	0	0	0
4	S	1	0	0	1	0
4	T	1	0	0	2	0
4	U	1	0	0	0	0
4	W	1	0	0	0	0
4	Z	1	0	0	0	0
5	I	1	0	0	0	0
5	Q	2	0	0	0	0
5	U	1	0	0	0	0
6	J	3	0	0	0	0
7	N	7	0	10	3	0
7	T	7	0	10	2	0
8	1	76	0	0	3	0
8	2	41	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	52	0	0	3	0
8	B	95	0	0	0	0
8	C	83	0	0	1	0
8	D	85	0	0	1	0
8	E	81	0	0	1	0
8	F	59	0	0	2	0
8	G	55	0	0	2	0
8	H	33	0	0	1	0
8	I	51	0	0	3	0
8	J	50	0	0	0	0
8	K	57	0	0	1	0
8	L	71	0	0	2	0
8	M	63	0	0	1	0
8	N	54	0	0	0	0
8	O	44	0	0	0	0
8	P	86	0	0	0	0
8	Q	52	0	0	1	0
8	R	63	0	0	1	0
8	S	40	0	0	0	0
8	T	56	0	0	0	0
8	U	46	0	0	1	0
8	V	57	0	0	1	0
8	W	74	0	0	1	0
8	X	83	0	0	5	0
8	Y	102	0	0	0	0
8	Z	81	0	0	3	0
All	All	52945	0	50796	539	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (539) 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)
1:2:31:ARG:HH21	1:2:210:ARG:HH12	1.11	0.94
1:1:64:ARG:NH2	4:1:302:CL:CL	2.38	0.94
1:F:31:ARG:NH2	3:F:301:EDO:O2	2.00	0.93
1:2:184:ARG:NH2	8:2:401:HOH:O	2.01	0.93
1:Q:64:ARG:NH2	4:Q:301:CL:CL	2.45	0.87
2:Z:301:SO4:O4	8:Z:401:HOH:O	1.93	0.87
1:S:160:ARG:HD2	1:T:229:LEU:HD23	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:ARG:NH2	4:C:302:CL:CL	2.50	0.82
1:G:87:LEU:HD22	1:G:130:ILE:HG13	1.61	0.80
1:I:229:LEU:HD21	1:J:229:LEU:HD21	1.62	0.80
1:N:141:GLN:HG3	7:N:301:PEG:H11	1.61	0.80
1:Z:64:ARG:HG2	1:Z:64:ARG:HH21	1.46	0.78
1:E:229:LEU:HD21	1:F:229:LEU:HD21	1.64	0.77
1:X:20:THR:OG1	1:X:32:LYS:NZ	2.19	0.75
1:X:6:MET:HE3	1:X:13:ALA:HB3	1.69	0.74
1:S:191:LEU:HD23	1:S:193:LEU:HD13	1.68	0.73
1:L:141:GLN:H	3:L:301:EDO:H11	1.53	0.72
1:2:1:THR:OG1	1:2:32:LYS:NZ	2.22	0.72
1:T:64:ARG:NH2	4:T:301:CL:CL	2.59	0.71
1:I:80:MET:HE1	1:I:116:LEU:HG	1.72	0.71
1:N:196:MET:HE2	1:N:198:TYR:HB2	1.72	0.70
2:X:302:SO4:O4	8:X:401:HOH:O	2.09	0.70
1:G:42:ARG:NH2	1:G:77:VAL:O	2.24	0.69
1:N:7:ARG:HH12	7:N:301:PEG:H12	1.57	0.68
1:G:3:CYS:SG	1:G:16:SER:HB3	2.34	0.68
1:E:80:MET:HB3	1:E:126:ARG:HD3	1.76	0.68
1:O:108:THR:O	1:O:111:ASN:ND2	2.26	0.67
1:K:35:LEU:HD21	1:K:196:MET:HE1	1.77	0.67
1:A:123:GLU:OE2	1:A:126:ARG:NH1	2.26	0.67
1:2:80:MET:HB2	1:2:126:ARG:HD3	1.77	0.67
1:I:19:ARG:HH11	1:I:19:ARG:HG3	1.59	0.67
1:C:87:LEU:HD12	1:C:116:LEU:HD22	1.77	0.66
1:U:172:MET:HB3	1:V:239:LEU:HD11	1.78	0.66
2:X:302:SO4:O3	8:X:402:HOH:O	2.10	0.66
1:T:219:MET:O	1:T:223:LYS:HG2	1.96	0.65
1:D:19:ARG:HH11	1:D:19:ARG:HG3	1.61	0.65
1:V:239:LEU:HD22	1:V:241:LEU:HD11	1.77	0.65
1:1:31:ARG:NH1	8:1:401:HOH:O	2.30	0.64
1:2:64:ARG:NH2	2:2:301:SO4:O1	2.30	0.64
1:S:220:MET:HG3	1:S:223:LYS:HE2	1.79	0.64
1:H:37:GLN:NE2	1:H:42:ARG:O	2.31	0.64
1:S:80:MET:HB3	1:S:126:ARG:HD3	1.79	0.63
1:S:179:MET:HG2	1:S:193:LEU:HD21	1.79	0.63
1:O:80:MET:HA	1:O:80:MET:HE2	1.81	0.63
1:G:221:ILE:HD11	1:H:236:LEU:HD13	1.81	0.62
1:O:123:GLU:OE2	1:O:126:ARG:NH1	2.31	0.62
1:M:193:LEU:HB2	1:M:211:ILE:HB	1.81	0.62
1:O:193:LEU:HB2	1:O:211:ILE:HB	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:38:GLN:HB2	1:R:75:MET:HE1	1.80	0.62
1:F:31:ARG:HH22	3:F:301:EDO:HO2	1.46	0.62
1:W:152:LYS:HG2	1:X:153:TYR:CZ	2.34	0.62
1:I:193:LEU:HB2	1:I:211:ILE:HB	1.83	0.61
1:Y:54:THR:O	1:Y:58:ILE:HG12	2.00	0.61
1:J:228:GLY:O	1:J:232:ILE:HG12	2.01	0.61
1:C:193:LEU:HB2	1:C:211:ILE:HB	1.82	0.60
1:I:233:PHE:HA	1:I:236:LEU:HD13	1.84	0.60
1:M:34:HIS:ND1	8:M:403:HOH:O	2.31	0.60
1:Y:59:VAL:O	1:Y:63:GLN:HG2	2.02	0.60
1:I:167:PRO:HG2	1:I:170:GLN:HG2	1.84	0.59
1:A:34:HIS:ND1	8:A:401:HOH:O	2.31	0.59
1:Y:218:PHE:O	1:Y:222:ARG:HG3	2.03	0.59
1:I:160:ARG:NH2	8:I:403:HOH:O	2.34	0.59
1:T:123:GLU:OE2	1:T:126:ARG:NH1	2.35	0.59
1:T:80:MET:HB3	1:T:126:ARG:HD3	1.84	0.59
1:B:35:LEU:HD21	1:B:45:VAL:HG22	1.85	0.58
1:R:239:LEU:HD22	1:R:241:LEU:HD13	1.85	0.58
1:W:38:GLN:HB3	1:W:42:ARG:HG2	1.85	0.58
1:W:236:LEU:HD13	1:X:221:ILE:HD11	1.83	0.58
1:E:31:ARG:NH2	8:E:403:HOH:O	2.36	0.58
1:I:123:GLU:OE2	1:I:126:ARG:NH1	2.33	0.58
1:O:172:MET:HB3	1:P:239:LEU:HD11	1.85	0.58
1:A:237:PRO:HG3	1:B:220:MET:HE2	1.85	0.58
1:D:170:GLN:NE2	8:D:404:HOH:O	2.34	0.57
1:E:80:MET:HG2	1:E:126:ARG:HB2	1.86	0.57
1:E:177:ILE:HD11	1:F:236:LEU:HD11	1.86	0.57
1:G:172:MET:HB3	1:H:239:LEU:HD21	1.85	0.57
1:D:1:THR:OG1	1:D:32:LYS:NZ	2.34	0.57
1:U:168:LEU:HG	1:U:197:ILE:HG23	1.86	0.57
1:W:152:LYS:HG2	1:X:153:TYR:CE1	2.39	0.57
1:Z:20:THR:HG21	1:Z:52:LEU:HD22	1.85	0.57
1:I:191:LEU:HD23	1:I:193:LEU:HG	1.85	0.57
1:2:47:GLN:HB2	1:2:115:LEU:HB2	1.86	0.57
1:S:172:MET:HB2	1:S:197:ILE:HD11	1.86	0.57
1:G:42:ARG:HG2	1:G:120:ILE:HG12	1.87	0.57
1:L:38:GLN:HB2	1:L:75:MET:HE1	1.86	0.56
1:Q:38:GLN:HB3	1:Q:42:ARG:HG2	1.87	0.56
1:W:80:MET:HE1	1:W:116:LEU:HG	1.87	0.56
1:E:225:TRP:CH2	1:F:229:LEU:HD22	2.40	0.56
1:Z:65:ARG:NH1	1:Z:71:GLN:OE1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:64:ARG:NH2	2:V:301:SO4:O1	2.38	0.56
1:H:218:PHE:HA	1:H:221:ILE:HG22	1.87	0.56
1:X:80:MET:HB3	1:X:126:ARG:HD3	1.88	0.56
1:A:57:SER:OG	1:N:70:GLU:OE2	2.21	0.56
1:M:191:LEU:HD23	1:M:193:LEU:HG	1.87	0.56
1:A:193:LEU:HB2	1:A:211:ILE:HB	1.88	0.56
1:D:218:PHE:CE2	1:D:222:ARG:HD2	2.40	0.56
1:S:38:GLN:HB2	1:S:75:MET:HE1	1.87	0.56
1:A:1:THR:HG21	1:A:49:ALA:HA	1.86	0.56
1:W:191:LEU:HD23	1:W:193:LEU:HG	1.88	0.56
1:H:193:LEU:HB2	1:H:211:ILE:HB	1.87	0.55
1:T:141:GLN:HG3	7:T:302:PEG:H12	1.89	0.55
1:W:221:ILE:HD11	1:X:236:LEU:HD13	1.88	0.55
1:N:80:MET:HG2	1:N:126:ARG:HB2	1.88	0.55
3:F:301:EDO:H22	1:H:141:GLN:H	1.71	0.55
1:N:44:LEU:HG	1:N:80:MET:HE1	1.89	0.55
1:Y:193:LEU:HB2	1:Y:211:ILE:HB	1.88	0.55
1:K:34:HIS:HD2	8:K:412:HOH:O	1.90	0.55
1:S:123:GLU:OE1	1:S:126:ARG:NH1	2.40	0.55
1:H:64:ARG:NH2	8:H:301:HOH:O	2.26	0.54
1:L:66:CYS:SG	1:L:75:MET:HG2	2.46	0.54
1:R:218:PHE:CE2	1:R:222:ARG:HD2	2.42	0.54
1:O:64:ARG:HD2	1:2:68:ASP:HB2	1.89	0.54
3:D:301:EDO:H11	1:F:140:THR:HB	1.90	0.54
1:L:193:LEU:HB2	1:L:211:ILE:HB	1.89	0.54
1:M:119:GLN:NE2	1:M:201:ASP:OD1	2.36	0.54
1:O:80:MET:HG3	1:O:126:ARG:HB2	1.88	0.54
1:R:80:MET:HB3	1:R:126:ARG:HD3	1.89	0.54
1:G:232:ILE:HG12	1:H:232:ILE:HD11	1.89	0.54
1:Q:20:THR:OG1	1:Q:32:LYS:NZ	2.29	0.54
1:R:80:MET:HG2	1:R:126:ARG:HB2	1.90	0.54
1:S:141:GLN:HG3	4:S:301:CL:CL	2.44	0.54
1:V:80:MET:HB3	1:V:126:ARG:HD3	1.89	0.54
1:G:220:MET:HE2	1:H:237:PRO:HG2	1.90	0.54
1:N:191:LEU:HD23	1:N:193:LEU:HG	1.90	0.54
1:G:233:PHE:HA	1:G:236:LEU:HD13	1.90	0.53
1:1:80:MET:HG2	1:1:126:ARG:HB2	1.89	0.53
1:H:170:GLN:N	1:H:170:GLN:OE1	2.42	0.53
1:M:80:MET:HB3	1:M:126:ARG:HD3	1.89	0.53
1:T:64:ARG:NH1	4:T:301:CL:CL	2.77	0.53
1:F:65:ARG:HG2	1:F:71:GLN:NE2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:218:PHE:CE2	1:H:222:ARG:HD2	2.44	0.53
1:Q:42:ARG:NH1	1:Q:74:LEU:O	2.42	0.53
1:F:31:ARG:NH2	3:F:301:EDO:HO2	2.03	0.52
1:I:142:ASP:O	8:I:401:HOH:O	2.19	0.52
1:O:1:THR:HG23	1:O:32:LYS:HD3	1.90	0.52
1:Q:170:GLN:OE1	1:Q:170:GLN:N	2.41	0.52
1:S:220:MET:HA	1:S:223:LYS:HE2	1.91	0.52
1:Y:142:ASP:CG	1:1:210:ARG:HH22	2.17	0.52
1:P:123:GLU:OE2	1:P:126:ARG:NH1	2.43	0.52
1:1:193:LEU:HB2	1:1:211:ILE:HB	1.90	0.52
1:E:123:GLU:OE2	1:E:126:ARG:NH1	2.41	0.52
1:H:37:GLN:HE21	1:H:37:GLN:HA	1.73	0.52
1:G:87:LEU:HD21	1:G:114:LEU:HD12	1.91	0.52
1:H:239:LEU:O	1:H:240:LYS:HD3	2.10	0.52
1:P:193:LEU:HB2	1:P:211:ILE:HB	1.91	0.52
1:R:38:GLN:HB3	1:R:42:ARG:HG2	1.91	0.52
1:R:239:LEU:HD22	1:R:241:LEU:CD1	2.39	0.52
1:E:239:LEU:HD12	1:F:217:TYR:CE2	2.44	0.52
1:W:20:THR:HG21	1:W:52:LEU:HD22	1.91	0.52
1:W:35:LEU:HD21	1:W:45:VAL:HG22	1.92	0.52
1:H:47:GLN:HB2	1:H:115:LEU:HB2	1.92	0.51
1:O:140:THR:HB	3:O:301:EDO:H22	1.91	0.51
1:I:228:GLY:O	1:I:232:ILE:HG12	2.10	0.51
1:L:80:MET:HG2	1:L:126:ARG:HB2	1.92	0.51
1:1:80:MET:HB3	1:1:126:ARG:HD3	1.92	0.51
1:X:79:SER:OG	8:X:403:HOH:O	2.19	0.51
1:R:17:ASP:HA	1:R:193:LEU:HD23	1.93	0.51
1:U:191:LEU:HD23	1:U:193:LEU:HG	1.93	0.51
1:W:192:PRO:HB2	1:W:210:ARG:HD2	1.92	0.51
1:X:191:LEU:HD23	1:X:193:LEU:HG	1.92	0.51
1:T:179:MET:HE2	1:T:193:LEU:HD21	1.92	0.51
1:Y:142:ASP:OD1	1:1:210:ARG:NH2	2.44	0.51
1:2:38:GLN:NE2	8:2:403:HOH:O	2.41	0.51
1:G:119:GLN:HB2	1:G:125:LEU:HD23	1.93	0.51
1:1:153:TYR:CZ	1:2:152:LYS:HG2	2.45	0.51
1:F:64:ARG:NH2	8:F:401:HOH:O	2.27	0.51
1:G:42:ARG:HH12	1:G:77:VAL:HG23	1.75	0.51
1:Q:172:MET:HB3	1:R:239:LEU:HD11	1.92	0.51
1:W:215:HIS:HE1	1:W:217:TYR:HB3	1.76	0.51
1:C:81:TYR:HB3	1:E:64:ARG:HH12	1.76	0.51
1:J:20:THR:HG21	1:J:52:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:229:LEU:HD11	1:T:229:LEU:HD11	1.91	0.51
1:G:80:MET:HG2	1:G:126:ARG:HB2	1.93	0.51
1:N:141:GLN:CG	7:N:301:PEG:H11	2.37	0.50
1:S:79:SER:OG	1:U:64:ARG:NH2	2.40	0.50
1:X:6:MET:HE1	1:X:175:ALA:HB2	1.93	0.50
1:L:80:MET:HB3	1:L:126:ARG:HD3	1.93	0.50
1:N:193:LEU:HB2	1:N:211:ILE:HB	1.92	0.50
1:N:34:HIS:C	1:N:35:LEU:HD12	2.37	0.50
1:R:40:GLY:N	8:R:408:HOH:O	2.44	0.50
1:U:218:PHE:HA	1:U:221:ILE:HG22	1.94	0.50
1:O:170:GLN:N	1:O:170:GLN:OE1	2.44	0.50
1:G:71:GLN:HG2	8:G:406:HOH:O	2.10	0.50
1:W:193:LEU:HB2	1:W:211:ILE:HB	1.94	0.50
1:2:152:LYS:HB2	8:2:411:HOH:O	2.12	0.50
1:H:205:THR:O	1:H:208:GLN:HG2	2.12	0.50
1:U:232:ILE:HD11	1:V:232:ILE:HG12	1.94	0.50
1:F:191:LEU:HD13	1:F:213:GLU:HA	1.93	0.50
1:N:77:VAL:HG21	1:N:83:ALA:HB2	1.93	0.50
1:C:81:TYR:HB3	1:E:64:ARG:NH1	2.27	0.50
1:N:238:GLY:O	1:N:240:LYS:HD2	2.12	0.50
1:K:18:SER:HB2	1:K:29:THR:HG23	1.93	0.49
1:O:191:LEU:HD23	1:O:193:LEU:HG	1.94	0.49
1:X:193:LEU:HB2	1:X:211:ILE:HB	1.94	0.49
1:B:29:THR:HG22	1:D:142:ASP:HB3	1.94	0.49
1:G:173:GLN:HG3	1:H:239:LEU:CD1	2.43	0.49
1:I:35:LEU:HD21	1:I:196:MET:SD	2.52	0.49
1:J:191:LEU:HD23	1:J:193:LEU:HG	1.95	0.49
1:Y:236:LEU:HD13	1:Z:221:ILE:HD11	1.93	0.49
1:L:147:GLN:OE1	8:L:401:HOH:O	2.19	0.49
1:O:20:THR:HG21	1:O:52:LEU:HD22	1.95	0.49
1:L:120:ILE:O	1:L:123:GLU:HG2	2.12	0.49
1:N:59:VAL:O	1:N:63:GLN:HG2	2.13	0.49
1:U:80:MET:HG2	1:U:126:ARG:HB2	1.95	0.49
1:T:18:SER:HB2	1:T:29:THR:HG23	1.93	0.49
1:W:221:ILE:HD12	1:X:236:LEU:HD22	1.94	0.49
1:X:228:GLY:O	1:X:232:ILE:HG12	2.13	0.49
1:B:35:LEU:CD2	1:B:45:VAL:HG22	2.43	0.49
1:E:179:MET:HG2	1:E:193:LEU:CD1	2.43	0.49
1:E:218:PHE:O	1:E:222:ARG:HG3	2.13	0.49
1:J:29:THR:OG1	1:L:142:ASP:HB3	2.13	0.49
1:V:119:GLN:HA	8:V:413:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:LEU:HD12	1:D:217:TYR:CE2	2.47	0.49
1:E:179:MET:HG2	1:E:193:LEU:HD11	1.95	0.49
1:C:80:MET:HB3	1:C:126:ARG:HD3	1.94	0.49
1:M:221:ILE:HD11	1:N:236:LEU:HD13	1.95	0.49
1:N:94:VAL:O	1:N:97:ARG:HG2	2.12	0.49
1:A:215:HIS:HE1	1:A:217:TYR:HB3	1.78	0.49
1:G:3:CYS:HB2	1:G:148:ILE:CG1	2.42	0.49
1:R:218:PHE:O	1:R:222:ARG:HG3	2.13	0.49
1:W:35:LEU:CD2	1:W:45:VAL:HG22	2.43	0.49
1:2:130:ILE:HG13	1:2:136:PHE:HB3	1.95	0.49
1:I:20:THR:HG21	1:I:52:LEU:HD22	1.93	0.48
1:L:8:LEU:HD21	1:L:162:LEU:HD11	1.95	0.48
1:F:218:PHE:O	1:F:222:ARG:HG3	2.12	0.48
1:L:196:MET:HE2	1:L:198:TYR:HB2	1.94	0.48
1:D:179:MET:HE2	1:D:193:LEU:HD21	1.96	0.48
1:I:168:LEU:HD11	1:I:199:PRO:HA	1.95	0.48
1:W:218:PHE:HA	1:W:221:ILE:HG22	1.95	0.48
1:Y:58:ILE:HD12	1:Y:91:VAL:HA	1.95	0.48
1:P:218:PHE:CE2	1:P:222:ARG:HD2	2.49	0.48
1:P:8:LEU:HD21	1:P:162:LEU:HD11	1.95	0.48
1:G:218:PHE:CE2	1:G:222:ARG:HD2	2.49	0.48
1:J:155:LYS:HE2	1:J:159:ASP:OD2	2.13	0.48
1:O:42:ARG:NH1	1:O:74:LEU:O	2.47	0.48
1:N:35:LEU:HD23	1:N:205:THR:HB	1.96	0.48
1:S:38:GLN:HB3	1:S:42:ARG:HG2	1.96	0.48
1:W:191:LEU:CD2	1:W:193:LEU:HG	2.43	0.48
1:A:222:ARG:NH2	8:A:405:HOH:O	2.47	0.47
1:O:80:MET:HE3	1:O:120:ILE:HG13	1.96	0.47
1:2:31:ARG:HH21	1:2:210:ARG:NH1	1.94	0.47
1:U:18:SER:HB2	1:U:29:THR:HG23	1.96	0.47
1:U:34:HIS:HD2	8:U:416:HOH:O	1.97	0.47
1:X:64:ARG:NH1	1:X:67:LEU:HB2	2.30	0.47
1:S:218:PHE:CE2	1:S:222:ARG:HD2	2.49	0.47
1:T:123:GLU:CD	1:T:126:ARG:HD2	2.39	0.47
1:Y:38:GLN:HB3	1:Y:42:ARG:HG2	1.95	0.47
1:2:216:PRO:HG2	8:2:427:HOH:O	2.13	0.47
1:J:80:MET:HB3	1:J:126:ARG:HD3	1.97	0.47
1:O:64:ARG:NH1	2:2:301:SO4:O4	2.43	0.47
1:U:80:MET:HB3	1:U:126:ARG:HD3	1.95	0.47
1:X:96:ASN:ND2	8:X:406:HOH:O	2.47	0.47
1:J:193:LEU:HB2	1:J:211:ILE:HB	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:MET:HG2	1:C:126:ARG:HB2	1.96	0.47
1:N:217:TYR:OH	1:N:221:ILE:HD12	2.15	0.47
1:O:80:MET:HB2	1:O:126:ARG:HD3	1.96	0.47
1:T:193:LEU:HB2	1:T:211:ILE:HB	1.97	0.47
1:V:9:SER:HB3	1:V:164:TYR:CE2	2.49	0.47
1:Z:193:LEU:HB2	1:Z:211:ILE:HB	1.96	0.47
1:1:34:HIS:HD2	8:1:412:HOH:O	1.98	0.47
1:Y:153:TYR:OH	1:Y:186:ASN:ND2	2.45	0.47
1:M:215:HIS:HE1	1:M:217:TYR:HB3	1.80	0.47
1:X:6:MET:CE	1:X:175:ALA:HB2	2.45	0.47
1:Z:80:MET:HG2	1:Z:126:ARG:HB2	1.96	0.47
1:1:218:PHE:O	1:1:222:ARG:HG3	2.15	0.47
1:T:218:PHE:O	1:T:222:ARG:HG3	2.14	0.47
1:U:193:LEU:HB2	1:U:211:ILE:HB	1.98	0.47
1:Z:218:PHE:O	1:Z:222:ARG:HG3	2.15	0.47
1:A:215:HIS:CE1	1:A:217:TYR:HB3	2.50	0.46
1:E:228:GLY:O	1:E:232:ILE:HG12	2.15	0.46
1:G:218:PHE:HA	1:G:221:ILE:HG22	1.97	0.46
1:I:229:LEU:HD22	1:J:225:TRP:CH2	2.49	0.46
1:Q:218:PHE:CE2	1:Q:222:ARG:HD2	2.51	0.46
1:U:218:PHE:O	1:U:222:ARG:HG3	2.14	0.46
1:2:64:ARG:NH2	2:2:301:SO4:O3	2.47	0.46
1:P:218:PHE:O	1:P:222:ARG:HG3	2.15	0.46
1:R:7:ARG:HA	1:R:12:LEU:HD23	1.97	0.46
1:V:218:PHE:O	1:V:222:ARG:HG3	2.15	0.46
1:A:19:ARG:NH1	1:A:187:LEU:O	2.40	0.46
1:M:237:PRO:HG3	1:N:220:MET:HE2	1.95	0.46
1:Q:35:LEU:HD21	1:Q:196:MET:SD	2.56	0.46
1:Q:87:LEU:HD22	1:Q:116:LEU:HD22	1.98	0.46
1:V:239:LEU:HD22	1:V:241:LEU:CD1	2.46	0.46
1:W:58:ILE:HD13	1:W:91:VAL:HG22	1.97	0.46
1:2:43:THR:C	1:2:44:LEU:HD12	2.41	0.46
1:L:141:GLN:HG3	3:L:301:EDO:H11	1.98	0.46
1:Q:218:PHE:O	1:Q:222:ARG:HG3	2.16	0.46
1:T:140:THR:HB	7:T:302:PEG:H41	1.98	0.46
1:U:20:THR:HG21	1:U:52:LEU:HD22	1.96	0.46
1:B:47:GLN:HB2	1:B:115:LEU:HB2	1.98	0.46
1:L:34:HIS:HD2	8:L:413:HOH:O	1.98	0.46
1:N:19:ARG:NH1	1:N:187:LEU:O	2.44	0.46
1:S:152:LYS:HD2	1:T:152:LYS:HD2	1.97	0.46
1:U:43:THR:O	1:U:118:GLY:HA3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:35:LEU:HD11	1:U:208:GLN:OE1	2.15	0.46
1:X:58:ILE:HD13	1:X:91:VAL:HG22	1.97	0.46
1:B:64:ARG:O	1:B:64:ARG:NH1	2.49	0.46
1:H:8:LEU:HD21	1:H:162:LEU:HD11	1.98	0.46
1:X:87:LEU:HD23	1:X:130:ILE:HG13	1.98	0.46
1:Z:80:MET:HB3	1:Z:126:ARG:HD3	1.98	0.46
1:H:35:LEU:HD11	1:H:208:GLN:OE1	2.16	0.46
1:S:130:ILE:HD13	1:S:136:PHE:HB3	1.96	0.46
1:K:130:ILE:HD13	1:K:136:PHE:HB3	1.98	0.45
1:O:44:LEU:HD21	1:O:80:MET:HE1	1.98	0.45
1:O:71:GLN:NE2	2:2:301:SO4:O1	2.49	0.45
1:W:215:HIS:CE1	1:W:217:TYR:HB3	2.51	0.45
1:B:130:ILE:HG13	1:B:136:PHE:HB3	1.98	0.45
1:E:229:LEU:HD21	1:F:229:LEU:CD2	2.41	0.45
1:R:19:ARG:NH1	1:R:187:LEU:O	2.42	0.45
1:S:3:CYS:HB2	1:S:148:ILE:CG1	2.46	0.45
1:J:229:LEU:HD23	1:J:229:LEU:HA	1.66	0.45
1:E:229:LEU:HD22	1:F:225:TRP:CH2	2.52	0.45
1:Z:168:LEU:HD12	1:Z:168:LEU:HA	1.60	0.45
1:F:223:LYS:NZ	1:F:227:GLU:OE2	2.32	0.45
1:K:91:VAL:O	1:K:95:ILE:HG12	2.16	0.45
1:U:239:LEU:HD12	1:V:217:TYR:CE2	2.52	0.45
1:X:217:TYR:OH	1:X:221:ILE:HD13	2.16	0.45
1:2:168:LEU:HG	1:2:197:ILE:HG23	1.98	0.45
1:2:218:PHE:CE2	1:2:222:ARG:HD2	2.51	0.45
1:D:193:LEU:HB2	1:D:211:ILE:HB	1.99	0.45
1:K:229:LEU:HD23	1:K:229:LEU:HA	1.78	0.45
1:O:61:LEU:HD23	1:O:64:ARG:HH11	1.81	0.45
1:Q:80:MET:HG2	1:Q:126:ARG:HB2	1.98	0.45
1:U:65:ARG:HG2	1:U:71:GLN:OE1	2.17	0.45
1:A:223:LYS:HA	1:A:223:LYS:HD3	1.68	0.45
1:C:141:GLN:H	3:C:301:EDO:H11	1.81	0.45
1:C:218:PHE:O	1:C:222:ARG:HG3	2.16	0.45
1:H:80:MET:HB3	1:H:126:ARG:HD3	1.99	0.45
1:M:215:HIS:CE1	1:M:217:TYR:HB3	2.52	0.45
1:S:80:MET:HG2	1:S:126:ARG:HB2	1.99	0.45
1:B:38:GLN:HB3	1:B:42:ARG:HB3	1.98	0.45
1:C:38:GLN:HB3	1:C:42:ARG:HG2	1.98	0.45
1:O:220:MET:HE2	1:P:237:PRO:HG2	1.98	0.45
1:X:10:SER:HB3	8:X:431:HOH:O	2.17	0.45
1:E:217:TYR:OH	1:E:221:ILE:HD12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:193:LEU:HB2	1:F:211:ILE:HB	1.99	0.45
1:I:80:MET:HE3	1:I:80:MET:HB3	1.80	0.45
1:T:38:GLN:HA	1:T:39:PRO:HD2	1.83	0.45
1:I:229:LEU:HD23	1:I:229:LEU:HA	1.75	0.45
1:N:119:GLN:NE2	1:N:201:ASP:OD1	2.42	0.45
1:S:42:ARG:NH1	1:S:74:LEU:O	2.49	0.45
1:Y:179:MET:HE2	1:Y:193:LEU:HD21	1.98	0.45
1:C:79:SER:OG	1:E:64:ARG:NH2	2.50	0.44
1:N:227:GLU:O	1:N:230:VAL:HG22	2.17	0.44
1:O:111:ASN:H	1:O:111:ASN:HD22	1.65	0.44
1:S:35:LEU:CD2	1:S:45:VAL:HG22	2.47	0.44
1:2:229:LEU:HD23	1:2:229:LEU:HA	1.84	0.44
1:A:91:VAL:O	1:A:95:ILE:HG13	2.18	0.44
1:F:47:GLN:HB2	1:F:115:LEU:HB2	1.99	0.44
1:K:31:ARG:HG2	1:K:194:ASP:OD2	2.16	0.44
1:M:133:GLN:CD	1:M:133:GLN:H	2.25	0.44
1:Q:191:LEU:HD23	1:Q:193:LEU:HG	1.98	0.44
1:G:173:GLN:HG3	1:H:239:LEU:HD11	1.98	0.44
1:W:241:LEU:HD13	1:X:209:TYR:CD2	2.52	0.44
1:D:218:PHE:O	1:D:222:ARG:HG3	2.17	0.44
1:E:215:HIS:HA	1:E:216:PRO:HD3	1.89	0.44
1:G:87:LEU:HD21	1:G:114:LEU:CD1	2.48	0.44
1:I:218:PHE:CE2	1:I:222:ARG:HD2	2.52	0.44
1:M:218:PHE:HA	1:M:221:ILE:HG22	2.00	0.44
1:M:80:MET:HG2	1:M:126:ARG:HB2	2.00	0.44
1:N:218:PHE:HA	1:N:221:ILE:HG22	1.98	0.44
1:Q:43:THR:C	1:Q:44:LEU:HD12	2.43	0.44
1:N:63:GLN:O	1:N:66:CYS:HB2	2.18	0.44
1:K:35:LEU:HD11	1:K:196:MET:HE1	1.99	0.44
1:L:191:LEU:HD23	1:L:193:LEU:HG	1.99	0.44
1:T:18:SER:CB	1:T:29:THR:HG23	2.48	0.44
1:N:80:MET:HB3	1:N:126:ARG:HD3	2.00	0.43
1:G:218:PHE:O	1:G:222:ARG:HG3	2.18	0.43
1:I:218:PHE:O	1:I:222:ARG:HG3	2.18	0.43
1:R:58:ILE:HD13	1:R:91:VAL:HG22	1.99	0.43
1:S:232:ILE:HD11	1:T:232:ILE:HG12	1.99	0.43
1:T:215:HIS:CE1	1:T:217:TYR:HB3	2.53	0.43
1:H:114:LEU:HB2	1:H:130:ILE:HB	2.00	0.43
1:I:26:HIS:HB3	8:I:423:HOH:O	2.18	0.43
1:U:152:LYS:HD2	1:V:152:LYS:HD2	1.99	0.43
1:Y:236:LEU:HD22	1:Z:221:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ASN:ND2	1:A:110:PHE:HD1	2.17	0.43
1:I:167:PRO:HG2	1:I:170:GLN:CG	2.48	0.43
1:P:87:LEU:O	1:P:91:VAL:HG23	2.18	0.43
1:P:89:GLU:HG2	1:P:92:ARG:HH11	1.83	0.43
1:E:8:LEU:HD21	1:E:162:LEU:HD11	1.99	0.43
1:I:21:ASN:HA	1:I:27:ILE:HA	1.99	0.43
1:P:170:GLN:N	1:P:170:GLN:OE1	2.51	0.43
1:R:168:LEU:HD12	1:R:168:LEU:HA	1.86	0.43
1:1:9:SER:HB3	1:1:164:TYR:CE2	2.53	0.43
1:2:125:LEU:HG	1:2:200:LEU:HD13	2.00	0.43
1:I:223:LYS:NZ	1:I:227:GLU:OE2	2.26	0.43
1:M:218:PHE:O	1:M:222:ARG:HG3	2.19	0.43
1:C:58:ILE:HD13	1:C:91:VAL:HG22	2.01	0.43
1:S:35:LEU:HD23	1:S:45:VAL:HG22	2.01	0.43
1:W:168:LEU:HD12	1:W:168:LEU:HA	1.89	0.43
1:F:229:LEU:HA	1:F:229:LEU:HD23	1.63	0.43
1:V:35:LEU:HD23	1:V:45:VAL:HG22	2.00	0.43
1:2:194:ASP:OD1	1:2:210:ARG:NE	2.51	0.43
1:F:196:MET:HE2	1:F:198:TYR:HB2	2.00	0.43
1:K:192:PRO:HB2	1:K:210:ARG:HD2	2.01	0.43
1:L:218:PHE:O	1:L:222:ARG:HG3	2.19	0.43
1:M:38:GLN:OE1	1:M:39:PRO:HD2	2.17	0.43
1:O:204:SER:OG	1:O:206:GLU:HG2	2.19	0.43
1:U:221:ILE:HG13	1:V:236:LEU:HD13	2.00	0.43
1:W:150:GLU:OE1	8:W:401:HOH:O	2.21	0.43
1:Y:140:THR:HB	2:1:301:SO4:O3	2.19	0.43
1:O:191:LEU:CD2	1:O:193:LEU:HG	2.49	0.43
1:W:80:MET:HB2	1:W:126:ARG:HD3	2.00	0.43
1:1:109:ASP:HB2	1:1:110:PHE:H	1.68	0.43
1:C:87:LEU:HD23	1:C:87:LEU:HA	1.84	0.42
1:N:60:SER:HB3	1:N:64:ARG:NH1	2.34	0.42
1:Q:121:LYS:NZ	8:Q:409:HOH:O	2.47	0.42
1:Z:218:PHE:HA	1:Z:221:ILE:HG22	2.00	0.42
1:G:169:ASP:HA	1:H:239:LEU:HD22	2.01	0.42
1:P:229:LEU:HD23	1:P:229:LEU:HA	1.72	0.42
1:1:153:TYR:CE1	1:2:152:LYS:HG2	2.54	0.42
1:D:168:LEU:HD13	1:D:197:ILE:HG23	2.00	0.42
1:F:64:ARG:NH1	8:F:401:HOH:O	2.47	0.42
1:J:239:LEU:HD11	1:J:241:LEU:HD21	2.01	0.42
1:X:210:ARG:HH12	1:Z:142:ASP:CG	2.27	0.42
1:J:168:LEU:HG	1:J:197:ILE:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:THR:O	1:D:118:GLY:HA3	2.19	0.42
1:D:80:MET:HB3	1:D:126:ARG:HD3	2.01	0.42
1:N:63:GLN:HG2	1:N:63:GLN:H	1.74	0.42
1:O:218:PHE:O	1:O:222:ARG:HG3	2.19	0.42
1:D:36:PHE:HB3	1:D:75:MET:HE3	2.02	0.42
1:N:223:LYS:HE3	1:N:227:GLU:OE2	2.19	0.42
1:U:37:GLN:NE2	1:U:42:ARG:O	2.53	0.42
1:Y:228:GLY:O	1:Y:232:ILE:HG12	2.19	0.42
1:C:213:GLU:O	1:C:219:MET:HE3	2.20	0.42
1:E:193:LEU:HB2	1:E:211:ILE:HB	2.02	0.42
1:G:12:LEU:HD11	1:G:125:LEU:HB3	2.01	0.42
1:I:125:LEU:HG	1:I:200:LEU:HD13	2.02	0.42
1:L:182:THR:CG2	1:L:189:VAL:HG21	2.49	0.42
1:R:168:LEU:HG	1:R:197:ILE:HG23	2.01	0.42
1:X:35:LEU:CD2	1:X:45:VAL:HG22	2.49	0.42
1:2:1:THR:HG21	1:2:49:ALA:HA	2.02	0.42
1:D:19:ARG:O	1:D:32:LYS:NZ	2.53	0.42
1:G:232:ILE:CG1	1:H:232:ILE:HD11	2.50	0.42
1:H:215:HIS:HA	1:H:216:PRO:HD3	1.89	0.42
1:Z:187:LEU:HD23	8:Z:431:HOH:O	2.19	0.42
1:R:229:LEU:HD23	1:R:229:LEU:HA	1.87	0.42
1:Z:47:GLN:HB2	1:Z:115:LEU:HB2	2.02	0.42
1:Z:74:LEU:HD23	1:Z:74:LEU:HA	1.85	0.42
1:E:191:LEU:HD23	1:E:193:LEU:HG	2.02	0.42
1:W:152:LYS:CG	1:X:153:TYR:CZ	3.02	0.42
1:1:6:MET:O	1:1:12:LEU:HD23	2.19	0.42
1:A:51:ASN:CG	1:A:110:PHE:HD1	2.28	0.41
1:N:8:LEU:HD21	1:N:162:LEU:HD11	2.01	0.41
1:N:14:PHE:O	1:N:172:MET:HE1	2.20	0.41
1:P:196:MET:HE2	1:P:198:TYR:HB2	2.01	0.41
1:S:126:ARG:HH12	1:U:64:ARG:NH1	2.18	0.41
1:H:123:GLU:OE2	1:H:126:ARG:NH1	2.49	0.41
1:K:196:MET:HE2	1:K:208:GLN:HG3	2.01	0.41
1:O:79:SER:HB2	1:O:123:GLU:OE2	2.20	0.41
1:C:31:ARG:NH1	8:C:415:HOH:O	2.53	0.41
1:J:218:PHE:CE2	1:J:222:ARG:HD2	2.55	0.41
1:N:35:LEU:HD21	1:N:196:MET:SD	2.60	0.41
1:V:38:GLN:HB3	1:V:42:ARG:HG2	2.03	0.41
1:F:64:ARG:NH1	1:F:65:ARG:HE	2.18	0.41
1:I:204:SER:HB2	1:I:206:GLU:HG3	2.03	0.41
1:L:191:LEU:CD2	1:L:193:LEU:HG	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:168:LEU:HD12	1:U:168:LEU:HA	1.79	0.41
1:X:218:PHE:O	1:X:222:ARG:HG3	2.20	0.41
1:1:73:ASN:O	1:1:77:VAL:HG13	2.21	0.41
1:1:218:PHE:HA	1:1:221:ILE:HG22	2.02	0.41
1:I:2:TYR:CZ	1:I:4:VAL:HG22	2.55	0.41
1:K:193:LEU:HB2	1:K:211:ILE:HB	2.02	0.41
1:O:91:VAL:O	1:O:95:ILE:HG13	2.21	0.41
1:Y:18:SER:HB2	1:Y:29:THR:HG23	2.02	0.41
1:B:218:PHE:HA	1:B:221:ILE:HG22	2.02	0.41
1:F:31:ARG:HH22	3:F:301:EDO:C2	2.24	0.41
1:F:113:ASN:O	1:F:114:LEU:HD23	2.20	0.41
1:K:191:LEU:HB3	1:K:192:PRO:HA	2.02	0.41
1:U:191:LEU:CD2	1:U:193:LEU:HG	2.49	0.41
1:1:240:LYS:HE2	1:1:240:LYS:HB3	1.81	0.41
1:A:54:THR:OG1	1:A:110:PHE:HB3	2.21	0.41
1:F:215:HIS:HA	1:F:216:PRO:HD3	1.83	0.41
1:K:168:LEU:HD23	1:K:168:LEU:HA	1.81	0.41
1:X:64:ARG:HD2	1:X:67:LEU:HD12	2.02	0.41
1:1:239:LEU:HD12	1:2:217:TYR:CE2	2.56	0.41
1:2:38:GLN:HB3	1:2:42:ARG:HG2	2.02	0.41
1:L:129:HIS:CD2	1:L:129:HIS:C	2.99	0.41
1:L:215:HIS:HA	1:L:216:PRO:HD2	1.86	0.41
1:O:49:ALA:O	1:O:112:CYS:HB2	2.20	0.41
1:O:80:MET:HB3	1:O:128:PHE:HE1	1.85	0.41
1:S:233:PHE:HA	1:S:236:LEU:HD13	2.01	0.41
1:T:215:HIS:HE1	1:T:217:TYR:HB3	1.86	0.41
1:W:218:PHE:O	1:W:222:ARG:HG3	2.19	0.41
1:Z:17:ASP:O	8:Z:402:HOH:O	2.22	0.41
1:A:71:GLN:HG2	8:A:403:HOH:O	2.21	0.41
1:C:129:HIS:CD2	1:C:129:HIS:C	2.99	0.41
1:C:228:GLY:O	1:C:232:ILE:HG12	2.20	0.41
1:E:58:ILE:HD13	1:E:91:VAL:HG22	2.03	0.41
1:F:74:LEU:HD23	1:F:86:LEU:HD23	2.03	0.41
1:G:184:ARG:NH2	8:G:410:HOH:O	2.54	0.41
1:H:192:PRO:HB2	1:H:210:ARG:HD2	2.03	0.41
1:I:216:PRO:HG2	8:I:436:HOH:O	2.20	0.41
1:J:208:GLN:O	1:J:208:GLN:HG3	2.20	0.41
1:L:182:THR:HG22	1:L:189:VAL:HG21	2.02	0.41
1:L:215:HIS:CE1	1:L:217:TYR:HB3	2.56	0.41
1:N:168:LEU:HD23	1:N:168:LEU:HA	1.89	0.41
1:O:125:LEU:HG	1:O:200:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:80:MET:HG2	1:P:126:ARG:HB2	2.03	0.41
1:P:191:LEU:HD23	1:P:193:LEU:HG	2.02	0.41
1:R:2:TYR:O	1:R:179:MET:HE1	2.20	0.41
1:S:66:CYS:SG	1:S:75:MET:HG2	2.61	0.41
1:Y:66:CYS:SG	1:Y:75:MET:HG2	2.61	0.41
1:I:191:LEU:HB3	1:I:192:PRO:HA	2.03	0.41
1:J:2:TYR:O	1:J:179:MET:HE1	2.20	0.41
1:K:199:PRO:HD2	1:K:202:SER:OG	2.21	0.41
1:K:228:GLY:O	1:K:232:ILE:HG12	2.20	0.41
1:H:1:THR:HA	1:H:17:ASP:OD1	2.20	0.40
1:H:157:ILE:O	1:H:161:VAL:HB	2.21	0.40
1:T:218:PHE:HA	1:T:221:ILE:HG22	2.03	0.40
1:E:1:THR:OG1	1:E:32:LYS:HE2	2.21	0.40
1:F:179:MET:HG2	1:F:193:LEU:CD1	2.51	0.40
1:I:240:LYS:HD2	1:I:240:LYS:HA	1.73	0.40
1:K:42:ARG:NH1	1:K:74:LEU:O	2.51	0.40
1:Q:38:GLN:HA	1:Q:39:PRO:HD2	1.93	0.40
1:Q:191:LEU:CD2	1:Q:193:LEU:HG	2.51	0.40
1:T:80:MET:HE2	1:T:80:MET:HB2	1.85	0.40
1:X:1:THR:OG1	1:X:32:LYS:HE2	2.21	0.40
1:Z:80:MET:HE3	1:Z:118:GLY:C	2.46	0.40
1:Z:168:LEU:HG	1:Z:197:ILE:HG23	2.03	0.40
1:A:35:LEU:HD23	1:A:45:VAL:HG22	2.03	0.40
1:A:51:ASN:O	1:A:55:THR:HG23	2.22	0.40
1:I:47:GLN:HB2	1:I:115:LEU:HB2	2.02	0.40
1:I:66:CYS:SG	1:I:75:MET:HG2	2.61	0.40
1:M:218:PHE:CE2	1:M:222:ARG:HD2	2.57	0.40
1:Q:80:MET:HB3	1:Q:126:ARG:HD3	2.03	0.40
1:Q:196:MET:HA	1:Q:207:GLN:O	2.22	0.40
1:S:218:PHE:O	1:S:222:ARG:HG3	2.21	0.40
1:W:11:GLY:HA2	1:W:125:LEU:HD11	2.02	0.40
1:K:236:LEU:HA	1:K:237:PRO:HD3	1.96	0.40
1:L:10:SER:OG	1:L:168:LEU:HD13	2.22	0.40
1:F:91:VAL:O	1:F:95:ILE:HG12	2.21	0.40
1:J:80:MET:HG2	1:J:126:ARG:HB2	2.04	0.40
1:J:168:LEU:HD12	1:J:168:LEU:HA	1.96	0.40
1:K:3:CYS:HB2	1:K:148:ILE:CG1	2.50	0.40
1:R:193:LEU:HB2	1:R:211:ILE:HB	2.03	0.40
1:T:168:LEU:HD11	1:T:199:PRO:HA	2.04	0.40
1:W:239:LEU:HD12	1:X:217:TYR:CE2	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:LYS:NZ	1:L:234:ALA:O[2_656]	2.19	0.01

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	1	230/251 (92%)	225 (98%)	5 (2%)	0	100	100
1	2	214/251 (85%)	211 (99%)	3 (1%)	0	100	100
1	A	221/251 (88%)	217 (98%)	4 (2%)	0	100	100
1	B	229/251 (91%)	225 (98%)	4 (2%)	0	100	100
1	C	232/251 (92%)	228 (98%)	4 (2%)	0	100	100
1	D	230/251 (92%)	228 (99%)	2 (1%)	0	100	100
1	E	229/251 (91%)	226 (99%)	3 (1%)	0	100	100
1	F	230/251 (92%)	226 (98%)	4 (2%)	0	100	100
1	G	230/251 (92%)	225 (98%)	5 (2%)	0	100	100
1	H	230/251 (92%)	224 (97%)	6 (3%)	0	100	100
1	I	229/251 (91%)	224 (98%)	5 (2%)	0	100	100
1	J	231/251 (92%)	228 (99%)	3 (1%)	0	100	100
1	K	229/251 (91%)	223 (97%)	6 (3%)	0	100	100
1	L	233/251 (93%)	230 (99%)	3 (1%)	0	100	100
1	M	229/251 (91%)	225 (98%)	4 (2%)	0	100	100
1	N	220/251 (88%)	217 (99%)	2 (1%)	1 (0%)	24	43
1	O	219/251 (87%)	216 (99%)	3 (1%)	0	100	100
1	P	231/251 (92%)	225 (97%)	6 (3%)	0	100	100
1	Q	233/251 (93%)	229 (98%)	4 (2%)	0	100	100
1	R	233/251 (93%)	229 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	231/251 (92%)	227 (98%)	4 (2%)	0	100	100
1	T	231/251 (92%)	225 (97%)	6 (3%)	0	100	100
1	U	231/251 (92%)	227 (98%)	4 (2%)	0	100	100
1	V	230/251 (92%)	226 (98%)	4 (2%)	0	100	100
1	W	229/251 (91%)	225 (98%)	4 (2%)	0	100	100
1	X	232/251 (92%)	227 (98%)	5 (2%)	0	100	100
1	Y	230/251 (92%)	226 (98%)	4 (2%)	0	100	100
1	Z	232/251 (92%)	228 (98%)	4 (2%)	0	100	100
All	All	6408/7028 (91%)	6292 (98%)	115 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	97	ARG

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	1	202/217 (93%)	200 (99%)	2 (1%)	68	86
1	2	192/217 (88%)	188 (98%)	4 (2%)	47	74
1	A	198/217 (91%)	197 (100%)	1 (0%)	81	92
1	B	202/217 (93%)	201 (100%)	1 (0%)	81	92
1	C	203/217 (94%)	201 (99%)	2 (1%)	68	86
1	D	203/217 (94%)	202 (100%)	1 (0%)	81	92
1	E	203/217 (94%)	202 (100%)	1 (0%)	81	92
1	F	203/217 (94%)	202 (100%)	1 (0%)	81	92
1	G	203/217 (94%)	200 (98%)	3 (2%)	57	80
1	H	203/217 (94%)	199 (98%)	4 (2%)	48	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	202/217 (93%)	200 (99%)	2 (1%)	68	86
1	J	203/217 (94%)	201 (99%)	2 (1%)	68	86
1	K	203/217 (94%)	201 (99%)	2 (1%)	68	86
1	L	204/217 (94%)	202 (99%)	2 (1%)	68	86
1	M	202/217 (93%)	200 (99%)	2 (1%)	68	86
1	N	197/217 (91%)	196 (100%)	1 (0%)	81	92
1	O	196/217 (90%)	195 (100%)	1 (0%)	81	92
1	P	204/217 (94%)	203 (100%)	1 (0%)	81	92
1	Q	205/217 (94%)	201 (98%)	4 (2%)	48	75
1	R	205/217 (94%)	204 (100%)	1 (0%)	81	92
1	S	203/217 (94%)	200 (98%)	3 (2%)	57	80
1	T	203/217 (94%)	201 (99%)	2 (1%)	68	86
1	U	203/217 (94%)	202 (100%)	1 (0%)	81	92
1	V	203/217 (94%)	201 (99%)	2 (1%)	68	86
1	W	203/217 (94%)	202 (100%)	1 (0%)	81	92
1	X	203/217 (94%)	202 (100%)	1 (0%)	81	92
1	Y	203/217 (94%)	202 (100%)	1 (0%)	81	92
1	Z	203/217 (94%)	201 (99%)	2 (1%)	68	86
All	All	5657/6076 (93%)	5606 (99%)	51 (1%)	70	87

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	B	8	LEU
1	C	8	LEU
1	C	191	LEU
1	D	8	LEU
1	E	8	LEU
1	F	8	LEU
1	G	8	LEU
1	G	16	SER
1	G	129	HIS
1	H	8	LEU
1	H	37	GLN
1	H	55	THR

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Mol	Chain	Res	Type
1	H	161	VAL
1	I	4	VAL
1	I	8	LEU
1	J	8	LEU
1	J	161	VAL
1	K	8	LEU
1	K	31	ARG
1	L	8	LEU
1	L	64	ARG
1	M	8	LEU
1	M	168	LEU
1	N	8	LEU
1	O	111	ASN
1	P	8	LEU
1	Q	8	LEU
1	Q	35	LEU
1	Q	55	THR
1	Q	161	VAL
1	R	8	LEU
1	S	8	LEU
1	S	168	LEU
1	S	193	LEU
1	T	8	LEU
1	T	161	VAL
1	U	8	LEU
1	V	8	LEU
1	V	109	ASP
1	W	8	LEU
1	X	8	LEU
1	Y	8	LEU
1	Z	8	LEU
1	Z	64	ARG
1	1	8	LEU
1	1	241	LEU
1	2	8	LEU
1	2	35	LEU
1	2	61	LEU
1	2	98	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	207	GLN
1	C	21	ASN
1	C	37	GLN
1	C	235	GLN
1	D	26	HIS
1	D	113	ASN
1	E	26	HIS
1	E	113	ASN
1	F	71	GLN
1	F	111	ASN
1	G	207	GLN
1	H	37	GLN
1	H	147	GLN
1	I	147	GLN
1	J	173	GLN
1	L	21	ASN
1	L	26	HIS
1	L	34	HIS
1	M	207	GLN
1	N	170	GLN
1	N	208	GLN
1	O	111	ASN
1	O	141	GLN
1	O	207	GLN
1	Q	26	HIS
1	Q	147	GLN
1	R	37	GLN
1	R	71	GLN
1	S	34	HIS
1	S	113	ASN
1	T	37	GLN
1	T	71	GLN
1	T	141	GLN
1	T	170	GLN
1	V	37	GLN
1	V	207	GLN
1	W	26	HIS
1	W	113	ASN
1	W	147	GLN
1	X	26	HIS
1	X	71	GLN
1	Y	38	GLN
1	1	113	ASN

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Mol	Chain	Res	Type
1	1	147	GLN
1	1	207	GLN
1	2	37	GLN
1	2	147	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 47 ligands modelled in this entry, 17 are monoatomic and 4 are unknown - leaving 26 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	B	301	-	4,4,4	0.30	0	6,6,6	0.32	0
6	AZI	J	301	-	2,2,2	2.86	2 (100%)	0,1,1	-	-
2	SO4	B	302	-	4,4,4	0.26	0	6,6,6	0.16	0
2	SO4	P	302	-	4,4,4	0.29	0	6,6,6	0.22	0
3	EDO	K	301	-	3,3,3	0.45	0	2,2,2	0.56	0
2	SO4	E	302	-	4,4,4	0.27	0	6,6,6	0.12	0
2	SO4	V	301	-	4,4,4	0.24	0	6,6,6	0.10	0
2	SO4	X	301	-	4,4,4	0.28	0	6,6,6	0.09	0
2	SO4	E	301	-	4,4,4	0.29	0	6,6,6	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	F	301	-	3,3,3	0.57	0	2,2,2	0.34	0
3	EDO	L	301	-	3,3,3	0.40	0	2,2,2	0.34	0
2	SO4	2	301	-	4,4,4	0.28	0	6,6,6	0.31	0
3	EDO	C	301	-	3,3,3	0.42	0	2,2,2	0.34	0
3	EDO	D	301	-	3,3,3	0.37	0	2,2,2	0.49	0
2	SO4	X	303	-	4,4,4	0.26	0	6,6,6	0.19	0
2	SO4	1	301	-	4,4,4	0.38	0	6,6,6	0.20	0
7	PEG	T	302	-	6,6,6	0.44	0	5,5,5	0.51	0
3	EDO	O	301	-	3,3,3	0.51	0	2,2,2	0.33	0
2	SO4	P	301	-	4,4,4	0.29	0	6,6,6	0.20	0
2	SO4	L	302	-	4,4,4	0.25	0	6,6,6	0.18	0
7	PEG	N	301	-	6,6,6	0.49	0	5,5,5	0.56	0
2	SO4	X	302	-	4,4,4	0.32	0	6,6,6	0.17	0
2	SO4	Z	301	-	4,4,4	0.28	0	6,6,6	0.11	0
2	SO4	2	302	-	4,4,4	0.28	0	6,6,6	0.19	0
2	SO4	A	301	-	4,4,4	0.24	0	6,6,6	0.14	0
2	SO4	W	301	-	4,4,4	0.25	0	6,6,6	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PEG	N	301	-	-	3/4/4/4	-
3	EDO	L	301	-	-	0/1/1/1	-
3	EDO	K	301	-	-	1/1/1/1	-
3	EDO	C	301	-	-	1/1/1/1	-
3	EDO	D	301	-	-	1/1/1/1	-
7	PEG	T	302	-	-	0/4/4/4	-
3	EDO	F	301	-	-	1/1/1/1	-
3	EDO	O	301	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	301	AZI	N3-N2	-2.87	1.17	1.23
6	J	301	AZI	N1-N2	-2.84	1.17	1.23

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	N	301	PEG	O2-C3-C4-O4
3	F	301	EDO	O1-C1-C2-O2
3	K	301	EDO	O1-C1-C2-O2
7	N	301	PEG	O1-C1-C2-O2
7	N	301	PEG	C1-C2-O2-C3
3	C	301	EDO	O1-C1-C2-O2
3	D	301	EDO	O1-C1-C2-O2

There are no ring outliers.

12 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	V	301	SO4	1	0
3	F	301	EDO	5	0
3	L	301	EDO	2	0
2	2	301	SO4	4	0
3	C	301	EDO	1	0
3	D	301	EDO	1	0
2	1	301	SO4	1	0
7	T	302	PEG	2	0
3	O	301	EDO	1	0
7	N	301	PEG	3	0
2	X	302	SO4	2	0
2	Z	301	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	234/251 (93%)	-0.15	1 (0%) 88 86	41, 58, 82, 99	0
1	2	220/251 (87%)	0.03	3 (1%) 73 70	46, 69, 94, 124	0
1	A	225/251 (89%)	-0.01	6 (2%) 56 51	36, 63, 93, 123	2 (0%)
1	B	233/251 (92%)	-0.12	2 (0%) 81 78	43, 57, 85, 101	0
1	C	236/251 (94%)	-0.13	3 (1%) 75 71	39, 59, 85, 109	0
1	D	234/251 (93%)	-0.22	3 (1%) 75 71	37, 55, 77, 103	0
1	E	233/251 (92%)	-0.11	3 (1%) 75 71	42, 55, 83, 100	0
1	F	234/251 (93%)	-0.12	2 (0%) 81 78	38, 59, 86, 104	0
1	G	234/251 (93%)	0.05	0 100 100	50, 69, 96, 108	0
1	H	234/251 (93%)	0.09	1 (0%) 88 86	49, 71, 97, 113	0
1	I	233/251 (92%)	0.09	0 100 100	49, 71, 93, 110	0
1	J	235/251 (93%)	-0.01	3 (1%) 75 71	50, 65, 89, 110	0
1	K	233/251 (92%)	-0.08	0 100 100	46, 62, 88, 103	0
1	L	237/251 (94%)	-0.03	1 (0%) 88 86	45, 62, 88, 116	0
1	M	233/251 (92%)	-0.02	2 (0%) 81 78	48, 66, 89, 106	0
1	N	226/251 (90%)	0.05	4 (1%) 67 64	50, 66, 95, 120	0
1	O	225/251 (89%)	0.08	4 (1%) 67 64	46, 68, 96, 116	0
1	P	234/251 (93%)	-0.15	2 (0%) 81 78	26, 57, 81, 107	1 (0%)
1	Q	237/251 (94%)	0.04	4 (1%) 69 65	46, 64, 92, 111	0
1	R	236/251 (94%)	-0.09	5 (2%) 63 59	25, 59, 90, 110	1 (0%)
1	S	235/251 (93%)	0.13	3 (1%) 75 71	51, 70, 95, 107	0
1	T	235/251 (93%)	0.06	2 (0%) 81 78	49, 68, 93, 114	0
1	U	235/251 (93%)	0.03	2 (0%) 81 78	51, 67, 92, 110	0
1	V	234/251 (93%)	-0.07	2 (0%) 81 78	49, 66, 90, 116	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	W	233/251 (92%)	-0.11	3 (1%) 75 71	42, 61, 83, 99	0
1	X	236/251 (94%)	-0.09	1 (0%) 88 86	44, 58, 83, 99	0
1	Y	233/251 (92%)	-0.29	2 (0%) 81 78	27, 53, 80, 101	1 (0%)
1	Z	236/251 (94%)	-0.14	3 (1%) 75 71	41, 59, 87, 103	0
All	All	6523/7028 (92%)	-0.05	67 (1%) 79 76	25, 63, 90, 124	5 (0%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	2	110	PHE	5.0
1	V	24	VAL	4.8
1	P	24	VAL	4.4
1	N	22	ALA	4.3
1	J	242	GLY	4.2
1	A	20	THR	4.0
1	C	24	VAL	3.9
1	F	24	VAL	3.6
1	D	24	VAL	3.6
1	Q	24	VAL	3.5
1	C	242	GLY	3.4
1	O	30	PHE	3.3
1	O	20	THR	3.3
1	F	242	GLY	3.2
1	H	24	VAL	3.2
1	W	24	VAL	3.1
1	Z	242	GLY	3.0
1	D	99	SER	3.0
1	S	24	VAL	2.9
1	A	111[A]	ASN	2.9
1	O	242	GLY	2.9
1	A	30	PHE	2.8
1	Z	100	GLY	2.8
1	Y	24	VAL	2.8
1	1	24	VAL	2.7
1	A	110	PHE	2.7
1	J	24	VAL	2.7
1	U	24	VAL	2.6
1	W	108	THR	2.6
1	L	242	GLY	2.5
1	V	25	ASP	2.5
1	B	24	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	T	26	HIS	2.5
1	N	187	LEU	2.4
1	2	187	LEU	2.4
1	P	23	GLY	2.4
1	S	68	ASP	2.4
1	N	110	PHE	2.4
1	U	242	GLY	2.3
1	2	241	LEU	2.3
1	M	242	GLY	2.3
1	N	30	PHE	2.3
1	R	240	LYS	2.3
1	B	242	GLY	2.3
1	O	95	ILE	2.2
1	Q	36	PHE	2.2
1	S	242	GLY	2.2
1	E	99	SER	2.2
1	Y	100	GLY	2.2
1	Q	78	ALA	2.1
1	A	29	THR	2.1
1	A	187	LEU	2.1
1	C	100	GLY	2.1
1	E	23	GLY	2.1
1	X	100	GLY	2.1
1	W	241	LEU	2.1
1	Z	107	GLY	2.1
1	Q	23	GLY	2.1
1	R	25	ASP	2.1
1	E	24	VAL	2.1
1	R	241	LEU	2.1
1	D	242	GLY	2.1
1	J	99	SER	2.0
1	M	78	ALA	2.0
1	T	242	GLY	2.0
1	R	237	PRO	2.0
1	R	99	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	Z	301	5/5	0.67	0.34	54,62,72,75	5
5	UNX	Q	302	1/1	0.71	0.48	80,80,80,80	0
2	SO4	P	302	5/5	0.74	0.13	71,71,76,79	5
5	UNX	U	302	1/1	0.77	0.23	88,88,88,88	0
5	UNX	Q	303	1/1	0.78	0.43	77,77,77,77	0
2	SO4	B	302	5/5	0.79	0.12	86,112,114,119	0
2	SO4	X	301	5/5	0.81	0.10	106,113,120,120	0
2	SO4	1	301	5/5	0.83	0.14	82,85,92,104	0
2	SO4	W	301	5/5	0.83	0.12	72,86,96,111	0
2	SO4	E	301	5/5	0.84	0.13	65,65,69,75	5
3	EDO	O	301	4/4	0.85	0.21	78,78,79,80	0
2	SO4	L	302	5/5	0.85	0.09	105,109,118,121	0
7	PEG	N	301	7/7	0.85	0.16	74,78,91,91	0
2	SO4	2	302	5/5	0.86	0.11	89,93,100,100	0
2	SO4	E	302	5/5	0.86	0.12	58,69,70,71	5
2	SO4	V	301	5/5	0.87	0.08	111,111,112,113	0
2	SO4	X	302	5/5	0.88	0.20	61,62,74,77	5
2	SO4	X	303	5/5	0.88	0.15	54,71,77,79	5
3	EDO	K	301	4/4	0.89	0.23	66,67,67,75	0
2	SO4	P	301	5/5	0.89	0.13	81,103,108,110	0
6	AZI	J	301	3/3	0.89	0.18	64,64,68,77	0
2	SO4	B	301	5/5	0.89	0.11	80,92,102,110	0
4	CL	T	301	1/1	0.90	0.09	82,82,82,82	0
3	EDO	C	301	4/4	0.91	0.22	54,55,64,64	0
7	PEG	T	302	7/7	0.91	0.15	60,69,76,79	0
3	EDO	F	301	4/4	0.92	0.19	60,63,67,68	0
4	CL	K	302	1/1	0.92	0.14	87,87,87,87	0
4	CL	R	301	1/1	0.92	0.12	82,82,82,82	0
3	EDO	D	301	4/4	0.92	0.21	53,57,59,60	0
3	EDO	L	301	4/4	0.92	0.19	55,61,61,70	0
4	CL	S	301	1/1	0.93	0.14	80,80,80,80	0
4	CL	G	301	1/1	0.94	0.17	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CL	K	303	1/1	0.94	0.18	87,87,87,87	0
4	CL	L	303	1/1	0.94	0.17	86,86,86,86	0
4	CL	U	301	1/1	0.95	0.17	90,90,90,90	0
4	CL	W	302	1/1	0.95	0.14	84,84,84,84	0
4	CL	P	303	1/1	0.95	0.12	79,79,79,79	0
2	SO4	2	301	5/5	0.95	0.09	68,78,84,103	0
4	CL	M	301	1/1	0.96	0.18	85,85,85,85	0
4	CL	1	302	1/1	0.96	0.13	82,82,82,82	0
4	CL	Q	301	1/1	0.97	0.10	77,77,77,77	0
2	SO4	A	301	5/5	0.97	0.06	57,66,68,75	0
4	CL	C	302	1/1	0.97	0.09	78,78,78,78	0
5	UNX	I	301	1/1	0.97	0.19	54,54,54,54	0
4	CL	D	302	1/1	0.97	0.12	78,78,78,78	0
4	CL	Z	302	1/1	0.98	0.08	73,73,73,73	0
4	CL	D	303	1/1	0.99	0.04	60,60,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.