



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:47 PM GMT

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

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

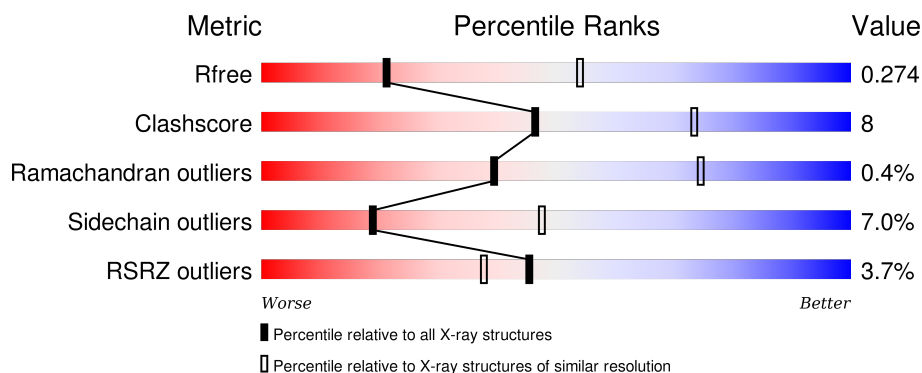
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



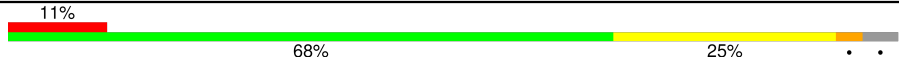
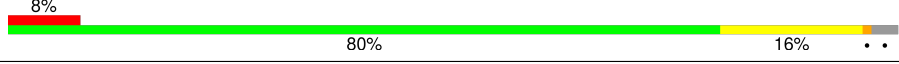



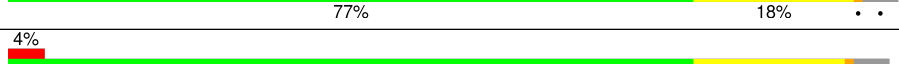
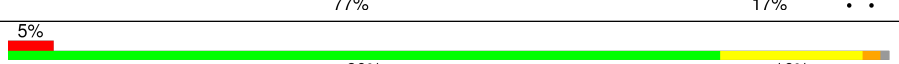
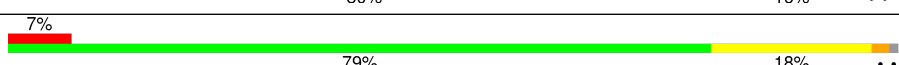
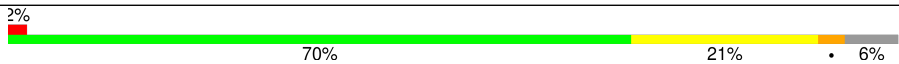
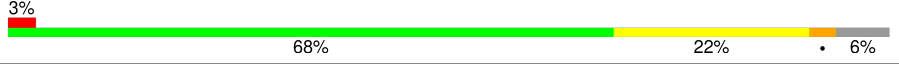
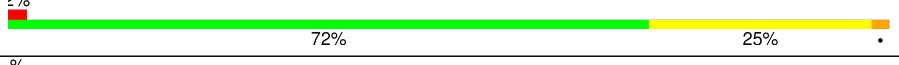
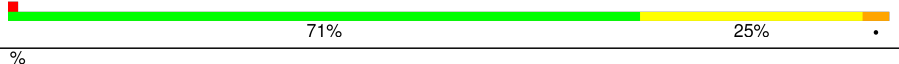
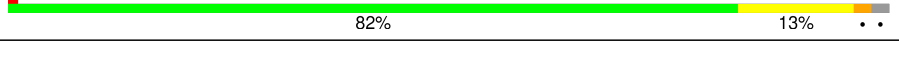

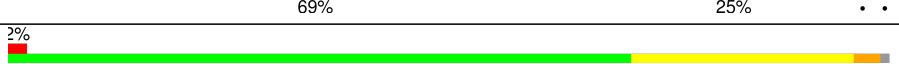



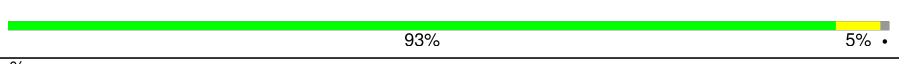

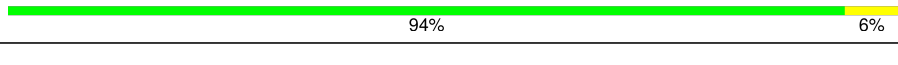

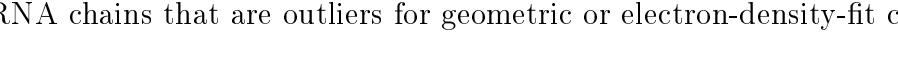
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	234	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>24%</div> <div>• •</div> </div> </div>
1	O	234	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>21%</div> <div>• •</div> </div> </div>
2	B	261	<div> <div>6%</div> <div> <div></div> <div>75%</div> <div>18%</div> <div>• 5%</div> </div> </div>
2	P	261	<div> <div>5%</div> <div> <div></div> <div>76%</div> <div>17%</div> <div>• 5%</div> </div> </div>
3	C	248	<div> <div>13%</div> <div> <div></div> <div>67%</div> <div>25%</div> <div>• •</div> </div> </div>

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Mol	Chain	Length	Quality of chain
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	
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	

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
16	K	I	302	-	-	-	X
16	K	L	303	-	-	-	X
16	K	S	303	-	-	-	X
16	K	a	305	-	-	-	X
16	K	b	203	-	-	-	X
17	04C	K	301	-	-	-	X
17	04C	N	201	-	-	-	X
17	04C	Y	301	-	-	-	X
17	04C	b	201	-	-	-	X

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 49805 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

- 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
			1592	1013	265	295	19			
9	W	204	Total	C	N	O	S	0	0	0
			1592	1013	265	295	19			

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

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

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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
			1654	1047	284	313	10			
12	Z	213	Total	C	N	O	S	0	0	0
			1654	1047	284	313	10			

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	P	1	Total	Cl	0	0
			1	1		
15	J	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	Q	4	Total 4	Cl 4	0	0
15	D	1	Total 1	Cl 1	0	0
15	a	4	Total 4	Cl 4	0	0
15	E	1	Total 1	Cl 1	0	0
15	H	1	Total 1	Cl 1	0	0
15	I	1	Total 1	Cl 1	0	0
15	V	4	Total 4	Cl 4	0	0
15	W	1	Total 1	Cl 1	0	0
15	Z	1	Total 1	Cl 1	0	0
15	A	3	Total 3	Cl 3	0	0
15	N	1	Total 1	Cl 1	0	0
15	U	1	Total 1	Cl 1	0	0
15	X	3	Total 3	Cl 3	0	0
15	O	2	Total 2	Cl 2	0	0
15	R	3	Total 3	Cl 3	0	0
15	L	2	Total 2	Cl 2	0	0
15	S	2	Total 2	Cl 2	0	0
15	M	4	Total 4	Cl 4	0	0

- Molecule 16 is POTASSIUM ION (three-letter code: K) (formula: K).

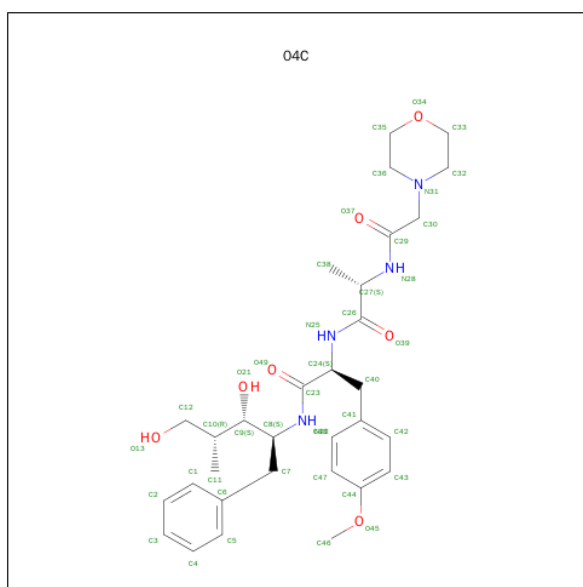
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	G	1	Total 1	K 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	K	1	Total K 1 1	0	0
16	b	1	Total K 1 1	0	0
16	B	1	Total K 1 1	0	0
16	I	1	Total K 1 1	0	0
16	Z	3	Total K 3 3	0	0
16	a	1	Total K 1 1	0	0
16	X	1	Total K 1 1	0	0
16	L	1	Total K 1 1	0	0
16	S	1	Total K 1 1	0	0
16	M	1	Total K 1 1	0	0

- Molecule 17 is 1,2,4-TRIDEOXY-4-METHYL-2-{[N-(MORPHOLIN-4-YLACETYL)-L-ALANYL-O-METHYL-L-TYROSYL]AMINO}-1-PHENYL-D-XYLITOL (three-letter code: 04C) (formula: $C_{31}H_{44}N_4O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	H	1	Total	C	N	O	0	0
			42	31	4	7		
17	K	1	Total	C	N	O	0	0
			42	31	4	7		
17	N	1	Total	C	N	O	0	0
			42	31	4	7		
17	V	1	Total	C	N	O	0	0
			42	31	4	7		
17	Y	1	Total	C	N	O	0	0
			42	31	4	7		
17	b	1	Total	C	N	O	0	0
			42	31	4	7		

- Molecule 18 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	K	1	Total	I	0	0
			1	1		
18	H	1	Total	I	0	0
			1	1		
18	b	1	Total	I	0	0
			1	1		
18	V	1	Total	I	0	0
			1	1		
18	N	1	Total	I	0	0
			1	1		
18	Y	1	Total	I	0	0
			1	1		

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	43	Total	O	0	0
			43	43		
19	B	42	Total	O	0	0
			42	42		
19	C	29	Total	O	0	0
			29	29		
19	D	24	Total	O	0	0
			24	24		
19	E	39	Total	O	0	0
			39	39		
19	F	37	Total	O	0	0
			37	37		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	G	44	Total O 44 44	0	0
19	H	40	Total O 40 40	0	0
19	I	25	Total O 25 25	0	0
19	J	28	Total O 28 28	0	0
19	K	32	Total O 32 32	0	0
19	L	43	Total O 43 43	0	0
19	M	50	Total O 50 50	0	0
19	N	29	Total O 29 29	0	0
19	O	44	Total O 44 44	0	0
19	P	38	Total O 38 38	0	0
19	Q	13	Total O 13 13	0	0
19	R	24	Total O 24 24	0	0
19	S	40	Total O 40 40	0	0
19	T	32	Total O 32 32	0	0
19	U	38	Total O 38 38	0	0
19	V	39	Total O 39 39	0	0
19	W	39	Total O 39 39	0	0
19	X	20	Total O 20 20	0	0
19	Y	36	Total O 36 36	0	0
19	Z	49	Total O 49 49	0	0
19	a	35	Total O 35 35	0	0

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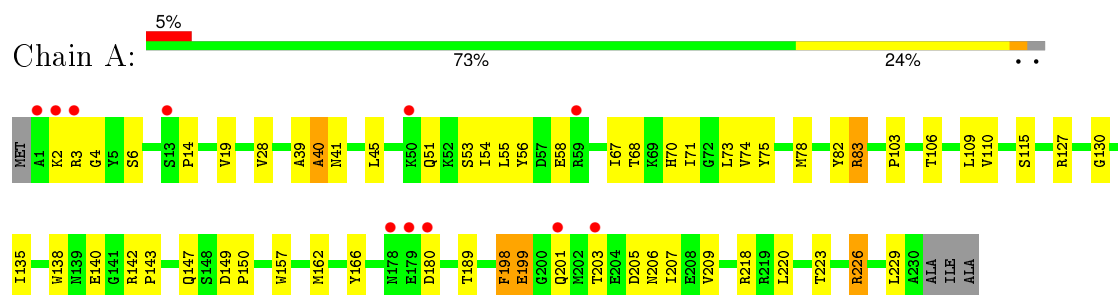
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	b	33	Total	O	0	0
			33	33		

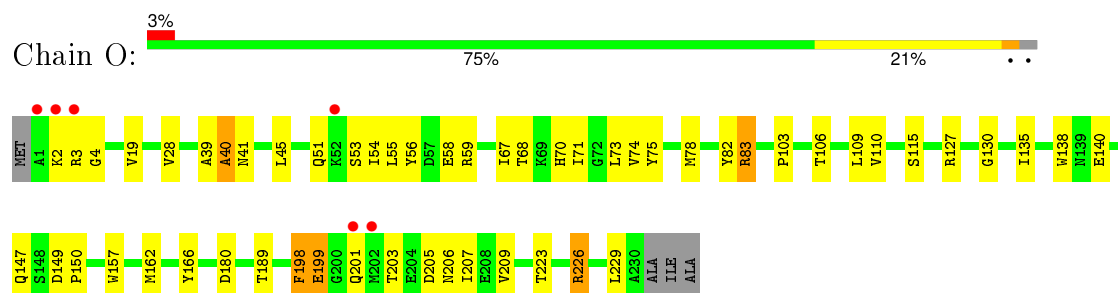
3 Residue-property plots [i](#)

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

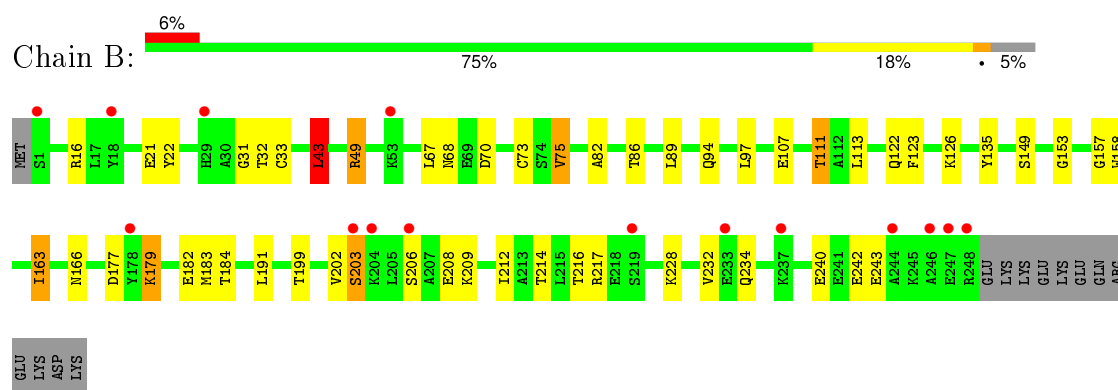
- Molecule 1: Proteasome subunit alpha type-2



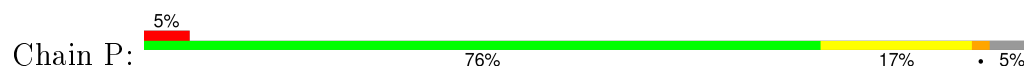
- Molecule 1: Proteasome subunit alpha type-2

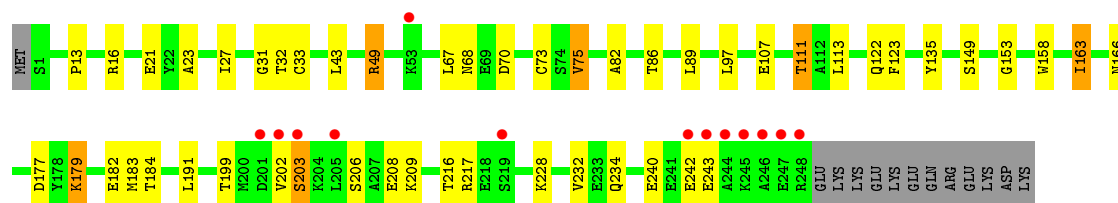


- Molecule 2: Proteasome subunit alpha type-4

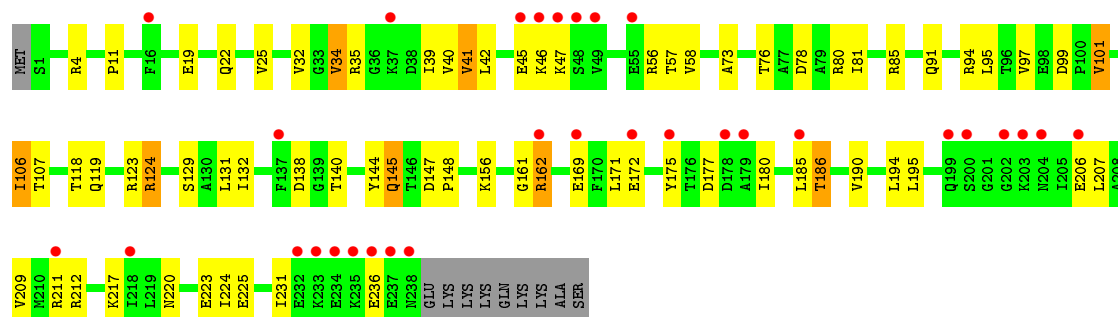


- Molecule 2: Proteasome subunit alpha type-4

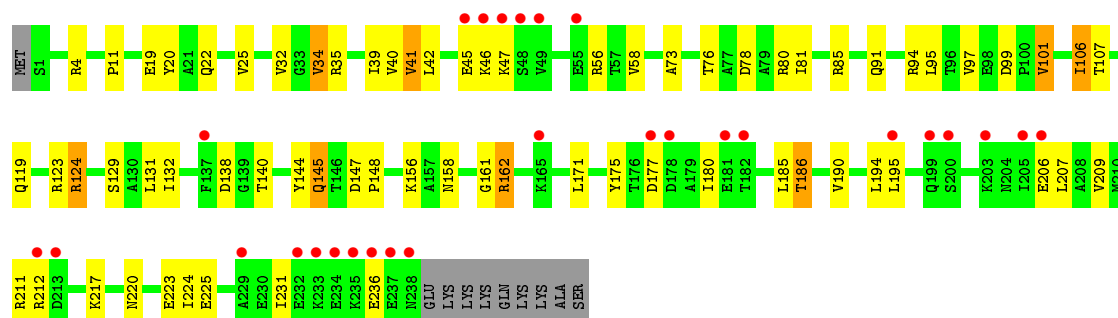




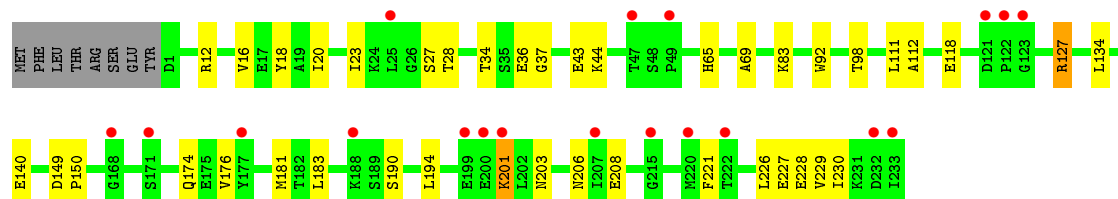
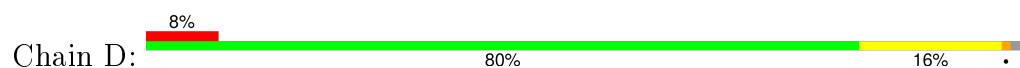
• Molecule 3: Proteasome subunit alpha type-7



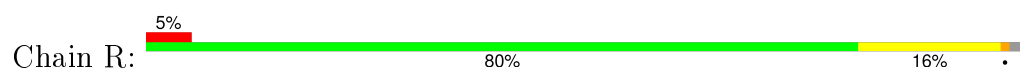
• Molecule 3: Proteasome subunit alpha type-7

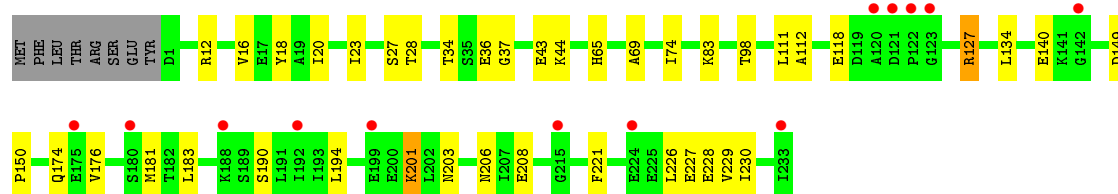


• Molecule 4: Proteasome subunit alpha type-5

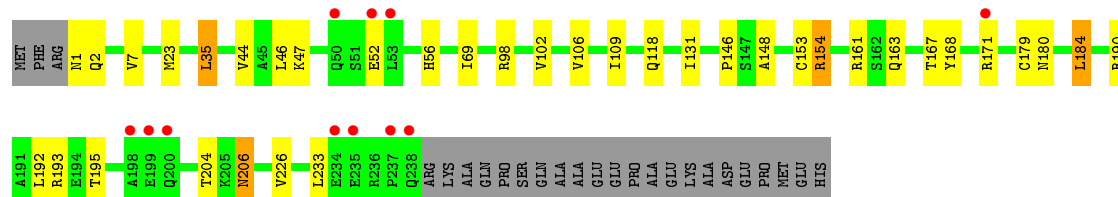
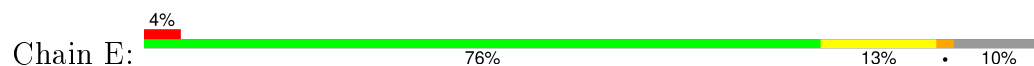


• Molecule 4: Proteasome subunit alpha type-5

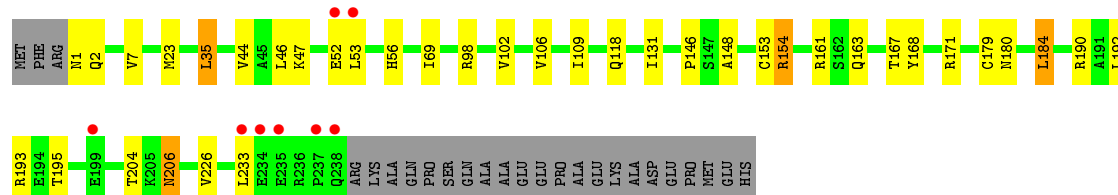
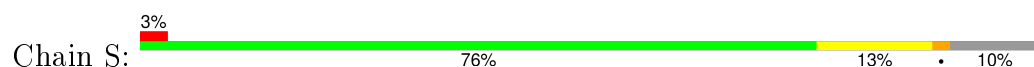




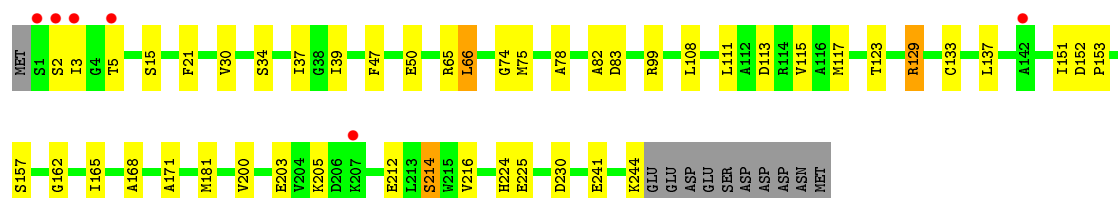
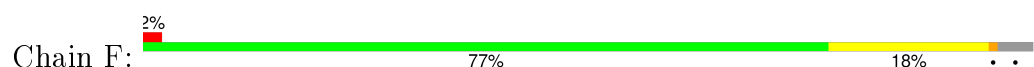
• Molecule 5: Proteasome subunit alpha type-1



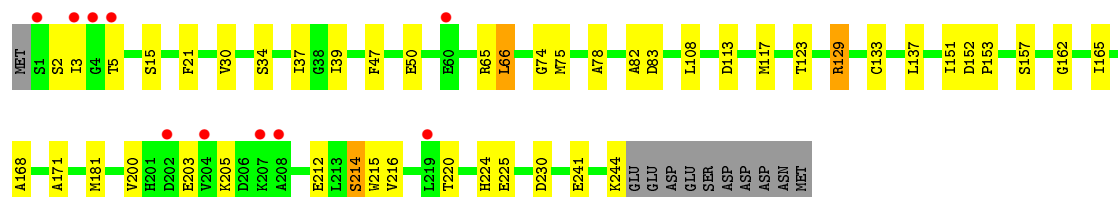
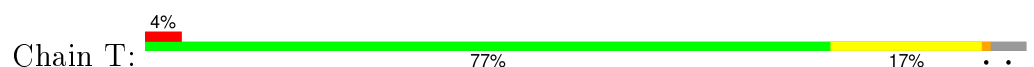
• Molecule 5: Proteasome subunit alpha type-1



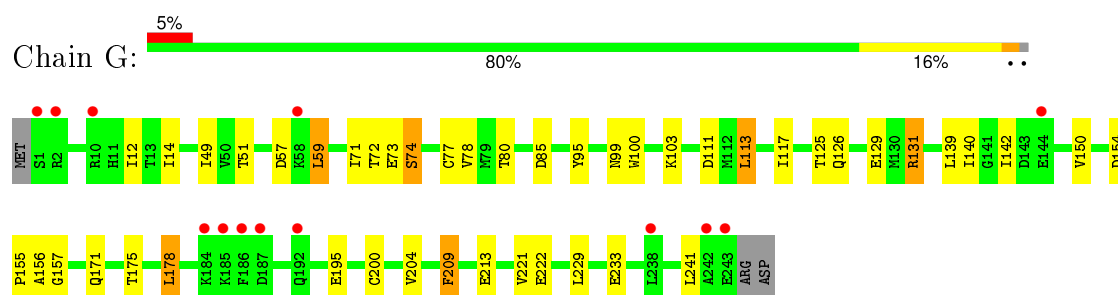
• Molecule 6: Proteasome subunit alpha type-3



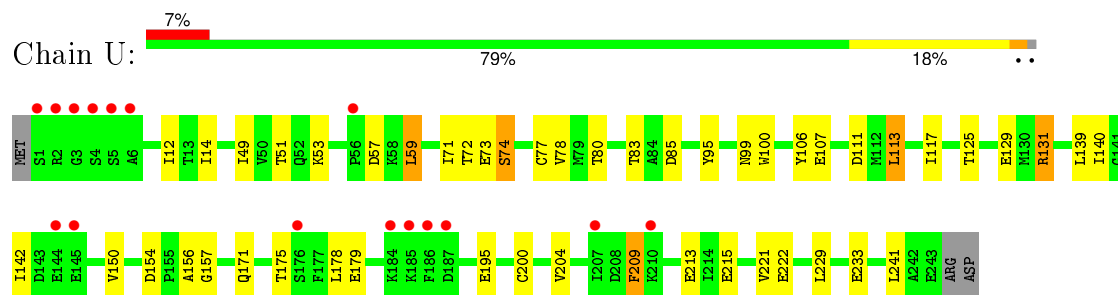
• Molecule 6: Proteasome subunit alpha type-3



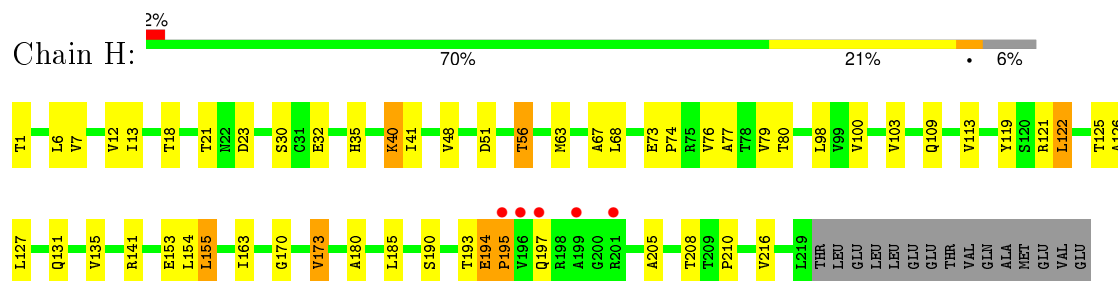
• Molecule 7: Proteasome subunit alpha type-6



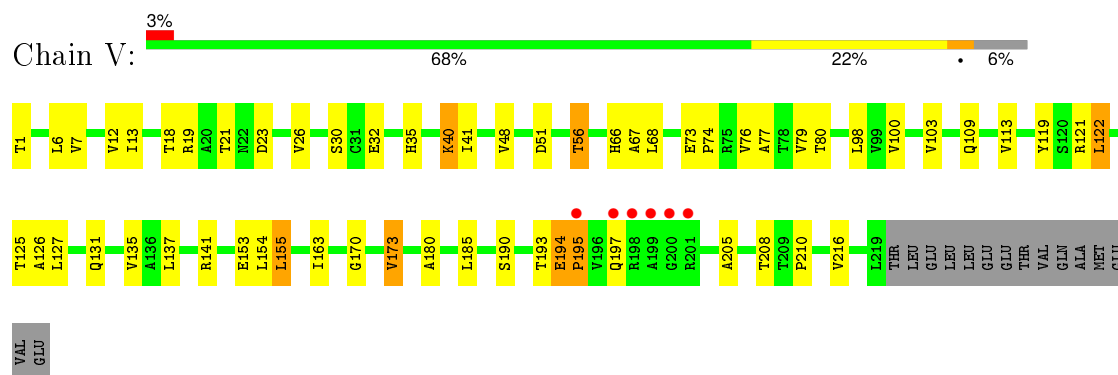
• Molecule 7: Proteasome subunit alpha type-6



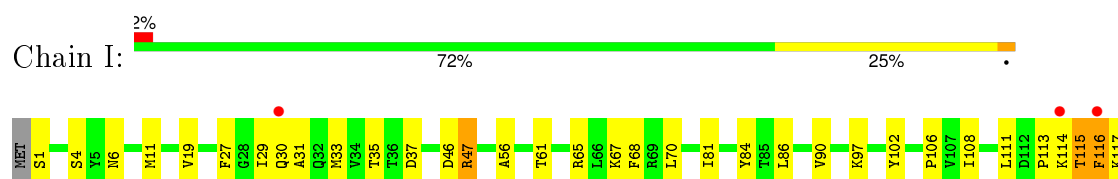
• Molecule 8: Proteasome subunit beta type-10

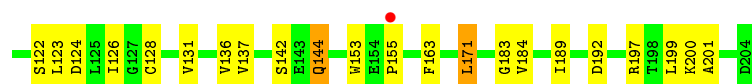


• Molecule 8: Proteasome subunit beta type-10

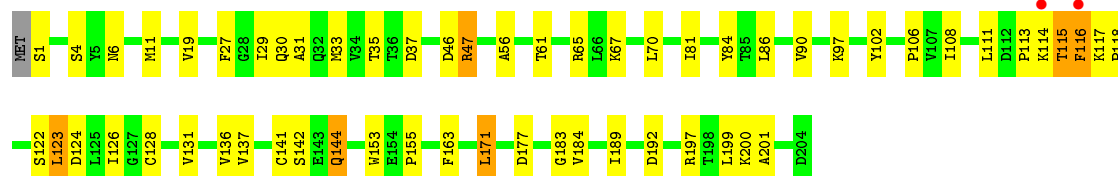
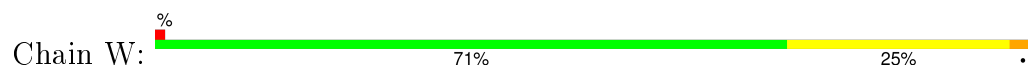


• Molecule 9: Proteasome subunit beta type-3

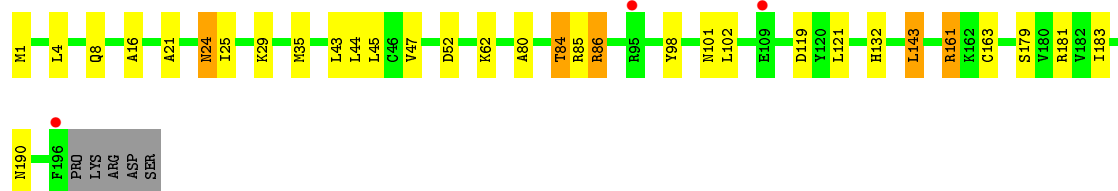
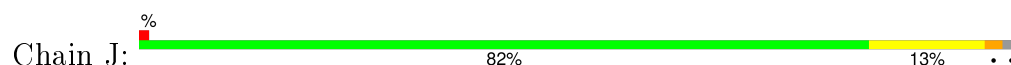




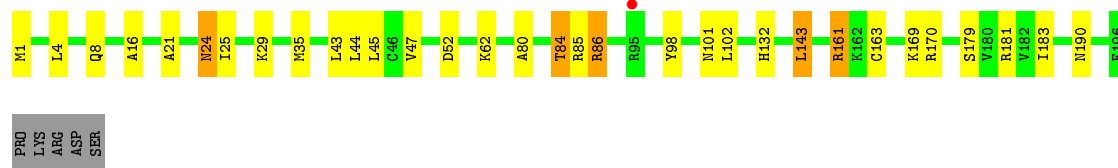
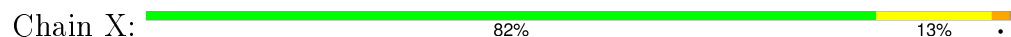
• Molecule 9: Proteasome subunit beta type-3



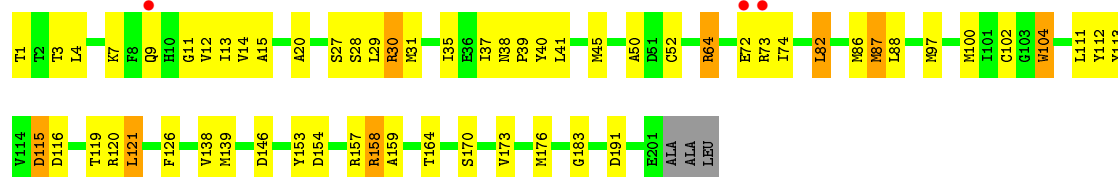
• Molecule 10: Proteasome subunit beta type-2



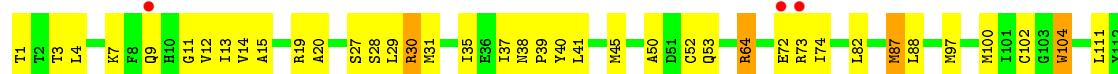
• Molecule 10: Proteasome subunit beta type-2



• Molecule 11: Proteasome subunit beta type-8

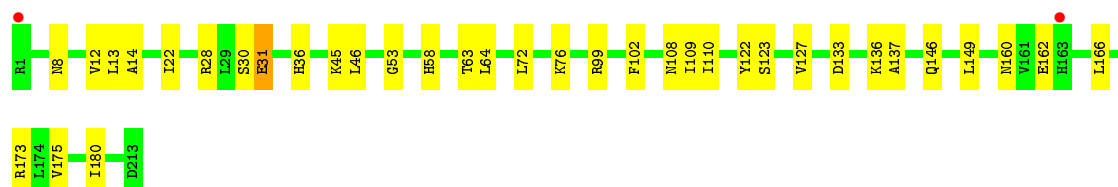
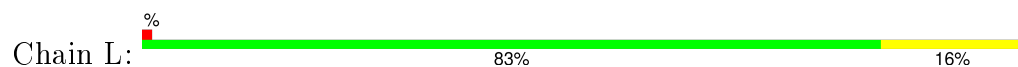


• Molecule 11: Proteasome subunit beta type-8

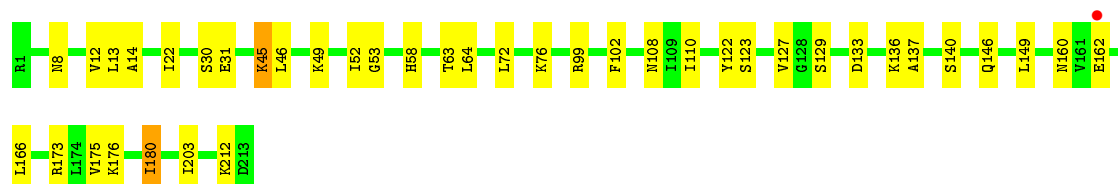
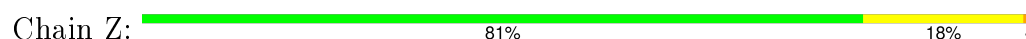




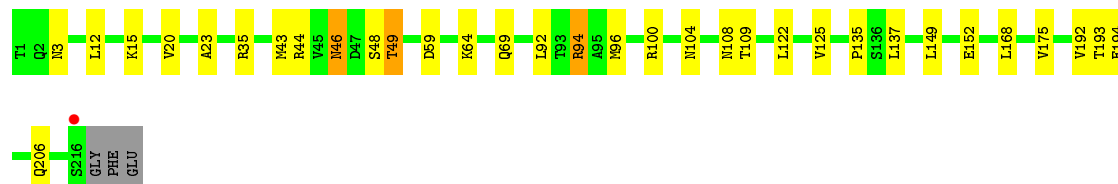
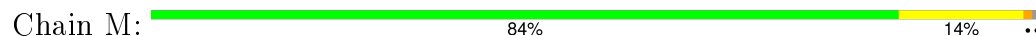
- Molecule 12: Proteasome subunit beta type-1



- Molecule 12: Proteasome subunit beta type-1



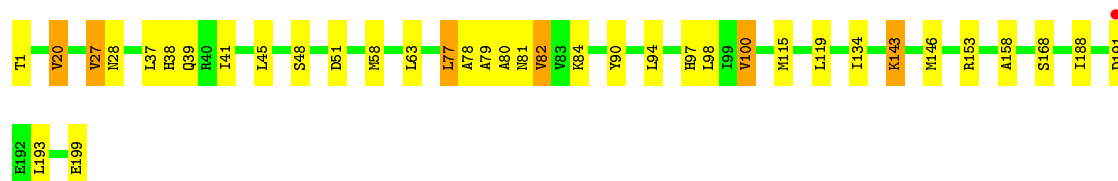
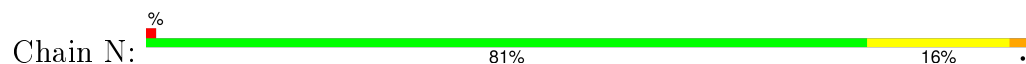
- Molecule 13: Proteasome subunit beta type-4



- Molecule 13: Proteasome subunit beta type-4



- Molecule 14: Proteasome subunit beta type-9



- Molecule 14: Proteasome subunit beta type-9

Chain b:  94% 6% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	117.30Å 194.60Å 157.70Å 90.00° 107.10° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 29.79 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.1 (15.00-2.90) 97.2 (29.79-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.6.0119	Depositor
R, R_{free}	0.235 , 0.275 0.233 , 0.274	Depositor DCC
R_{free} test set	7209 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	46.1	Xtriage
Anisotropy	0.520	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 53.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	2 of 145087 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	49805	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.47 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.5201e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: K, IOD, 04C, 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	0.39	1/1840 (0.1%)	0.50	0/2491
1	O	0.39	1/1840 (0.1%)	0.50	0/2491
2	B	0.37	1/1980 (0.1%)	0.51	1/2667 (0.0%)
2	P	0.37	1/1980 (0.1%)	0.51	0/2667
3	C	0.34	0/1903	0.51	0/2569
3	Q	0.34	0/1903	0.51	0/2569
4	D	0.36	1/1805 (0.1%)	0.47	0/2437
4	R	0.36	0/1805	0.47	0/2437
5	E	0.38	0/1907	0.51	0/2578
5	S	0.37	0/1907	0.51	0/2578
6	F	0.38	0/1938	0.49	0/2608
6	T	0.38	0/1938	0.49	0/2608
7	G	0.37	1/1924 (0.1%)	0.49	0/2600
7	U	0.37	1/1924 (0.1%)	0.49	0/2600
8	H	0.36	1/1645 (0.1%)	0.53	0/2235
8	V	0.37	1/1645 (0.1%)	0.53	0/2235
9	I	0.34	0/1621	0.50	0/2185
9	W	0.34	0/1621	0.50	0/2185
10	J	0.33	0/1602	0.50	0/2167
10	X	0.33	0/1602	0.49	0/2167
11	K	0.43	1/1597 (0.1%)	0.55	0/2151
11	Y	0.43	1/1597 (0.1%)	0.55	0/2151
12	L	0.32	0/1685	0.49	0/2271
12	Z	0.32	0/1685	0.50	0/2271
13	M	0.40	0/1718	0.50	0/2325
13	a	0.40	1/1718 (0.1%)	0.50	0/2325
14	N	0.37	0/1526	0.51	0/2071
14	b	0.37	0/1526	0.51	1/2071 (0.0%)
All	All	0.37	12/49382 (0.0%)	0.50	2/66710 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying

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

Mol	Chain	#Chirality outliers	#Planarity outliers
11	K	0	1
11	Y	0	1
14	N	0	2
14	b	0	1
All	All	0	5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	V	1	THR	C-N	5.77	1.47	1.34
8	H	1	THR	C-N	5.51	1.46	1.34
11	Y	104	TRP	CD2-CE2	5.05	1.47	1.41
7	U	100	TRP	CD2-CE2	5.04	1.47	1.41
1	A	138	TRP	CD2-CE2	5.04	1.47	1.41
11	K	104	TRP	CD2-CE2	5.03	1.47	1.41
7	G	100	TRP	CD2-CE2	5.03	1.47	1.41
1	O	138	TRP	CD2-CE2	5.03	1.47	1.41
2	P	158	TRP	CD2-CE2	5.02	1.47	1.41
4	D	92	TRP	CD2-CE2	5.01	1.47	1.41
13	a	209	TRP	CD2-CE2	5.00	1.47	1.41
2	B	158	TRP	CD2-CE2	5.00	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	1	THR	C-N-CA	5.78	136.14	121.70
2	B	43	LEU	CA-CB-CG	5.14	127.12	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	K	1	THR	Peptide
14	N	1	THR	Mainchain,Peptide
11	Y	1	THR	Peptide
14	b	1	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1801	0	1800	41	0
1	O	1801	0	1800	35	0
2	B	1950	0	1973	29	0
2	P	1950	0	1973	24	0
3	C	1876	0	1902	45	0
3	Q	1876	0	1902	43	0
4	D	1778	0	1767	25	0
4	R	1778	0	1767	27	0
5	E	1872	0	1859	24	0
5	S	1872	0	1859	24	0
6	F	1903	0	1894	30	0
6	T	1903	0	1894	29	0
7	G	1890	0	1900	28	0
7	U	1890	0	1900	31	0
8	H	1619	0	1640	27	0
8	V	1619	0	1640	30	0
9	I	1592	0	1612	32	0
9	W	1592	0	1612	32	0
10	J	1570	0	1573	19	0
10	X	1570	0	1573	18	0
11	K	1566	0	1516	41	1
11	Y	1566	0	1515	40	0
12	L	1654	0	1652	20	0
12	Z	1654	0	1651	25	0
13	M	1685	0	1664	17	1
13	a	1685	0	1664	0	0
14	N	1498	0	1476	20	0
14	b	1498	0	1476	0	0
15	A	3	0	0	0	0
15	D	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	J	1	0	0	0	0
15	L	2	0	0	0	0
15	M	4	0	0	0	0
15	N	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	O	2	0	0	0	0
15	P	1	0	0	0	0
15	Q	4	0	0	0	0
15	R	3	0	0	0	0
15	S	2	0	0	0	0
15	U	1	0	0	0	0
15	V	4	0	0	0	0
15	W	1	0	0	0	0
15	X	3	0	0	0	0
15	Z	1	0	0	0	0
15	a	4	0	0	0	0
16	B	1	0	0	0	0
16	G	1	0	0	0	0
16	I	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	S	1	0	0	0	0
16	X	1	0	0	0	0
16	Z	3	0	0	0	0
16	a	1	0	0	0	0
16	b	1	0	0	0	0
17	H	42	0	42	0	0
17	K	42	0	42	3	0
17	N	42	0	42	3	0
17	V	42	0	42	1	0
17	Y	42	0	42	3	0
17	b	42	0	42	0	0
18	H	1	0	0	0	0
18	K	1	0	0	1	0
18	N	1	0	0	0	0
18	V	1	0	0	1	0
18	Y	1	0	0	0	0
18	b	1	0	0	0	0
19	A	43	0	0	2	0
19	B	42	0	0	4	0
19	C	29	0	0	0	0
19	D	24	0	0	0	0
19	E	39	0	0	0	0
19	F	37	0	0	0	0
19	G	44	0	0	1	0
19	H	40	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	I	25	0	0	0	0
19	J	28	0	0	0	0
19	K	32	0	0	3	0
19	L	43	0	0	3	0
19	M	50	0	0	1	0
19	N	29	0	0	2	0
19	O	44	0	0	0	0
19	P	38	0	0	0	0
19	Q	13	0	0	0	0
19	R	24	0	0	0	0
19	S	40	0	0	0	0
19	T	32	0	0	0	0
19	U	38	0	0	3	0
19	V	39	0	0	0	0
19	W	39	0	0	0	0
19	X	20	0	0	0	0
19	Y	36	0	0	0	0
19	Z	49	0	0	5	0
19	a	35	0	0	0	0
19	b	33	0	0	0	0
All	All	49805	0	48706	700	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 8.

All (700) 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)
5:S:154:ARG:HH11	5:S:154:ARG:HG2	1.26	0.98
11:Y:31:MET:HG2	17:Y:301:04C:H42	1.45	0.98
5:E:154:ARG:HG2	5:E:154:ARG:HH11	1.27	0.96
5:E:2:GLN:HE22	6:F:5:THR:HA	1.29	0.96
3:C:162:ARG:HH11	3:C:162:ARG:HG2	1.31	0.95
3:Q:35:ARG:HH21	3:Q:156:LYS:HG3	1.32	0.93
3:Q:162:ARG:HG2	3:Q:162:ARG:HH11	1.31	0.93
3:C:35:ARG:HH21	3:C:156:LYS:HG3	1.32	0.92
12:Z:110:ILE:HA	19:Z:426:HOH:O	1.67	0.92
12:Z:49:LYS:HB3	19:Z:415:HOH:O	1.72	0.89
8:H:194:GLU:H	8:H:195:PRO:HD3	1.37	0.88
8:V:194:GLU:H	8:V:195:PRO:HD3	1.37	0.87
4:R:201:LYS:H	4:R:201:LYS:HE2	1.42	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:31:MET:HG2	17:K:301:04C:H42	1.57	0.84
12:Z:52:ILE:HA	19:Z:426:HOH:O	1.76	0.84
4:D:201:LYS:H	4:D:201:LYS:HE2	1.44	0.81
8:H:40:LYS:HE2	8:H:73:GLU:HG3	1.63	0.81
11:Y:53:GLN:OE1	12:Z:129:SER:HA	1.82	0.79
8:V:40:LYS:HE2	8:V:73:GLU:HG3	1.65	0.77
5:E:2:GLN:NE2	6:F:5:THR:HA	2.00	0.76
9:W:124:ASP:HB2	9:W:128:CYS:H	1.50	0.76
3:C:41:VAL:HB	3:C:209:VAL:HG12	1.68	0.75
3:C:162:ARG:HG2	3:C:162:ARG:NH1	1.95	0.75
5:S:2:GLN:HE22	6:T:5:THR:HA	1.51	0.75
3:Q:41:VAL:HB	3:Q:209:VAL:HG12	1.68	0.74
5:S:47:LYS:HB3	5:S:56:HIS:HB3	1.69	0.74
12:L:13:LEU:HD11	12:L:149:LEU:HD11	1.70	0.74
9:I:124:ASP:HB2	9:I:128:CYS:H	1.50	0.74
5:E:47:LYS:HB3	5:E:56:HIS:HB3	1.69	0.73
2:P:68:ASN:HD22	2:P:70:ASP:H	1.37	0.73
6:T:151:ILE:HG12	6:T:157:SER:HB3	1.70	0.73
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.70	0.73
12:Z:13:LEU:HD11	12:Z:149:LEU:HD11	1.70	0.72
2:B:68:ASN:HD22	2:B:70:ASP:H	1.37	0.72
6:F:151:ILE:HG12	6:F:157:SER:HB3	1.71	0.72
5:S:154:ARG:HG2	5:S:154:ARG:NH1	2.02	0.71
3:Q:162:ARG:HG2	3:Q:162:ARG:NH1	1.95	0.71
8:V:131:GLN:O	8:V:135:VAL:HG23	1.90	0.71
8:H:131:GLN:O	8:H:135:VAL:HG23	1.91	0.70
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.73	0.70
1:O:83:ARG:HG2	1:O:83:ARG:HH11	1.56	0.69
9:W:115:THR:O	9:W:116:PHE:CD2	2.46	0.69
2:P:166:ASN:HB2	2:P:199:THR:HG23	1.73	0.69
9:I:115:THR:O	9:I:116:PHE:CD2	2.46	0.69
11:Y:138:VAL:HG21	11:Y:159:ALA:HA	1.75	0.69
11:Y:64:ARG:HH11	11:Y:64:ARG:HG3	1.57	0.68
2:B:212:ILE:HG22	19:B:434:HOH:O	1.92	0.68
1:O:45:LEU:HB3	1:O:74:VAL:HG21	1.76	0.68
1:A:45:LEU:HB3	1:A:74:VAL:HG21	1.76	0.68
1:A:83:ARG:HH11	1:A:83:ARG:HG2	1.57	0.68
2:B:166:ASN:HB2	2:B:199:THR:HG23	1.73	0.68
4:D:221:PHE:HB3	4:D:226:LEU:CD1	2.24	0.68
4:R:221:PHE:HB3	4:R:226:LEU:CD1	2.25	0.67
8:H:194:GLU:N	8:H:195:PRO:HD3	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:138:VAL:HG21	11:K:159:ALA:HA	1.75	0.67
1:A:127:ARG:HH21	7:G:125:THR:HG22	1.58	0.67
5:E:2:GLN:HE22	6:F:5:THR:CA	2.06	0.66
12:Z:110:ILE:HG12	19:Z:426:HOH:O	1.93	0.66
8:V:194:GLU:N	8:V:195:PRO:HD3	2.09	0.66
10:J:52:ASP:HB3	10:J:98:TYR:HD2	1.61	0.66
5:E:154:ARG:NH1	5:E:154:ARG:HG2	2.03	0.66
11:Y:41:LEU:HB2	11:Y:73:ARG:HH22	1.60	0.66
5:E:148:ALA:HB3	6:F:82:ALA:HB1	1.77	0.66
8:V:40:LYS:H	8:V:40:LYS:HD3	1.61	0.66
6:T:39:ILE:HG22	6:T:162:GLY:HA2	1.77	0.65
5:S:148:ALA:HB3	6:T:82:ALA:HB1	1.77	0.65
11:K:41:LEU:HB2	11:K:73:ARG:HH22	1.60	0.65
1:O:203:THR:H	1:O:206:ASN:HD22	1.43	0.65
1:A:203:THR:H	1:A:206:ASN:HD22	1.43	0.65
4:R:176:VAL:O	4:R:176:VAL:HG12	1.96	0.65
4:R:34:THR:HG22	4:R:36:GLU:H	1.62	0.65
10:X:52:ASP:HB3	10:X:98:TYR:HD2	1.61	0.65
4:D:176:VAL:HG12	4:D:176:VAL:O	1.96	0.65
3:Q:101:VAL:HG11	3:Q:106:ILE:HG12	1.80	0.64
6:F:39:ILE:HG22	6:F:162:GLY:HA2	1.78	0.64
12:Z:8:ASN:HD22	12:Z:58:HIS:H	1.45	0.64
8:H:40:LYS:H	8:H:40:LYS:HD3	1.61	0.64
2:B:135:TYR:HE1	2:B:149:SER:HB2	1.63	0.64
9:W:144:GLN:H	9:W:144:GLN:HE21	1.46	0.64
8:V:205:ALA:O	8:V:208:THR:HG23	1.97	0.64
4:D:227:GLU:HA	4:D:230:ILE:HG22	1.79	0.63
13:M:59:ASP:HB3	13:M:108:ASN:HD21	1.62	0.63
1:O:149:ASP:HB2	1:O:150:PRO:HD2	1.80	0.63
2:P:135:TYR:HE1	2:P:149:SER:HB2	1.63	0.63
3:C:101:VAL:HG11	3:C:106:ILE:HG12	1.80	0.63
11:K:30:ARG:HG2	11:K:30:ARG:O	1.99	0.63
9:I:144:GLN:HE21	9:I:144:GLN:H	1.47	0.63
12:L:8:ASN:HD22	12:L:58:HIS:H	1.45	0.63
4:D:34:THR:HG22	4:D:36:GLU:H	1.62	0.63
8:H:205:ALA:O	8:H:208:THR:HG23	1.98	0.62
8:H:13:ILE:HG12	8:H:155:LEU:HD22	1.80	0.62
14:N:20:VAL:CG2	14:N:27:VAL:HG22	2.28	0.62
1:O:67:ILE:HD11	1:O:73:LEU:HD12	1.81	0.62
11:K:7:LYS:HB3	11:K:12:VAL:HG22	1.81	0.62
1:A:149:ASP:HB2	1:A:150:PRO:HD2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:162:ARG:HH11	3:C:162:ARG:CG	2.10	0.62
4:R:227:GLU:HA	4:R:230:ILE:HG22	1.80	0.62
12:Z:12:VAL:HG21	12:Z:53:GLY:HA3	1.82	0.61
11:Y:7:LYS:HB3	11:Y:12:VAL:HG22	1.81	0.61
1:A:67:ILE:HD11	1:A:73:LEU:HD12	1.81	0.61
11:Y:30:ARG:O	11:Y:30:ARG:HG2	2.00	0.61
4:R:221:PHE:HB3	4:R:226:LEU:HD12	1.83	0.61
9:I:86:LEU:O	9:I:90:VAL:HG23	2.01	0.61
12:L:14:ALA:HA	12:L:22:ILE:O	2.01	0.60
9:W:86:LEU:O	9:W:90:VAL:HG23	2.01	0.60
3:C:41:VAL:HG22	3:C:190:VAL:HG21	1.83	0.60
12:Z:14:ALA:HA	12:Z:22:ILE:O	2.01	0.60
11:K:64:ARG:HG2	11:K:64:ARG:HH11	1.66	0.60
3:C:35:ARG:NH2	3:C:156:LYS:HG3	2.11	0.60
1:O:127:ARG:HH21	7:U:125:THR:HG22	1.67	0.60
1:O:4:GLY:HA2	7:U:129:GLU:HG2	1.82	0.60
3:Q:41:VAL:HG22	3:Q:190:VAL:HG21	1.83	0.59
3:Q:162:ARG:CG	3:Q:162:ARG:HH11	2.10	0.59
4:D:221:PHE:HB3	4:D:226:LEU:HD12	1.83	0.59
6:T:168:ALA:HB3	6:T:200:VAL:HG13	1.84	0.59
6:F:47:PHE:HB2	6:F:214:SER:HB2	1.85	0.59
1:A:45:LEU:HD13	1:A:74:VAL:HG23	1.85	0.59
12:L:12:VAL:HG21	12:L:53:GLY:HA3	1.84	0.59
10:J:86:ARG:HA	10:J:86:ARG:HE	1.67	0.58
4:D:44:LYS:HE2	4:D:208:GLU:HG3	1.85	0.58
1:O:45:LEU:HD13	1:O:74:VAL:HG23	1.85	0.58
6:F:66:LEU:HD22	6:F:212:GLU:HB3	1.85	0.58
10:X:86:ARG:HA	10:X:86:ARG:HE	1.67	0.58
14:N:80:ALA:HB1	14:N:119:LEU:HD11	1.85	0.58
6:T:47:PHE:HB2	6:T:214:SER:HB2	1.85	0.58
6:T:66:LEU:HD22	6:T:212:GLU:HB3	1.85	0.58
11:K:73:ARG:HD2	11:K:74:ILE:H	1.69	0.58
6:F:168:ALA:HB3	6:F:200:VAL:HG13	1.84	0.58
4:R:44:LYS:HE2	4:R:208:GLU:HG3	1.85	0.58
8:V:13:ILE:HG12	8:V:155:LEU:HD22	1.86	0.57
3:Q:35:ARG:NH2	3:Q:156:LYS:HG3	2.11	0.57
3:Q:39:ILE:HG22	3:Q:211:ARG:HA	1.87	0.57
8:V:41:ILE:HG21	8:V:79:VAL:HG21	1.87	0.57
11:Y:38:ASN:HB2	11:Y:73:ARG:NH2	2.20	0.57
11:Y:73:ARG:HD2	11:Y:74:ILE:H	1.70	0.57
1:A:45:LEU:HB3	1:A:74:VAL:CG2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:38:ASN:HB2	11:K:73:ARG:NH2	2.19	0.56
3:Q:45:GLU:OE2	3:Q:194:LEU:HB3	2.06	0.56
3:C:45:GLU:OE2	3:C:194:LEU:HB3	2.06	0.56
3:C:39:ILE:HG22	3:C:211:ARG:HA	1.87	0.56
5:S:2:GLN:NE2	6:T:5:THR:HA	2.19	0.56
8:V:141:ARG:HB2	8:V:154:LEU:HD13	1.87	0.56
1:A:218:ARG:HG3	19:A:430:HOH:O	2.04	0.56
8:H:41:ILE:HG21	8:H:79:VAL:HG21	1.88	0.56
9:I:184:VAL:HB	9:I:199:LEU:HD12	1.88	0.56
2:P:135:TYR:CE1	2:P:149:SER:HB2	2.41	0.56
13:M:92:LEU:O	13:M:96:MET:HG2	2.06	0.56
9:W:184:VAL:HB	9:W:199:LEU:HD12	1.88	0.56
5:E:161:ARG:HD2	5:E:195:THR:O	2.06	0.56
1:O:45:LEU:HB3	1:O:74:VAL:CG2	2.35	0.55
5:S:161:ARG:HD2	5:S:195:THR:O	2.07	0.55
11:Y:3:THR:HG22	11:Y:100:MET:CE	2.36	0.55
11:Y:37:ILE:HG22	11:Y:38:ASN:HD22	1.71	0.55
11:K:37:ILE:HG22	11:K:38:ASN:HD22	1.72	0.55
17:N:201:04C:H8	17:N:201:04C:H22	1.88	0.55
14:N:98:LEU:HD21	19:N:310:HOH:O	2.05	0.55
8:V:109:GLN:HG2	8:V:121:ARG:HH11	1.71	0.55
11:K:3:THR:HG22	11:K:100:MET:CE	2.36	0.55
3:C:25:VAL:HG21	3:C:129:SER:HB2	1.87	0.55
2:B:135:TYR:CE1	2:B:149:SER:HB2	2.41	0.55
4:R:174:GLN:HE21	5:S:52:GLU:HG2	1.72	0.55
8:H:194:GLU:N	8:H:195:PRO:CD	2.70	0.55
8:H:141:ARG:HB2	8:H:154:LEU:HD13	1.88	0.55
2:P:153:GLY:O	3:Q:80:ARG:NH2	2.34	0.55
3:Q:25:VAL:HG21	3:Q:129:SER:HB2	1.87	0.55
8:H:109:GLN:HG2	8:H:121:ARG:HH11	1.70	0.55
5:E:44:VAL:HG12	5:E:192:LEU:HD22	1.89	0.55
7:U:57:ASP:OD2	7:U:59:LEU:HB2	2.06	0.55
8:V:35:HIS:CG	8:V:56:THR:HG21	2.42	0.54
2:B:75:VAL:HG21	2:B:82:ALA:HB1	1.89	0.54
5:S:193:ARG:HH22	5:S:233:LEU:HD12	1.73	0.54
7:G:57:ASP:OD2	7:G:59:LEU:HB2	2.07	0.54
3:Q:32:VAL:HG12	3:Q:194:LEU:HD21	1.88	0.54
3:C:32:VAL:HG12	3:C:194:LEU:HD21	1.87	0.54
11:K:112:TYR:HB3	19:K:406:HOH:O	2.06	0.54
1:A:39:ALA:O	1:A:41:ASN:N	2.36	0.54
8:V:40:LYS:N	8:V:40:LYS:HD3	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:58:VAL:O	3:C:58:VAL:HG12	2.07	0.54
2:P:75:VAL:HG21	2:P:82:ALA:HB1	1.90	0.54
7:U:95:TYR:O	7:U:99:ASN:HB2	2.08	0.54
5:E:193:ARG:HH22	5:E:233:LEU:HD12	1.73	0.54
6:T:152:ASP:HB2	6:T:153:PRO:HD2	1.90	0.54
3:C:19:GLU:HA	3:C:22:GLN:HE21	1.72	0.54
7:G:95:TYR:O	7:G:99:ASN:HB2	2.08	0.54
8:V:98:LEU:HB2	8:V:113:VAL:HG13	1.90	0.54
3:Q:58:VAL:O	3:Q:58:VAL:HG12	2.07	0.53
2:B:212:ILE:CG2	19:B:434:HOH:O	2.53	0.53
13:M:15:LYS:HB3	13:M:20:VAL:HG22	1.88	0.53
3:Q:19:GLU:HA	3:Q:22:GLN:HE21	1.72	0.53
8:V:194:GLU:N	8:V:195:PRO:CD	2.70	0.53
4:D:221:PHE:HB3	4:D:226:LEU:HD11	1.89	0.53
11:K:153:TYR:O	11:K:157:ARG:HB2	2.09	0.53
14:N:45:LEU:HD23	17:N:201:O4C:H44	1.89	0.53
6:T:34:SER:HB2	6:T:50:GLU:HG3	1.90	0.53
5:S:44:VAL:HG12	5:S:192:LEU:HD22	1.89	0.53
4:R:221:PHE:HB3	4:R:226:LEU:HD11	1.90	0.53
12:L:109:ILE:HB	19:L:442:HOH:O	2.08	0.53
8:H:35:HIS:CG	8:H:56:THR:HG21	2.44	0.53
6:F:152:ASP:HB2	6:F:153:PRO:HD2	1.90	0.53
4:D:203:ASN:HB3	4:D:206:ASN:HB2	1.91	0.53
3:Q:81:ILE:O	3:Q:85:ARG:HG2	2.09	0.53
14:N:20:VAL:HG23	14:N:27:VAL:HG22	1.91	0.53
13:M:15:LYS:HE2	13:M:135:PRO:HA	1.91	0.53
9:I:171:LEU:HD21	9:I:199:LEU:HD13	1.91	0.53
3:C:95:LEU:HG	10:J:62:LYS:HG2	1.89	0.53
11:Y:153:TYR:O	11:Y:157:ARG:HB2	2.09	0.52
3:Q:180:ILE:HA	3:Q:186:THR:HG23	1.91	0.52
4:R:16:VAL:O	4:R:20:ILE:HG12	2.09	0.52
3:C:81:ILE:O	3:C:85:ARG:HG2	2.09	0.52
6:F:34:SER:HB2	6:F:50:GLU:HG3	1.90	0.52
10:X:35:MET:HG2	10:X:45:LEU:HD22	1.92	0.52
9:I:11:MET:HG3	9:I:137:VAL:HG12	1.91	0.52
11:Y:3:THR:HG22	11:Y:100:MET:HE1	1.90	0.52
4:D:16:VAL:O	4:D:20:ILE:HG12	2.09	0.52
11:Y:97:MET:H	11:Y:116:ASP:HB3	1.74	0.52
12:L:99:ARG:HD2	12:L:102:PHE:O	2.10	0.52
9:W:171:LEU:HD21	9:W:199:LEU:HD13	1.91	0.52
4:D:27:SER:HB2	4:D:43:GLU:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:11:MET:HG3	9:W:137:VAL:HG12	1.91	0.52
2:P:31:GLY:HA2	2:P:49:ARG:NH1	2.25	0.52
11:Y:38:ASN:HB2	11:Y:73:ARG:CZ	2.39	0.52
11:K:40:TYR:HB3	11:K:183:GLY:HA2	1.91	0.52
11:K:40:TYR:HE1	11:K:73:ARG:HG2	1.75	0.52
7:G:77:CYS:HB3	7:G:139:LEU:HD23	1.92	0.52
14:N:84:LYS:HG3	14:N:119:LEU:HB2	1.92	0.52
8:V:210:PRO:HB2	9:W:200:LYS:HB3	1.92	0.52
2:B:31:GLY:HA2	2:B:49:ARG:NH1	2.25	0.52
7:U:77:CYS:HB3	7:U:139:LEU:HD23	1.92	0.52
6:F:123:THR:O	7:G:131:ARG:NH1	2.43	0.52
8:H:40:LYS:N	8:H:40:LYS:HD3	2.23	0.52
11:K:138:VAL:CG2	11:K:159:ALA:HA	2.40	0.52
11:Y:40:TYR:HB3	11:Y:183:GLY:HA2	1.91	0.52
10:X:21:ALA:HB3	10:X:29:LYS:HB2	1.92	0.52
6:F:78:ALA:HB3	6:F:165:ILE:HD12	1.92	0.52
8:H:98:LEU:HB2	8:H:113:VAL:HG13	1.92	0.52
11:K:74:ILE:HD11	19:K:422:HOH:O	2.10	0.51
4:R:203:ASN:HB3	4:R:206:ASN:HB2	1.91	0.51
12:Z:99:ARG:HD2	12:Z:102:PHE:O	2.10	0.51
3:Q:78:ASP:OD1	3:Q:124:ARG:NH2	2.43	0.51
11:K:115:ASP:HB2	11:K:119:THR:HB	1.92	0.51
11:K:97:MET:H	11:K:116:ASP:HB3	1.74	0.51
3:C:78:ASP:OD1	3:C:124:ARG:NH2	2.44	0.51
2:B:153:GLY:O	3:C:80:ARG:NH2	2.36	0.51
8:V:103:VAL:HG11	8:V:180:ALA:HA	1.91	0.51
1:O:198:PHE:O	1:O:199:GLU:CB	2.59	0.51
12:Z:110:ILE:HB	12:Z:122:TYR:HB2	1.92	0.51
11:Y:138:VAL:CG2	11:Y:159:ALA:HA	2.41	0.51
11:K:38:ASN:HB2	11:K:73:ARG:CZ	2.41	0.51
11:K:100:MET:SD	11:K:126:PHE:HB2	2.51	0.51
4:R:174:GLN:HA	5:S:53:LEU:HD21	1.92	0.51
11:Y:115:ASP:HB2	11:Y:119:THR:HB	1.92	0.51
10:J:35:MET:HG2	10:J:45:LEU:HD22	1.92	0.51
11:Y:40:TYR:HE1	11:Y:73:ARG:HG2	1.76	0.51
3:C:180:ILE:HA	3:C:186:THR:HG23	1.91	0.51
11:Y:100:MET:SD	11:Y:126:PHE:HB2	2.51	0.51
6:T:78:ALA:HB3	6:T:165:ILE:HD12	1.92	0.51
1:O:39:ALA:O	1:O:41:ASN:N	2.36	0.51
2:B:67:LEU:HD11	2:B:73:CYS:HB3	1.93	0.51
8:H:103:VAL:HG11	8:H:180:ALA:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:GLN:HE21	9:I:68:PHE:HA	1.76	0.51
13:M:92:LEU:HD23	13:M:125:VAL:HG21	1.93	0.50
4:R:27:SER:HB2	4:R:43:GLU:HG3	1.91	0.50
6:F:241:GLU:HA	6:F:244:LYS:NZ	2.25	0.50
8:H:67:ALA:HB2	8:H:74:PRO:HG3	1.93	0.50
1:A:198:PHE:O	1:A:199:GLU:CB	2.59	0.50
1:A:51:GLN:HG2	1:A:56:TYR:CD2	2.46	0.50
9:W:47:ARG:HG2	9:W:111:LEU:HB2	1.94	0.50
12:L:8:ASN:ND2	12:L:58:HIS:H	2.09	0.50
1:A:4:GLY:HA2	7:G:129:GLU:HG2	1.94	0.50
3:Q:95:LEU:HG	10:X:62:LYS:HG2	1.93	0.50
10:X:101:ASN:HB3	10:X:132:HIS:CE1	2.46	0.50
11:Y:87:MET:HG3	11:Y:116:ASP:HA	1.93	0.50
1:O:147:GLN:HG3	1:O:162:MET:HE1	1.93	0.50
2:P:31:GLY:HA2	2:P:49:ARG:HH11	1.77	0.50
10:J:101:ASN:HB3	10:J:132:HIS:CE1	2.46	0.50
9:I:46:ASP:O	9:I:47:ARG:CB	2.59	0.50
2:P:206:SER:HB3	2:P:209:LYS:HD2	1.94	0.49
11:K:72:GLU:O	11:K:72:GLU:HG2	2.12	0.49
4:R:34:THR:HB	4:R:37:GLY:O	2.12	0.49
9:W:46:ASP:O	9:W:47:ARG:CB	2.59	0.49
2:P:67:LEU:HD11	2:P:73:CYS:HB3	1.93	0.49
10:J:21:ALA:HB3	10:J:29:LYS:HB2	1.93	0.49
11:Y:40:TYR:CE1	11:Y:73:ARG:HG2	2.47	0.49
4:D:34:THR:HB	4:D:37:GLY:O	2.12	0.49
8:V:67:ALA:HB2	8:V:74:PRO:HG3	1.94	0.49
11:Y:31:MET:CG	17:Y:301:04C:H42	2.32	0.49
3:C:35:ARG:HA	3:C:40:VAL:HG13	1.95	0.49
14:N:63:LEU:HD21	14:N:79:ALA:HA	1.93	0.49
1:A:220:LEU:HD23	19:A:430:HOH:O	2.12	0.49
7:G:171:GLN:O	7:G:175:THR:HG23	2.12	0.49
1:A:106:THR:O	1:A:110:VAL:HG23	2.13	0.49
12:L:22:ILE:HG21	12:L:175:VAL:HG21	1.95	0.49
6:T:74:GLY:HA3	6:T:224:HIS:CD2	2.48	0.49
2:B:206:SER:HB3	2:B:209:LYS:HD2	1.94	0.49
9:I:47:ARG:HG2	9:I:111:LEU:HB2	1.94	0.49
2:P:13:PRO:HA	3:Q:20:TYR:CE2	2.46	0.49
3:Q:35:ARG:HA	3:Q:40:VAL:HG13	1.95	0.49
9:I:124:ASP:HB3	9:I:126:ILE:H	1.78	0.49
12:L:8:ASN:HA	12:L:30:SER:O	2.13	0.49
7:U:171:GLN:O	7:U:175:THR:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:40:TYR:CE1	11:K:73:ARG:HG2	2.47	0.48
3:C:131:LEU:HD23	3:C:145:GLN:HB3	1.95	0.48
1:O:106:THR:O	1:O:110:VAL:HG23	2.13	0.48
11:K:87:MET:HG3	11:K:116:ASP:HA	1.94	0.48
4:R:34:THR:HG23	4:R:181:MET:O	2.14	0.48
12:Z:8:ASN:ND2	12:Z:58:HIS:H	2.09	0.48
7:U:107:GLU:HG3	19:U:424:HOH:O	2.12	0.48
11:Y:173:VAL:HG12	11:Y:191:ASP:HA	1.95	0.48
6:F:74:GLY:HA3	6:F:224:HIS:CD2	2.48	0.48
9:W:124:ASP:HB3	9:W:126:ILE:H	1.78	0.48
11:Y:72:GLU:O	11:Y:72:GLU:HG2	2.12	0.48
4:R:149:ASP:HB2	4:R:150:PRO:CD	2.43	0.48
1:O:51:GLN:HG2	1:O:56:TYR:CD2	2.49	0.48
4:D:149:ASP:HB2	4:D:150:PRO:CD	2.42	0.48
2:B:31:GLY:HA2	2:B:49:ARG:HH11	1.77	0.48
3:Q:91:GLN:HE21	10:X:62:LYS:HG3	1.79	0.48
11:K:173:VAL:HG12	11:K:191:ASP:HA	1.95	0.48
4:D:34:THR:HG23	4:D:181:MET:O	2.13	0.48
8:H:210:PRO:HB2	9:I:200:LYS:HB3	1.95	0.48
10:X:44:LEU:HD11	10:X:102:LEU:HD13	1.96	0.48
11:K:3:THR:HG22	11:K:100:MET:HE1	1.94	0.48
7:G:72:THR:HG22	7:G:74:SER:H	1.79	0.48
5:S:2:GLN:HE22	6:T:5:THR:H	1.62	0.48
9:W:46:ASP:O	9:W:47:ARG:HB2	2.14	0.48
9:I:46:ASP:O	9:I:47:ARG:HB2	2.13	0.48
6:T:108:LEU:HD11	6:T:137:LEU:HB3	1.96	0.48
2:B:89:LEU:HG	2:B:113:LEU:HD13	1.96	0.48
12:Z:22:ILE:HG21	12:Z:175:VAL:HG21	1.95	0.47
6:T:152:ASP:HB2	6:T:153:PRO:CD	2.44	0.47
1:O:147:GLN:HE21	1:O:157:TRP:HE1	1.62	0.47
9:I:113:PRO:O	9:I:114:LYS:HB2	2.14	0.47
4:D:65:HIS:CE1	4:D:98:THR:HB	2.49	0.47
10:J:181:ARG:HG2	10:J:190:ASN:HA	1.96	0.47
6:F:152:ASP:HB2	6:F:153:PRO:CD	2.45	0.47
10:X:143:LEU:HD13	10:X:163:CYS:SG	2.55	0.47
5:S:2:GLN:HE22	6:T:5:THR:CA	2.23	0.47
11:K:72:GLU:O	11:K:73:ARG:HB3	2.14	0.47
3:Q:175:TYR:CZ	3:Q:180:ILE:HD11	2.50	0.47
7:U:12:ILE:HG13	7:U:14:ILE:HG12	1.96	0.47
12:L:110:ILE:HB	12:L:122:TYR:HB2	1.96	0.47
6:F:168:ALA:HB1	6:F:171:ALA:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:122:SER:HB3	9:I:136:VAL:HB	1.96	0.47
10:J:80:ALA:O	10:J:84:THR:HG23	2.13	0.47
14:N:38:HIS:CD2	14:N:39:GLN:H	2.33	0.47
12:Z:8:ASN:HA	12:Z:30:SER:O	2.13	0.47
10:J:143:LEU:HD13	10:J:163:CYS:SG	2.55	0.47
3:Q:131:LEU:HD23	3:Q:145:GLN:HB3	1.95	0.47
6:F:108:LEU:HD11	6:F:137:LEU:HB3	1.96	0.47
9:W:113:PRO:O	9:W:114:LYS:HB2	2.15	0.47
2:P:89:LEU:HG	2:P:113:LEU:HD13	1.97	0.47
4:R:65:HIS:CE1	4:R:98:THR:HB	2.49	0.47
7:G:12:ILE:HG13	7:G:14:ILE:HG12	1.96	0.47
12:L:137:ALA:H	12:L:146:GLN:HE21	1.63	0.47
12:L:46:LEU:HB3	12:L:72:LEU:HD11	1.97	0.47
9:W:122:SER:HB3	9:W:136:VAL:HB	1.97	0.47
5:S:206:ASN:HD22	5:S:206:ASN:C	2.18	0.47
6:T:168:ALA:HB1	6:T:171:ALA:HB3	1.96	0.47
14:N:168:SER:O	17:N:201:O4C:H33	2.14	0.47
3:Q:19:GLU:HA	3:Q:22:GLN:NE2	2.30	0.47
2:B:122:GLN:HG3	3:C:124:ARG:HG3	1.95	0.47
1:A:40:ALA:HB2	1:A:180:ASP:HA	1.97	0.47
12:Z:46:LEU:HB3	12:Z:72:LEU:HD11	1.96	0.47
9:I:61:THR:O	9:I:65:ARG:HG3	2.14	0.47
5:S:168:TYR:OH	5:S:190:ARG:HD2	2.15	0.47
11:Y:72:GLU:O	11:Y:73:ARG:HB3	2.14	0.47
2:P:86:THR:HA	2:P:89:LEU:HD12	1.97	0.47
12:Z:137:ALA:H	12:Z:146:GLN:HE21	1.63	0.47
9:W:61:THR:O	9:W:65:ARG:HG3	2.14	0.47
5:S:167:THR:O	5:S:171:ARG:HG3	2.15	0.46
1:A:147:GLN:HE21	1:A:157:TRP:HE1	1.62	0.46
5:E:106:VAL:HA	5:E:109:ILE:HD12	1.96	0.46
3:Q:11:PRO:HA	4:R:18:TYR:CD2	2.51	0.46
14:N:188:ILE:HG22	14:N:193:LEU:HD12	1.97	0.46
3:C:175:TYR:CZ	3:C:180:ILE:HD11	2.50	0.46
1:A:147:GLN:HG3	1:A:162:MET:HE1	1.95	0.46
5:S:106:VAL:HA	5:S:109:ILE:HD12	1.96	0.46
5:E:206:ASN:HD22	5:E:206:ASN:C	2.18	0.46
10:J:161:ARG:HE	10:J:161:ARG:HB2	1.52	0.46
11:K:20:ALA:HB3	11:K:28:SER:HB3	1.97	0.46
4:D:149:ASP:HB2	4:D:150:PRO:HD2	1.98	0.46
2:B:86:THR:HA	2:B:89:LEU:HD12	1.97	0.46
14:N:90:TYR:HB2	14:N:94:LEU:HD12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:44:LEU:HD11	10:J:102:LEU:HD13	1.96	0.46
10:X:181:ARG:HG2	10:X:190:ASN:HA	1.97	0.46
10:X:80:ALA:O	10:X:84:THR:HG23	2.14	0.46
14:N:97:HIS:CG	14:N:115:MET:HB3	2.50	0.46
5:E:167:THR:O	5:E:171:ARG:HG3	2.15	0.46
11:Y:19:ARG:O	17:Y:301:04C:H34	2.16	0.46
3:C:19:GLU:HA	3:C:22:GLN:NE2	2.30	0.46
7:G:140:ILE:HG22	7:G:150:VAL:HG22	1.98	0.46
9:I:153:TRP:CH2	9:I:155:PRO:HA	2.51	0.46
7:U:49:ILE:HG13	19:U:413:HOH:O	2.15	0.46
7:G:142:ILE:HD13	7:G:221:VAL:HA	1.98	0.46
11:Y:20:ALA:HB3	11:Y:28:SER:HB3	1.97	0.46
14:N:134:ILE:HG21	14:N:158:ALA:O	2.15	0.46
6:F:3:ILE:HD12	6:F:15:SER:HB2	1.97	0.46
12:L:64:LEU:CD2	12:L:108:ASN:HD21	2.28	0.46
1:A:70:HIS:CE1	1:A:103:PRO:HB3	2.51	0.46
12:Z:64:LEU:CD2	12:Z:108:ASN:HD21	2.28	0.46
11:Y:154:ASP:O	11:Y:158:ARG:HB2	2.16	0.46
1:O:70:HIS:CE1	1:O:103:PRO:HB3	2.51	0.46
9:W:97:LYS:HG3	9:W:102:TYR:CE1	2.50	0.46
11:Y:4:LEU:CD2	11:Y:159:ALA:HB3	2.46	0.46
8:H:153:GLU:HG3	8:H:154:LEU:N	2.31	0.46
7:U:229:LEU:O	7:U:233:GLU:HB2	2.16	0.46
11:K:11:GLY:HA2	11:K:104:TRP:HZ3	1.81	0.46
9:I:97:LYS:HG3	9:I:102:TYR:CE1	2.51	0.46
1:A:75:TYR:HB3	1:A:82:TYR:CD1	2.51	0.46
6:T:34:SER:OG	6:T:65:ARG:NH1	2.49	0.46
13:M:46:ASN:ND2	13:M:49:THR:H	2.14	0.46
9:I:163:PHE:CE1	9:I:197:ARG:HD3	2.51	0.46
1:O:40:ALA:HB2	1:O:180:ASP:HA	1.98	0.46
7:G:229:LEU:O	7:G:233:GLU:HB2	2.16	0.46
1:O:75:TYR:HB3	1:O:82:TYR:CD1	2.51	0.45
9:I:47:ARG:HG3	9:I:189:ILE:CG2	2.47	0.45
13:M:46:ASN:ND2	13:M:48:SER:H	2.13	0.45
11:K:50:ALA:CB	12:L:127:VAL:HG12	2.46	0.45
8:H:48:VAL:HB	8:H:51:ASP:HB2	1.99	0.45
9:I:35:THR:HG22	9:I:37:ASP:H	1.82	0.45
1:O:149:ASP:HB2	1:O:150:PRO:CD	2.46	0.45
5:E:168:TYR:OH	5:E:190:ARG:HD2	2.15	0.45
1:A:149:ASP:HB2	1:A:150:PRO:CD	2.46	0.45
7:U:72:THR:HG22	7:U:74:SER:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:149:ASP:HB2	4:R:150:PRO:HD2	1.98	0.45
6:T:75:MET:HE2	6:T:137:LEU:HD21	1.99	0.45
9:W:35:THR:HG22	9:W:37:ASP:H	1.81	0.45
7:U:140:ILE:HG22	7:U:150:VAL:HG22	1.98	0.45
3:C:97:VAL:HG12	3:C:99:ASP:H	1.82	0.45
14:N:48:SER:HB3	14:N:51:ASP:HB2	1.98	0.45
8:V:48:VAL:HB	8:V:51:ASP:HB2	1.97	0.45
6:F:34:SER:OG	6:F:65:ARG:NH1	2.50	0.45
7:G:71:ILE:HG21	7:G:113:LEU:HD11	1.99	0.45
10:X:24:ASN:CG	10:X:25:ILE:H	2.20	0.45
6:T:2:SER:HA	6:T:21:PHE:CE2	2.52	0.45
9:W:153:TRP:CH2	9:W:155:PRO:HA	2.51	0.45
2:B:214:THR:HG22	19:B:434:HOH:O	2.17	0.45
1:A:83:ARG:NH2	7:G:157:GLY:O	2.50	0.45
6:T:3:ILE:HD12	6:T:15:SER:HB2	1.99	0.45
11:K:154:ASP:O	11:K:158:ARG:HB2	2.16	0.45
7:U:142:ILE:HD13	7:U:221:VAL:HA	1.97	0.45
12:Z:45:LYS:HB2	12:Z:203:ILE:HD13	1.97	0.45
11:K:4:LEU:CD2	11:K:159:ALA:HB3	2.46	0.45
1:A:73:LEU:HD21	1:A:135:ILE:HG12	1.99	0.45
7:U:72:THR:HG22	7:U:73:GLU:N	2.32	0.45
7:U:154:ASP:HB3	7:U:156:ALA:H	1.82	0.45
4:D:83:LYS:HD2	4:D:111:LEU:HD11	1.99	0.45
7:U:195:GLU:HG2	7:U:241:LEU:HG	1.99	0.45
14:N:78:ALA:O	14:N:82:VAL:HG13	2.17	0.45
5:E:2:GLN:HE22	6:F:5:THR:N	2.14	0.45
2:B:43:LEU:HB2	19:B:434:HOH:O	2.16	0.45
1:A:53:SER:HB3	1:A:56:TYR:CD1	2.52	0.45
12:L:123:SER:CB	12:L:136:LYS:HG2	2.47	0.45
5:E:35:LEU:HD13	5:E:184:LEU:HD22	1.99	0.45
7:G:200:CYS:O	7:G:204:VAL:HG23	2.17	0.45
11:Y:113:TYR:HD2	11:Y:121:LEU:HD12	1.82	0.45
2:P:32:THR:HG21	2:P:199:THR:HG21	1.99	0.44
12:Z:123:SER:CB	12:Z:136:LYS:HG2	2.47	0.44
9:W:163:PHE:CE1	9:W:197:ARG:HD3	2.51	0.44
3:C:107:THR:HG21	3:C:144:TYR:HB3	1.99	0.44
9:W:171:LEU:CD2	9:W:199:LEU:HD13	2.47	0.44
9:W:47:ARG:HG3	9:W:189:ILE:CG2	2.46	0.44
7:U:200:CYS:O	7:U:204:VAL:HG23	2.17	0.44
13:M:12:LEU:HB2	13:M:23:ALA:HB3	1.99	0.44
11:Y:11:GLY:HA2	11:Y:104:TRP:HZ3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:71:ILE:HG21	7:U:113:LEU:HD11	1.99	0.44
13:M:149:LEU:HD11	13:M:175:VAL:HG21	1.99	0.44
6:F:2:SER:HA	6:F:21:PHE:CE2	2.52	0.44
13:M:193:THR:OG1	13:M:194:GLU:N	2.50	0.44
11:K:113:TYR:HD2	11:K:121:LEU:HD12	1.82	0.44
13:M:59:ASP:CB	13:M:108:ASN:HD21	2.27	0.44
8:V:153:GLU:HG3	8:V:154:LEU:N	2.31	0.44
12:L:76:LYS:HE3	12:L:76:LYS:HB2	1.87	0.44
6:T:83:ASP:OD2	6:T:129:ARG:NH2	2.51	0.44
5:E:154:ARG:NH1	5:E:154:ARG:CG	2.77	0.44
7:U:72:THR:HG21	19:U:424:HOH:O	2.18	0.44
3:C:119:GLN:HG3	4:D:127:ARG:HG3	1.99	0.44
9:I:171:LEU:CD2	9:I:199:LEU:HD13	2.47	0.44
9:W:27:PHE:HB3	9:W:35:THR:HB	1.99	0.44
3:C:107:THR:HG23	3:C:132:ILE:HD13	1.99	0.44
3:Q:97:VAL:HG12	3:Q:99:ASP:H	1.82	0.44
2:P:16:ARG:HD2	2:P:21:GLU:OE2	2.18	0.44
2:B:32:THR:HG21	2:B:199:THR:HG21	1.99	0.44
1:O:53:SER:HB3	1:O:56:TYR:CD1	2.52	0.44
17:V:301:O4C:H37	18:V:302:IOD:I	2.88	0.44
3:Q:107:THR:HG21	3:Q:144:TYR:HB3	1.99	0.44
7:G:195:GLU:HG2	7:G:241:LEU:HG	2.00	0.44
2:P:202:VAL:O	2:P:203:SER:HB3	2.18	0.44
9:W:106:PRO:HG2	9:W:123:LEU:HB2	1.99	0.44
4:D:69:ALA:HB3	4:D:134:LEU:HB2	2.00	0.44
10:J:24:ASN:CG	10:J:25:ILE:H	2.20	0.44
2:B:107:GLU:O	2:B:111:THR:OG1	2.34	0.44
2:B:16:ARG:HD2	2:B:21:GLU:OE2	2.18	0.44
3:Q:224:ILE:HG13	3:Q:225:GLU:N	2.33	0.44
3:Q:119:GLN:HG3	4:R:127:ARG:HG3	2.00	0.44
5:S:2:GLN:HE22	6:T:5:THR:N	2.16	0.43
14:N:80:ALA:HA	14:N:100:VAL:HG11	1.98	0.43
4:R:83:LYS:HD2	4:R:111:LEU:HD11	2.00	0.43
3:Q:34:VAL:CG1	3:Q:190:VAL:HG22	2.48	0.43
1:A:71:ILE:HG21	1:A:109:LEU:HD22	2.01	0.43
1:A:6:SER:O	2:B:126:LYS:NZ	2.51	0.43
7:G:155:PRO:HD3	19:G:425:HOH:O	2.17	0.43
11:K:14:VAL:O	11:K:176:MET:HA	2.18	0.43
8:H:63:MET:CE	8:H:74:PRO:HB3	2.48	0.43
9:I:19:VAL:HG23	9:I:189:ILE:HB	2.01	0.43
1:O:68:THR:HG23	1:O:70:HIS:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:123:PHE:HB3	3:Q:123:ARG:HB3	2.00	0.43
11:K:164:THR:HG22	11:K:170:SER:HB3	2.01	0.43
13:M:104:ASN:ND2	19:M:437:HOH:O	2.50	0.43
1:O:78:MET:CE	1:O:130:GLY:HA3	2.48	0.43
12:Z:140:SER:HB2	19:Z:423:HOH:O	2.17	0.43
2:B:202:VAL:O	2:B:203:SER:HB3	2.18	0.43
1:A:78:MET:CE	1:A:130:GLY:HA3	2.48	0.43
1:A:83:ARG:HH11	1:A:83:ARG:CG	2.30	0.43
3:C:25:VAL:HG23	3:C:73:ALA:O	2.19	0.43
1:A:68:THR:HG23	1:A:70:HIS:H	1.83	0.43
9:I:27:PHE:HB3	9:I:35:THR:HB	1.99	0.43
2:P:107:GLU:O	2:P:111:THR:OG1	2.34	0.43
6:T:123:THR:O	7:U:131:ARG:NH1	2.52	0.43
6:T:241:GLU:HA	6:T:244:LYS:NZ	2.33	0.43
6:F:83:ASP:OD2	6:F:129:ARG:NH2	2.52	0.43
3:C:11:PRO:HA	4:D:18:TYR:CD2	2.53	0.43
5:S:35:LEU:HD13	5:S:184:LEU:HD22	1.99	0.43
1:A:58:GLU:HG2	1:A:205:ASP:HB3	2.01	0.43
8:V:18:THR:HB	8:V:30:SER:HA	2.01	0.43
3:C:34:VAL:CG1	3:C:190:VAL:HG22	2.48	0.43
1:A:110:VAL:HG22	1:A:135:ILE:HD13	2.00	0.43
3:Q:25:VAL:O	3:Q:161:GLY:HA2	2.19	0.43
1:O:162:MET:HA	1:O:166:TYR:HB2	2.00	0.43
11:K:15:ALA:HB2	11:K:176:MET:HG3	2.00	0.43
5:S:23:MET:HA	5:S:146:PRO:HG2	2.01	0.43
2:P:122:GLN:HG3	3:Q:124:ARG:HG3	2.01	0.43
9:I:29:ILE:O	9:I:31:ALA:N	2.52	0.43
11:Y:38:ASN:HB3	11:Y:39:PRO:HD2	2.01	0.43
1:O:73:LEU:HD21	1:O:135:ILE:HG12	1.99	0.43
3:C:25:VAL:O	3:C:161:GLY:HA2	2.19	0.43
7:G:85:ASP:OD1	7:G:131:ARG:NH2	2.52	0.43
17:K:301:04C:H41	17:K:301:04C:H29	1.85	0.42
3:Q:107:THR:HG23	3:Q:132:ILE:HD13	1.99	0.42
7:U:85:ASP:OD1	7:U:131:ARG:NH2	2.52	0.42
2:B:228:LYS:O	2:B:232:VAL:HG23	2.19	0.42
11:Y:14:VAL:O	11:Y:176:MET:HA	2.18	0.42
11:Y:15:ALA:HB2	11:Y:176:MET:HG3	2.00	0.42
2:B:123:PHE:HB3	3:C:123:ARG:HB3	2.00	0.42
11:Y:45:MET:HG2	11:Y:52:CYS:HB3	2.01	0.42
4:R:69:ALA:HB3	4:R:134:LEU:HB2	2.00	0.42
1:A:55:LEU:HD21	7:G:178:LEU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:23:MET:HA	5:E:146:PRO:HG2	2.01	0.42
13:M:94:ARG:NE	13:M:94:ARG:HA	2.34	0.42
10:J:16:ALA:HA	10:J:179:SER:O	2.18	0.42
1:A:127:ARG:HG3	7:G:126:GLN:HG3	2.01	0.42
5:E:102:VAL:O	5:E:106:VAL:HG23	2.19	0.42
2:P:228:LYS:O	2:P:232:VAL:HG23	2.19	0.42
9:W:70:LEU:HD11	9:W:81:ILE:HG21	2.01	0.42
9:W:19:VAL:HG23	9:W:189:ILE:HB	2.01	0.42
5:S:102:VAL:O	5:S:106:VAL:HG23	2.18	0.42
4:D:190:SER:O	4:D:194:LEU:HB2	2.19	0.42
9:I:70:LEU:HD11	9:I:81:ILE:HG21	2.01	0.42
8:V:122:LEU:HD13	8:V:125:THR:HB	2.01	0.42
3:C:224:ILE:HG13	3:C:225:GLU:N	2.33	0.42
4:R:190:SER:O	4:R:194:LEU:HB2	2.19	0.42
10:X:16:ALA:HA	10:X:179:SER:O	2.19	0.42
1:O:110:VAL:HG22	1:O:135:ILE:HD13	2.00	0.42
2:B:33:CYS:HB3	2:B:163:ILE:HD12	2.02	0.42
7:G:72:THR:HG22	7:G:73:GLU:N	2.34	0.42
1:O:55:LEU:HG	7:U:179:GLU:HG3	2.01	0.42
7:U:113:LEU:O	7:U:117:ILE:HG12	2.19	0.42
2:P:13:PRO:HA	3:Q:20:TYR:CD2	2.53	0.42
7:G:154:ASP:HB3	7:G:156:ALA:H	1.83	0.42
11:Y:164:THR:HG22	11:Y:170:SER:HB3	2.01	0.42
6:F:99:ARG:NH1	13:M:69:GLN:OE1	2.52	0.42
7:U:71:ILE:HD11	7:U:77:CYS:SG	2.60	0.42
3:Q:11:PRO:HA	4:R:18:TYR:CE2	2.54	0.42
3:C:147:ASP:HB2	3:C:148:PRO:HD2	2.01	0.42
11:Y:102:CYS:SG	11:Y:111:LEU:HD13	2.60	0.42
2:P:33:CYS:HB3	2:P:163:ILE:HD12	2.02	0.42
1:O:58:GLU:HG2	1:O:205:ASP:HB3	2.01	0.42
11:Y:64:ARG:HA	11:Y:64:ARG:HD3	1.88	0.42
3:Q:25:VAL:HG23	3:Q:73:ALA:O	2.19	0.42
1:A:198:PHE:O	1:A:199:GLU:HB2	2.20	0.42
1:A:147:GLN:HG3	1:A:162:MET:CE	2.50	0.42
1:A:162:MET:HA	1:A:166:TYR:HB2	2.00	0.42
7:U:49:ILE:HG21	7:U:78:VAL:HB	2.01	0.42
9:W:29:ILE:O	9:W:31:ALA:N	2.52	0.42
8:H:18:THR:HB	8:H:30:SER:HA	2.01	0.42
17:K:301:O4C:O13	18:K:302:IOD:I	3.08	0.42
5:S:69:ILE:HG22	5:S:131:ILE:HG12	2.02	0.42
9:I:6:ASN:ND2	9:I:56:ALA:H	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:71:ILE:HD11	7:G:77:CYS:SG	2.60	0.42
7:U:49:ILE:CG2	7:U:78:VAL:HB	2.50	0.42
5:S:118:GLN:HG3	6:T:129:ARG:HG3	2.02	0.42
5:E:118:GLN:HG3	6:F:129:ARG:HG3	2.01	0.42
8:H:77:ALA:O	8:H:80:THR:HG22	2.19	0.42
5:E:46:LEU:HB2	5:E:192:LEU:HD11	2.02	0.42
10:J:4:LEU:HB2	10:J:132:HIS:HB2	2.02	0.42
6:F:75:MET:HE2	6:F:137:LEU:HD21	2.02	0.42
9:W:6:ASN:ND2	9:W:56:ALA:H	2.18	0.42
3:Q:147:ASP:HB2	3:Q:148:PRO:HD2	2.01	0.42
9:I:183:GLY:HA2	9:I:201:ALA:HB3	2.02	0.42
12:L:136:LYS:HA	12:L:146:GLN:HE22	1.85	0.41
8:V:77:ALA:O	8:V:80:THR:HG22	2.20	0.41
8:H:126:ALA:HB3	8:H:135:VAL:HG22	2.02	0.41
4:R:20:ILE:HA	4:R:23:ILE:HD12	2.01	0.41
8:H:122:LEU:CD1	8:H:125:THR:HB	2.50	0.41
9:I:1:SER:HB3	9:I:4:SER:HB2	2.02	0.41
8:V:173:VAL:HG13	8:V:190:SER:HB3	2.01	0.41
1:O:83:ARG:NH2	7:U:157:GLY:O	2.53	0.41
1:A:74:VAL:HG12	1:A:75:TYR:H	1.85	0.41
6:F:39:ILE:HG22	6:F:162:GLY:CA	2.46	0.41
5:S:46:LEU:HB2	5:S:192:LEU:HD11	2.02	0.41
3:C:94:ARG:HB3	10:J:62:LYS:CE	2.51	0.41
7:G:113:LEU:O	7:G:117:ILE:HG12	2.19	0.41
10:X:4:LEU:HB2	10:X:132:HIS:HB2	2.02	0.41
1:O:71:ILE:HG21	1:O:109:LEU:HD22	2.01	0.41
8:V:122:LEU:CD1	8:V:125:THR:HB	2.49	0.41
14:N:77:LEU:HD22	14:N:81:ASN:ND2	2.35	0.41
7:G:209:PHE:HB2	7:G:213:GLU:HB2	2.01	0.41
13:M:122:LEU:HG	13:M:137:LEU:HD12	2.02	0.41
11:K:3:THR:HG22	11:K:100:MET:HE2	2.02	0.41
13:M:46:ASN:HD21	13:M:49:THR:CG2	2.33	0.41
11:K:102:CYS:SG	11:K:111:LEU:HD13	2.60	0.41
6:F:113:ASP:O	6:F:117:MET:HG2	2.20	0.41
5:E:2:GLN:HE22	6:F:5:THR:H	1.68	0.41
11:K:38:ASN:HB3	11:K:39:PRO:HD2	2.01	0.41
9:I:90:VAL:HG21	9:I:108:ILE:HD11	2.03	0.41
4:R:20:ILE:HD13	4:R:150:PRO:HD2	2.02	0.41
7:U:53:LYS:HB2	7:U:215:GLU:HG3	2.03	0.41
7:U:106:TYR:OH	8:V:66:HIS:HE1	2.04	0.41
11:Y:50:ALA:CB	12:Z:127:VAL:HG12	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:106:PRO:HG2	9:I:123:LEU:HB2	2.02	0.41
1:O:83:ARG:CG	1:O:83:ARG:HH11	2.29	0.41
6:T:39:ILE:HG22	6:T:162:GLY:CA	2.45	0.41
3:Q:94:ARG:HB3	10:X:62:LYS:CE	2.51	0.41
8:V:7:VAL:HG22	8:V:12:VAL:HG12	2.02	0.41
3:C:42:LEU:O	3:C:207:LEU:HB2	2.21	0.41
3:Q:42:LEU:O	3:Q:207:LEU:HB2	2.21	0.41
3:C:25:VAL:HG21	3:C:129:SER:CB	2.50	0.41
1:A:142:ARG:HA	1:A:143:PRO:HD3	1.95	0.41
7:U:209:PHE:HB2	7:U:213:GLU:HB2	2.01	0.41
11:K:45:MET:HG2	11:K:52:CYS:HB3	2.01	0.41
9:W:117:LYS:HA	9:W:118:PRO:HD3	1.92	0.41
7:G:49:ILE:HG21	7:G:78:VAL:HB	2.02	0.41
7:G:51:THR:OG1	7:G:78:VAL:HG21	2.20	0.41
9:W:183:GLY:HA2	9:W:201:ALA:HB3	2.03	0.41
12:L:28:ARG:NH2	19:L:425:HOH:O	2.52	0.41
4:D:174:GLN:HE21	5:E:52:GLU:HG2	1.85	0.41
2:B:157:GLY:HA3	3:C:57:THR:HG21	2.02	0.41
3:C:47:LYS:HE3	3:C:206:GLU:HB2	2.03	0.41
8:H:173:VAL:HG13	8:H:190:SER:HB3	2.02	0.41
1:O:74:VAL:HG12	1:O:75:TYR:H	1.85	0.41
9:I:144:GLN:HE21	9:I:144:GLN:N	2.16	0.41
9:W:90:VAL:HG21	9:W:108:ILE:HD11	2.03	0.41
14:N:41:ILE:HD13	14:N:79:ALA:HB2	2.02	0.41
7:U:51:THR:OG1	7:U:78:VAL:HG21	2.21	0.41
1:O:68:THR:HG22	1:O:71:ILE:HB	2.03	0.41
13:M:43:MET:SD	13:M:64:LYS:HG3	2.60	0.41
10:J:43:LEU:HD12	10:J:183:ILE:HD11	2.02	0.41
10:J:119:ASP:HB3	10:J:121:LEU:H	1.85	0.41
2:P:179:LYS:O	2:P:183:MET:HG2	2.21	0.41
8:V:19:ARG:HG3	8:V:26:VAL:HG13	2.03	0.41
8:V:126:ALA:HB3	8:V:135:VAL:HG22	2.02	0.41
3:C:118:THR:O	4:D:127:ARG:NH1	2.54	0.41
3:C:169:GLU:HA	3:C:172:GLU:HG3	2.03	0.41
3:Q:47:LYS:HE3	3:Q:206:GLU:HB2	2.03	0.40
14:N:143:LYS:O	14:N:146:MET:HG3	2.21	0.40
8:H:7:VAL:HG22	8:H:12:VAL:HG12	2.03	0.40
11:K:82:LEU:O	11:K:86:MET:HG3	2.22	0.40
12:Z:76:LYS:HE3	12:Z:76:LYS:HB2	1.87	0.40
4:R:74:ILE:HD12	4:R:74:ILE:H	1.86	0.40
10:X:169:LYS:HG2	10:X:170:ARG:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:91:GLN:HE21	10:J:62:LYS:HG3	1.85	0.40
4:D:20:ILE:HA	4:D:23:ILE:HD12	2.01	0.40
1:O:147:GLN:HG3	1:O:162:MET:CE	2.50	0.40
12:L:180:ILE:HA	19:L:429:HOH:O	2.20	0.40
1:O:223:THR:HG23	1:O:226:ARG:HH21	1.86	0.40
10:X:43:LEU:HD12	10:X:183:ILE:HD11	2.03	0.40
1:A:223:THR:HG23	1:A:226:ARG:HH21	1.86	0.40
3:C:211:ARG:HG2	3:C:211:ARG:H	1.73	0.40
8:V:137:LEU:HD13	8:V:141:ARG:HE	1.86	0.40
14:N:45:LEU:HG	19:N:310:HOH:O	2.21	0.40
11:K:120:ARG:HG3	19:K:406:HOH:O	2.21	0.40
12:Z:136:LYS:HA	12:Z:146:GLN:HE22	1.85	0.40
7:G:49:ILE:CG2	7:G:78:VAL:HB	2.51	0.40
9:W:1:SER:HB3	9:W:4:SER:HB2	2.02	0.40
1:A:14:PRO:HA	2:B:22:TYR:CD2	2.57	0.40
2:B:179:LYS:O	2:B:183:MET:HG2	2.21	0.40
6:F:111:LEU:O	6:F:115:VAL:HG23	2.21	0.40
2:P:23:ALA:O	2:P:27:ILE:HD12	2.21	0.40
6:T:215:TRP:HB3	6:T:220:THR:HG21	2.04	0.40
12:Z:13:LEU:HD11	12:Z:149:LEU:CD1	2.47	0.40
4:D:20:ILE:HD13	4:D:150:PRO:HD2	2.02	0.40
3:Q:145:GLN:HG2	3:Q:158:ASN:HD22	1.86	0.40
1:A:68:THR:HG22	1:A:71:ILE:HB	2.03	0.40
6:T:113:ASP:O	6:T:117:MET:HG2	2.20	0.40
12:Z:176:LYS:O	12:Z:180:ILE:HG13	2.22	0.40
5:E:69:ILE:HG22	5:E:131:ILE:HG12	2.02	0.40
10:X:161:ARG:HE	10:X:161:ARG:HB2	1.49	0.40
3:C:94:ARG:HB3	10:J:62:LYS:HE3	2.03	0.40
1:O:198:PHE:O	1:O:199:GLU:HB2	2.20	0.40
12:L:31:GLU:HB2	12:L:36:HIS:CD2	2.56	0.40
9:W:141:CYS:HB3	9:W:177:ASP:HB2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:146:ASP:O	13:M:206:GLN:NE2[2_655]	2.08	0.12

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%)	217 (95%)	8 (4%)	3 (1%)	15	46
1	O	228/234 (97%)	217 (95%)	8 (4%)	3 (1%)	15	46
2	B	246/261 (94%)	240 (98%)	5 (2%)	1 (0%)	39	74
2	P	246/261 (94%)	240 (98%)	5 (2%)	1 (0%)	39	74
3	C	236/248 (95%)	222 (94%)	14 (6%)	0	100	100
3	Q	236/248 (95%)	221 (94%)	15 (6%)	0	100	100
4	D	231/241 (96%)	222 (96%)	8 (4%)	1 (0%)	39	74
4	R	231/241 (96%)	222 (96%)	8 (4%)	1 (0%)	39	74
5	E	236/263 (90%)	227 (96%)	9 (4%)	0	100	100
5	S	236/263 (90%)	227 (96%)	9 (4%)	0	100	100
6	F	242/255 (95%)	234 (97%)	7 (3%)	1 (0%)	39	74
6	T	242/255 (95%)	234 (97%)	7 (3%)	1 (0%)	39	74
7	G	241/246 (98%)	236 (98%)	5 (2%)	0	100	100
7	U	241/246 (98%)	237 (98%)	4 (2%)	0	100	100
8	H	217/234 (93%)	206 (95%)	9 (4%)	2 (1%)	21	57
8	V	217/234 (93%)	206 (95%)	9 (4%)	2 (1%)	21	57
9	I	202/205 (98%)	191 (95%)	9 (4%)	2 (1%)	19	54
9	W	202/205 (98%)	191 (95%)	9 (4%)	2 (1%)	19	54
10	J	194/201 (96%)	187 (96%)	6 (3%)	1 (0%)	34	71
10	X	194/201 (96%)	187 (96%)	6 (3%)	1 (0%)	34	71
11	K	199/204 (98%)	189 (95%)	10 (5%)	0	100	100
11	Y	199/204 (98%)	189 (95%)	10 (5%)	0	100	100
12	L	211/213 (99%)	206 (98%)	5 (2%)	0	100	100
12	Z	211/213 (99%)	205 (97%)	6 (3%)	0	100	100
13	M	214/219 (98%)	205 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	214/219 (98%)	205 (96%)	9 (4%)	0	100	100
14	N	197/199 (99%)	195 (99%)	2 (1%)	0	100	100
14	b	197/199 (99%)	195 (99%)	2 (1%)	0	100	100
All	All	6188/6446 (96%)	5953 (96%)	213 (3%)	22 (0%)	39	74

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	216	VAL
9	I	30	GLN
6	T	216	VAL
9	W	30	GLN
1	A	40	ALA
1	A	198	PHE
1	A	199	GLU
2	B	203	SER
10	J	24	ASN
1	O	40	ALA
1	O	198	PHE
1	O	199	GLU
2	P	203	SER
10	X	24	ASN
4	D	112	ALA
9	I	47	ARG
4	R	112	ALA
9	W	47	ARG
8	H	195	PRO
8	V	195	PRO
8	H	194	GLU
8	V	194	GLU

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%)	175 (93%)	14 (7%)	17	44
1	O	189/191 (99%)	174 (92%)	15 (8%)	15	41
2	B	208/221 (94%)	190 (91%)	18 (9%)	13	36
2	P	208/221 (94%)	190 (91%)	18 (9%)	13	36
3	C	202/211 (96%)	178 (88%)	24 (12%)	6	19
3	Q	202/211 (96%)	178 (88%)	24 (12%)	6	19
4	D	195/203 (96%)	186 (95%)	9 (5%)	33	69
4	R	195/203 (96%)	186 (95%)	9 (5%)	33	69
5	E	204/224 (91%)	191 (94%)	13 (6%)	22	53
5	S	204/224 (91%)	191 (94%)	13 (6%)	22	53
6	F	200/211 (95%)	189 (94%)	11 (6%)	27	61
6	T	200/211 (95%)	189 (94%)	11 (6%)	27	61
7	G	207/210 (99%)	197 (95%)	10 (5%)	31	67
7	U	207/210 (99%)	197 (95%)	10 (5%)	31	67
8	H	169/183 (92%)	151 (89%)	18 (11%)	8	24
8	V	169/183 (92%)	151 (89%)	18 (11%)	8	24
9	I	174/175 (99%)	163 (94%)	11 (6%)	22	54
9	W	174/175 (99%)	163 (94%)	11 (6%)	22	54
10	J	166/171 (97%)	158 (95%)	8 (5%)	31	67
10	X	166/171 (97%)	158 (95%)	8 (5%)	31	67
11	K	165/166 (99%)	151 (92%)	14 (8%)	13	37
11	Y	165/166 (99%)	151 (92%)	14 (8%)	13	37
12	L	178/178 (100%)	170 (96%)	8 (4%)	34	70
12	Z	178/178 (100%)	168 (94%)	10 (6%)	26	60
13	M	178/180 (99%)	167 (94%)	11 (6%)	23	55
13	a	178/180 (99%)	167 (94%)	11 (6%)	23	55
14	N	155/155 (100%)	143 (92%)	12 (8%)	16	42
14	b	155/155 (100%)	144 (93%)	11 (7%)	18	47
All	All	5180/5358 (97%)	4816 (93%)	364 (7%)	19	47

All (364) 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	54	ILE
1	A	83	ARG
1	A	115	SER
1	A	140	GLU
1	A	189	THR
1	A	201	GLN
1	A	207	ILE
1	A	209	VAL
1	A	226	ARG
1	A	229	LEU
2	B	43	LEU
2	B	49	ARG
2	B	75	VAL
2	B	97	LEU
2	B	111	THR
2	B	163	ILE
2	B	177	ASP
2	B	179	LYS
2	B	182	GLU
2	B	184	THR
2	B	191	LEU
2	B	208	GLU
2	B	216	THR
2	B	217	ARG
2	B	234	GLN
2	B	240	GLU
2	B	242	GLU
2	B	243	GLU
3	C	4	ARG
3	C	34	VAL
3	C	41	VAL
3	C	46	LYS
3	C	56	ARG
3	C	76	THR
3	C	101	VAL
3	C	106	ILE
3	C	124	ARG
3	C	138	ASP
3	C	140	THR

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Mol	Chain	Res	Type
3	C	145	GLN
3	C	162	ARG
3	C	171	LEU
3	C	177	ASP
3	C	185	LEU
3	C	186	THR
3	C	195	LEU
3	C	212	ARG
3	C	217	LYS
3	C	220	ASN
3	C	223	GLU
3	C	231	ILE
3	C	236	GLU
4	D	12	ARG
4	D	28	THR
4	D	118	GLU
4	D	127	ARG
4	D	140	GLU
4	D	183	LEU
4	D	201	LYS
4	D	228	GLU
4	D	229	VAL
5	E	1	ASN
5	E	7	VAL
5	E	35	LEU
5	E	98	ARG
5	E	153	CYS
5	E	154	ARG
5	E	163	GLN
5	E	179	CYS
5	E	180	ASN
5	E	184	LEU
5	E	204	THR
5	E	206	ASN
5	E	226	VAL
6	F	30	VAL
6	F	37	ILE
6	F	66	LEU
6	F	129	ARG
6	F	133	CYS
6	F	181	MET
6	F	203	GLU

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Mol	Chain	Res	Type
6	F	205	LYS
6	F	214	SER
6	F	225	GLU
6	F	230	ASP
7	G	59	LEU
7	G	74	SER
7	G	80	THR
7	G	103	LYS
7	G	111	ASP
7	G	113	LEU
7	G	131	ARG
7	G	178	LEU
7	G	209	PHE
7	G	222	GLU
8	H	6	LEU
8	H	21	THR
8	H	23	ASP
8	H	32	GLU
8	H	40	LYS
8	H	56	THR
8	H	68	LEU
8	H	76	VAL
8	H	100	VAL
8	H	119	TYR
8	H	122	LEU
8	H	127	LEU
8	H	155	LEU
8	H	173	VAL
8	H	185	LEU
8	H	193	THR
8	H	197	GLN
8	H	216	VAL
9	I	33	MET
9	I	67	LYS
9	I	84	TYR
9	I	115	THR
9	I	116	PHE
9	I	117	LYS
9	I	131	VAL
9	I	142	SER
9	I	144	GLN
9	I	171	LEU

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Mol	Chain	Res	Type
9	I	192	ASP
10	J	1	MET
10	J	8	GLN
10	J	47	VAL
10	J	84	THR
10	J	85	ARG
10	J	86	ARG
10	J	143	LEU
10	J	161	ARG
11	K	9	GLN
11	K	13	ILE
11	K	27	SER
11	K	29	LEU
11	K	30	ARG
11	K	35	ILE
11	K	64	ARG
11	K	82	LEU
11	K	87	MET
11	K	88	LEU
11	K	115	ASP
11	K	121	LEU
11	K	139	MET
11	K	158	ARG
12	L	31	GLU
12	L	45	LYS
12	L	63	THR
12	L	133	ASP
12	L	160	ASN
12	L	162	GLU
12	L	166	LEU
12	L	173	ARG
13	M	3	ASN
13	M	35	ARG
13	M	44	ARG
13	M	46	ASN
13	M	49	THR
13	M	94	ARG
13	M	100	ARG
13	M	109	THR
13	M	152	GLU
13	M	168	LEU
13	M	192	VAL

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Mol	Chain	Res	Type
14	N	20	VAL
14	N	27	VAL
14	N	28	ASN
14	N	37	LEU
14	N	58	MET
14	N	77	LEU
14	N	82	VAL
14	N	100	VAL
14	N	143	LYS
14	N	153	ARG
14	N	191	ASP
14	N	199	GLU
1	O	2	LYS
1	O	3	ARG
1	O	19	VAL
1	O	28	VAL
1	O	54	ILE
1	O	59	ARG
1	O	83	ARG
1	O	115	SER
1	O	140	GLU
1	O	189	THR
1	O	201	GLN
1	O	207	ILE
1	O	209	VAL
1	O	226	ARG
1	O	229	LEU
2	P	43	LEU
2	P	49	ARG
2	P	75	VAL
2	P	97	LEU
2	P	111	THR
2	P	163	ILE
2	P	177	ASP
2	P	179	LYS
2	P	182	GLU
2	P	184	THR
2	P	191	LEU
2	P	208	GLU
2	P	216	THR
2	P	217	ARG
2	P	234	GLN

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Mol	Chain	Res	Type
2	P	240	GLU
2	P	242	GLU
2	P	243	GLU
3	Q	4	ARG
3	Q	34	VAL
3	Q	41	VAL
3	Q	46	LYS
3	Q	56	ARG
3	Q	76	THR
3	Q	101	VAL
3	Q	106	ILE
3	Q	124	ARG
3	Q	138	ASP
3	Q	140	THR
3	Q	145	GLN
3	Q	162	ARG
3	Q	171	LEU
3	Q	177	ASP
3	Q	185	LEU
3	Q	186	THR
3	Q	195	LEU
3	Q	212	ARG
3	Q	217	LYS
3	Q	220	ASN
3	Q	223	GLU
3	Q	231	ILE
3	Q	236	GLU
4	R	12	ARG
4	R	28	THR
4	R	118	GLU
4	R	127	ARG
4	R	140	GLU
4	R	183	LEU
4	R	201	LYS
4	R	228	GLU
4	R	229	VAL
5	S	1	ASN
5	S	7	VAL
5	S	35	LEU
5	S	98	ARG
5	S	153	CYS
5	S	154	ARG

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Mol	Chain	Res	Type
5	S	163	GLN
5	S	179	CYS
5	S	180	ASN
5	S	184	LEU
5	S	204	THR
5	S	206	ASN
5	S	226	VAL
6	T	30	VAL
6	T	37	ILE
6	T	66	LEU
6	T	129	ARG
6	T	133	CYS
6	T	181	MET
6	T	203	GLU
6	T	205	LYS
6	T	214	SER
6	T	225	GLU
6	T	230	ASP
7	U	59	LEU
7	U	74	SER
7	U	80	THR
7	U	83	THR
7	U	111	ASP
7	U	113	LEU
7	U	131	ARG
7	U	178	LEU
7	U	209	PHE
7	U	222	GLU
8	V	6	LEU
8	V	21	THR
8	V	23	ASP
8	V	32	GLU
8	V	40	LYS
8	V	56	THR
8	V	68	LEU
8	V	76	VAL
8	V	100	VAL
8	V	119	TYR
8	V	122	LEU
8	V	127	LEU
8	V	155	LEU
8	V	173	VAL

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Mol	Chain	Res	Type
8	V	185	LEU
8	V	193	THR
8	V	197	GLN
8	V	216	VAL
9	W	33	MET
9	W	67	LYS
9	W	84	TYR
9	W	115	THR
9	W	116	PHE
9	W	123	LEU
9	W	131	VAL
9	W	142	SER
9	W	144	GLN
9	W	171	LEU
9	W	192	ASP
10	X	1	MET
10	X	8	GLN
10	X	47	VAL
10	X	84	THR
10	X	85	ARG
10	X	86	ARG
10	X	143	LEU
10	X	161	ARG
11	Y	9	GLN
11	Y	13	ILE
11	Y	27	SER
11	Y	29	LEU
11	Y	30	ARG
11	Y	35	ILE
11	Y	64	ARG
11	Y	82	LEU
11	Y	87	MET
11	Y	88	LEU
11	Y	115	ASP
11	Y	121	LEU
11	Y	139	MET
11	Y	158	ARG
12	Z	31	GLU
12	Z	45	LYS
12	Z	63	THR
12	Z	133	ASP
12	Z	160	ASN

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Mol	Chain	Res	Type
12	Z	162	GLU
12	Z	166	LEU
12	Z	173	ARG
12	Z	180	ILE
12	Z	212	LYS
13	a	3	ASN
13	a	35	ARG
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
13	a	192	VAL
14	b	27	VAL
14	b	28	ASN
14	b	37	LEU
14	b	58	MET
14	b	77	LEU
14	b	82	VAL
14	b	100	VAL
14	b	143	LYS
14	b	153	ARG
14	b	191	ASP
14	b	199	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (117) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	139	ASN
1	A	147	GLN
1	A	165	ASN
1	A	206	ASN
2	B	39	ASN
2	B	68	ASN
2	B	87	ASN
2	B	94	GLN
2	B	122	GLN
2	B	154	ASN

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Mol	Chain	Res	Type
2	B	176	GLN
3	C	22	GLN
3	C	91	GLN
3	C	174	ASN
3	C	220	ASN
4	D	106	GLN
4	D	174	GLN
4	D	196	GLN
4	D	213	GLN
5	E	2	GLN
5	E	40	HIS
5	E	143	GLN
5	E	163	GLN
5	E	172	HIS
7	G	89	GLN
7	G	126	GLN
8	H	66	HIS
8	H	106	ASN
8	H	143	GLN
8	H	186	GLN
9	I	6	ASN
9	I	39	GLN
9	I	64	GLN
9	I	144	GLN
10	J	8	GLN
10	J	27	GLN
10	J	32	HIS
10	J	61	GLN
10	J	174	ASN
11	K	10	HIS
11	K	117	ASN
11	K	124	GLN
12	L	8	ASN
12	L	58	HIS
12	L	108	ASN
12	L	146	GLN
12	L	152	GLN
12	L	159	GLN
13	M	46	ASN
13	M	104	ASN
13	M	108	ASN
13	M	157	GLN

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Mol	Chain	Res	Type
13	M	208	ASN
14	N	28	ASN
14	N	81	ASN
14	N	157	ASN
1	O	111	GLN
1	O	139	ASN
1	O	147	GLN
1	O	165	ASN
1	O	206	ASN
2	P	39	ASN
2	P	68	ASN
2	P	94	GLN
2	P	122	GLN
2	P	154	ASN
3	Q	22	GLN
3	Q	91	GLN
3	Q	174	ASN
3	Q	220	ASN
4	R	106	GLN
4	R	174	GLN
4	R	196	GLN
4	R	213	GLN
5	S	2	GLN
5	S	40	HIS
5	S	143	GLN
5	S	163	GLN
5	S	172	HIS
7	U	67	HIS
7	U	89	GLN
7	U	126	GLN
8	V	66	HIS
8	V	91	GLN
8	V	106	ASN
8	V	143	GLN
8	V	186	GLN
9	W	6	ASN
9	W	39	GLN
9	W	64	GLN
9	W	80	GLN
9	W	144	GLN
10	X	27	GLN
10	X	61	GLN

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Mol	Chain	Res	Type
10	X	132	HIS
10	X	174	ASN
11	Y	10	HIS
11	Y	38	ASN
11	Y	117	ASN
11	Y	124	GLN
12	Z	8	ASN
12	Z	58	HIS
12	Z	108	ASN
12	Z	146	GLN
12	Z	151	ASN
13	a	46	ASN
13	a	104	ASN
13	a	108	ASN
13	a	157	GLN
13	a	208	ASN
14	b	28	ASN
14	b	38	HIS
14	b	66	HIS
14	b	81	ASN
14	b	97	HIS
14	b	157	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 66 ligands modelled in this entry, 60 are monoatomic - leaving 6 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
17	04C	H	301	8	43,44,44	1.10	2 (4%)	55,58,58	1.00	3 (5%)
17	04C	K	301	11	43,44,44	1.15	2 (4%)	55,58,58	0.99	3 (5%)
17	04C	N	201	14	43,44,44	1.19	3 (6%)	55,58,58	1.19	6 (10%)
17	04C	V	301	8	43,44,44	1.13	2 (4%)	55,58,58	1.05	4 (7%)
17	04C	Y	301	11	43,44,44	1.20	2 (4%)	55,58,58	1.37	6 (10%)
17	04C	b	201	14	43,44,44	1.23	3 (6%)	55,58,58	1.17	6 (10%)

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
17	04C	H	301	8	-	0/44/52/52	0/3/3/3
17	04C	K	301	11	-	0/44/52/52	0/3/3/3
17	04C	N	201	14	-	0/44/52/52	0/3/3/3
17	04C	V	301	8	-	0/44/52/52	0/3/3/3
17	04C	Y	301	11	-	0/44/52/52	0/3/3/3
17	04C	b	201	14	-	0/44/52/52	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	201	04C	C7-C6	2.39	1.57	1.51
17	H	301	04C	C10-C9	2.46	1.58	1.53
17	N	201	04C	C12-C10	2.47	1.55	1.52
17	V	301	04C	C12-C10	2.55	1.55	1.52
17	V	301	04C	C10-C9	2.66	1.58	1.53
17	H	301	04C	C12-C10	2.66	1.56	1.52
17	Y	301	04C	C12-C10	2.69	1.56	1.52
17	b	201	04C	C7-C6	2.71	1.57	1.51
17	Y	301	04C	C10-C9	2.84	1.58	1.53
17	b	201	04C	C10-C9	2.90	1.59	1.53
17	b	201	04C	C12-C10	2.94	1.56	1.52
17	K	301	04C	C12-C10	2.97	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	301	04C	C10-C9	3.01	1.59	1.53
17	N	201	04C	C10-C9	3.20	1.59	1.53

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	201	04C	C11-C10-C12	-4.25	104.25	109.86
17	K	301	04C	C11-C10-C12	-4.20	104.33	109.86
17	N	201	04C	C11-C10-C12	-3.91	104.70	109.86
17	H	301	04C	C7-C8-N22	-3.61	106.19	110.14
17	V	301	04C	C7-C8-N22	-3.48	106.33	110.14
17	H	301	04C	C11-C10-C12	-3.27	105.55	109.86
17	Y	301	04C	C7-C8-N22	-3.21	106.63	110.14
17	V	301	04C	C11-C10-C12	-3.15	105.71	109.86
17	N	201	04C	C7-C8-N22	-2.81	107.07	110.14
17	Y	301	04C	C11-C10-C12	-2.74	106.25	109.86
17	b	201	04C	C7-C8-N22	-2.69	107.20	110.14
17	N	201	04C	C40-C24-N25	-2.61	105.33	110.80
17	K	301	04C	C7-C8-N22	-2.59	107.31	110.14
17	b	201	04C	C40-C24-N25	-2.32	105.94	110.80
17	N	201	04C	C7-C8-C9	-2.02	106.65	111.14
17	N	201	04C	C32-N31-C36	2.06	113.37	108.90
17	K	301	04C	C32-N31-C36	2.13	113.51	108.90
17	H	301	04C	C32-N31-C36	2.20	113.66	108.90
17	b	201	04C	C30-N31-C36	2.20	114.32	111.07
17	V	301	04C	C30-N31-C36	2.29	114.45	111.07
17	V	301	04C	C6-C7-C8	2.29	117.13	113.48
17	b	201	04C	C30-N31-C32	2.37	114.57	111.07
17	b	201	04C	C6-C7-C8	2.51	117.47	113.48
17	Y	301	04C	C6-C7-C8	2.77	117.88	113.48
17	N	201	04C	C6-C7-C8	3.70	119.37	113.48
17	Y	301	04C	C35-C36-N31	3.92	116.06	110.12
17	Y	301	04C	C33-C32-N31	4.26	116.58	110.12
17	Y	301	04C	C32-N31-C36	4.76	119.20	108.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	K	301	04C	3	0
17	N	201	04C	3	0
17	V	301	04C	1	0
17	Y	301	04C	3	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	A	230/234 (98%)	0.10	11 (4%) 34 28	44, 68, 95, 106	0
1	O	230/234 (98%)	0.04	6 (2%) 59 54	35, 52, 86, 96	0
2	B	248/261 (95%)	0.26	15 (6%) 25 18	45, 72, 121, 149	0
2	P	248/261 (95%)	0.01	13 (5%) 31 24	32, 57, 99, 142	0
3	C	238/248 (95%)	0.66	31 (13%) 5 3	51, 87, 150, 194	0
3	Q	238/248 (95%)	0.48	28 (11%) 6 4	41, 74, 132, 174	0
4	D	233/241 (96%)	0.57	19 (8%) 14 9	41, 91, 150, 200	0
4	R	233/241 (96%)	0.41	13 (5%) 28 21	43, 83, 125, 154	0
5	E	238/263 (90%)	0.21	11 (4%) 36 30	34, 66, 107, 128	0
5	S	238/263 (90%)	0.09	8 (3%) 49 41	35, 61, 102, 122	0
6	F	244/255 (95%)	0.18	6 (2%) 61 55	37, 67, 103, 117	0
6	T	244/255 (95%)	0.10	10 (4%) 41 34	34, 57, 93, 111	0
7	G	243/246 (98%)	0.21	13 (5%) 30 23	47, 70, 108, 129	0
7	U	243/246 (98%)	0.09	16 (6%) 22 16	32, 57, 99, 117	0
8	H	219/234 (93%)	-0.12	5 (2%) 64 59	11, 50, 94, 125	0
8	V	219/234 (93%)	-0.24	6 (2%) 58 52	4, 41, 78, 103	0
9	I	204/205 (99%)	-0.07	4 (1%) 68 64	33, 55, 82, 101	0
9	W	204/205 (99%)	-0.25	2 (0%) 84 82	27, 42, 64, 82	0
10	J	196/201 (97%)	-0.16	3 (1%) 76 74	38, 50, 72, 83	0
10	X	196/201 (97%)	-0.26	1 (0%) 91 90	32, 48, 67, 83	0
11	K	201/204 (98%)	-0.07	3 (1%) 76 74	9, 47, 72, 87	0
11	Y	201/204 (98%)	0.16	4 (1%) 68 64	5, 57, 82, 94	0
12	L	213/213 (100%)	-0.19	2 (0%) 85 84	29, 42, 64, 86	0
12	Z	213/213 (100%)	-0.13	1 (0%) 91 90	41, 49, 67, 96	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	216/219 (98%)	-0.30	1 (0%) 91 90	29, 38, 61, 82	0
13	a	216/219 (98%)	-0.23	1 (0%) 91 90	36, 44, 61, 82	0
14	N	199/199 (100%)	-0.18	1 (0%) 91 90	4, 43, 61, 72	0
14	b	199/199 (100%)	-0.20	0 100 100	3, 41, 61, 70	0
All	All	6244/6446 (96%)	0.06	234 (3%) 45 38	3, 56, 111, 200	0

All (234) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	49	VAL	7.8
6	F	5	THR	7.5
4	D	123	GLY	7.5
4	R	123	GLY	7.3
7	U	1	SER	6.7
4	R	122	PRO	6.6
6	F	1	SER	6.3
4	R	233	ILE	6.2
8	H	199	ALA	5.7
3	Q	236	GLU	5.6
13	M	216	SER	5.6
7	G	242	ALA	5.4
3	C	233	LYS	5.4
5	E	238	GLN	5.3
3	Q	238	ASN	5.3
3	C	200	SER	5.0
8	V	199	ALA	4.9
7	G	1	SER	4.9
4	D	233	ILE	4.9
3	C	203	LYS	4.9
3	C	238	ASN	4.8
3	Q	200	SER	4.7
2	B	247	GLU	4.7
2	B	237	LYS	4.6
1	A	1	ALA	4.6
5	S	52	GLU	4.6
3	C	237	GLU	4.5
7	G	187	ASP	4.5
4	D	232	ASP	4.4
3	Q	178	ASP	4.4
7	G	2	ARG	4.3
2	B	244	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
6	T	5	THR	4.3
3	Q	45	GLU	4.2
4	D	122	PRO	4.1
4	D	199	GLU	4.1
3	C	199	GLN	4.0
6	F	3	ILE	4.0
7	U	186	PHE	4.0
5	E	52	GLU	4.0
2	P	248	ARG	4.0
7	G	243	GLU	4.0
6	T	1	SER	4.0
4	D	201	LYS	3.9
3	Q	55	GLU	3.9
4	D	171	SER	3.9
5	S	238	GLN	3.9
3	Q	199	GLN	3.8
5	S	199	GLU	3.8
3	C	45	GLU	3.7
5	E	53	LEU	3.7
2	B	53	LYS	3.7
1	A	2	LYS	3.7
7	U	3	GLY	3.6
5	E	235	GLU	3.6
7	U	2	ARG	3.6
5	E	237	PRO	3.6
13	a	216	SER	3.6
3	C	48	SER	3.5
6	T	204	VAL	3.5
5	E	199	GLU	3.5
3	Q	232	GLU	3.5
7	G	185	LYS	3.4
3	Q	233	LYS	3.4
9	I	116	PHE	3.4
8	V	200	GLY	3.3
3	C	236	GLU	3.3
4	D	177	TYR	3.3
8	H	201	ARG	3.3
2	B	203	SER	3.3
1	O	2	LYS	3.3
2	B	204	LYS	3.3
8	V	201	ARG	3.3
6	T	207	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
2	P	203	SER	3.2
4	R	224	GLU	3.2
4	R	199	GLU	3.2
5	S	237	PRO	3.2
6	F	207	LYS	3.2
3	C	232	GLU	3.1
7	U	6	ALA	3.1
7	G	186	PHE	3.1
6	T	3	ILE	3.1
9	I	114	LYS	3.1
3	Q	182	THR	3.1
4	R	215	GLY	3.1
3	C	178	ASP	3.1
2	B	1	SER	3.1
3	Q	181	GLU	3.0
2	P	202	VAL	3.0
7	U	187	ASP	3.0
3	Q	203	LYS	3.0
4	R	192	ILE	3.0
5	E	234	GLU	3.0
3	C	47	LYS	3.0
3	Q	46	LYS	3.0
10	J	95	ARG	2.9
8	H	197	GLN	2.9
5	E	50	GLN	2.9
2	B	206	SER	2.9
1	O	3	ARG	2.9
1	A	178	ASN	2.9
2	P	244	ALA	2.9
4	D	215	GLY	2.9
3	C	234	GLU	2.9
3	Q	165	LYS	2.9
11	Y	9	GLN	2.8
7	U	185	LYS	2.8
3	C	137	PHE	2.8
3	C	185	LEU	2.8
2	P	219	SER	2.8
4	D	47	THR	2.8
8	H	196	VAL	2.8
1	A	3	ARG	2.8
7	U	4	SER	2.7
2	P	246	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
6	T	4	GLY	2.7
11	Y	200	GLY	2.7
3	C	211	ARG	2.7
4	D	121	ASP	2.7
1	A	59	ARG	2.7
6	T	219	LEU	2.7
4	R	175	GLU	2.7
3	Q	237	GLU	2.7
3	C	204	ASN	2.7
3	Q	47	LYS	2.7
4	R	180	SER	2.7
3	C	235	LYS	2.7
3	Q	48	SER	2.7
5	E	198	ALA	2.7
8	H	195	PRO	2.6
3	C	202	GLY	2.6
2	B	246	ALA	2.6
11	K	9	GLN	2.6
11	K	73	ARG	2.6
7	G	58	LYS	2.6
4	D	200	GLU	2.6
7	U	184	LYS	2.6
3	Q	177	ASP	2.6
6	T	208	ALA	2.6
5	E	200	GLN	2.6
5	S	234	GLU	2.6
4	D	49	PRO	2.6
3	Q	137	PHE	2.6
3	C	179	ALA	2.6
1	A	180	ASP	2.6
11	K	72	GLU	2.5
11	Y	73	ARG	2.5
6	T	60	GLU	2.5
2	P	243	GLU	2.5
12	Z	162	GLU	2.5
3	C	169	GLU	2.5
4	R	121	ASP	2.5
2	B	233	GLU	2.5
2	P	245	LYS	2.5
6	F	2	SER	2.5
5	S	53	LEU	2.5
1	O	201	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
3	C	55	GLU	2.5
3	C	206	GLU	2.4
3	C	37	LYS	2.4
9	W	114	LYS	2.4
4	D	222	THR	2.4
1	A	203	THR	2.4
2	B	178	TYR	2.4
2	P	247	GLU	2.4
5	S	233	LEU	2.4
3	C	162	ARG	2.4
2	B	248	ARG	2.4
1	O	1	ALA	2.4
4	D	220	MET	2.4
10	X	95	ARG	2.4
2	P	53	LYS	2.4
3	Q	212	ARG	2.3
7	G	184	LYS	2.3
3	Q	206	GLU	2.3
9	W	116	PHE	2.3
2	B	219	SER	2.3
5	S	235	GLU	2.3
12	L	163	HIS	2.3
6	T	202	ASP	2.3
10	J	109	GLU	2.3
1	A	201	GLN	2.3
3	C	46	LYS	2.3
3	Q	229	ALA	2.3
14	N	191	ASP	2.2
1	A	179	GLU	2.2
2	B	18	TYR	2.2
3	C	16	PHE	2.2
7	U	145	GLU	2.2
7	G	238	LEU	2.2
3	Q	213	ASP	2.2
6	F	142	ALA	2.2
1	A	50	LYS	2.2
7	G	144	GLU	2.2
7	U	207	ILE	2.2
4	R	188	LYS	2.2
7	U	56	PRO	2.2
3	Q	49	VAL	2.2
7	U	210	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
7	U	144	GLU	2.2
7	U	5	SER	2.2
7	U	176	SER	2.2
12	L	1	ARG	2.2
3	C	218	ILE	2.2
7	G	10	ARG	2.2
3	C	175	TYR	2.2
1	A	13	SER	2.1
4	D	188	LYS	2.1
11	Y	72	GLU	2.1
2	B	29	HIS	2.1
3	Q	234	GLU	2.1
4	R	142	GLY	2.1
9	I	155	PRO	2.1
7	G	192	GLN	2.1
9	I	30	GLN	2.1
4	D	25	LEU	2.1
2	P	201	ASP	2.1
4	D	168	GLY	2.1
8	V	195	PRO	2.1
8	V	197	GLN	2.1
8	V	198	ARG	2.1
3	C	172	GLU	2.1
3	Q	235	LYS	2.1
2	P	242	GLU	2.1
4	R	120	ALA	2.1
10	J	196	PHE	2.1
4	D	207	ILE	2.0
3	Q	205	ILE	2.0
3	Q	195	LEU	2.0
5	E	171	ARG	2.0
1	O	52	LYS	2.0
2	P	205	LEU	2.0
1	O	202	MET	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
16	K	L	303	1/1	0.70	0.68	23.23	31,31,31,31	0
16	K	b	203	1/1	0.85	0.36	11.81	45,45,45,45	0
16	K	a	305	1/1	0.96	0.45	10.44	37,37,37,37	0
16	K	I	302	1/1	0.97	0.46	7.76	41,41,41,41	0
17	04C	Y	301	42/42	0.89	0.30	3.20	2,16,29,34	0
17	04C	K	301	42/42	0.92	0.26	2.88	7,14,28,32	0
17	04C	N	201	42/42	0.91	0.23	2.43	2,3,8,11	0
17	04C	b	201	42/42	0.93	0.23	2.35	2,3,12,17	0
16	K	S	303	1/1	0.88	0.27	2.25	50,50,50,50	0
16	K	Z	304	1/1	0.91	0.21	1.36	40,40,40,40	0
17	04C	H	301	42/42	0.94	0.21	1.13	6,13,19,20	0
17	04C	V	301	42/42	0.94	0.16	0.38	3,5,24,25	0
15	CL	E	301	1/1	0.91	0.20	0.25	42,42,42,42	0
15	CL	R	302	1/1	0.85	0.22	0.07	59,59,59,59	0
15	CL	Z	301	1/1	0.98	0.19	-0.45	26,26,26,26	0
15	CL	S	301	1/1	0.97	0.17	-0.53	35,35,35,35	0
15	CL	U	301	1/1	0.83	0.13	-1.22	45,45,45,45	0
15	CL	M	302	1/1	0.98	0.14	-1.24	30,30,30,30	0
15	CL	Q	301	1/1	0.96	0.16	-1.44	39,39,39,39	0
15	CL	V	304	1/1	0.98	0.09	-1.60	33,33,33,33	0
15	CL	A	302	1/1	0.95	0.12	-1.94	32,32,32,32	0
15	CL	V	306	1/1	0.95	0.12	-1.97	40,40,40,40	0
15	CL	R	303	1/1	0.89	0.11	-2.27	45,45,45,45	0
15	CL	Q	302	1/1	0.96	0.10	-2.58	37,37,37,37	0
15	CL	N	203	1/1	0.98	0.08	-2.73	36,36,36,36	0
15	CL	Q	304	1/1	0.98	0.04	-4.27	29,29,29,29	0
15	CL	H	303	1/1	0.99	0.07	-4.51	31,31,31,31	0
15	CL	W	301	1/1	0.99	0.12	-	28,28,28,28	0
15	CL	I	301	1/1	0.98	0.06	-	28,28,28,28	0
18	IOD	N	202	1/1	0.99	0.02	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
16	K	B	301	1/1	0.73	0.32	-	55,55,55,55	0
15	CL	M	303	1/1	0.98	0.06	-	25,25,25,25	0
15	CL	O	301	1/1	0.98	0.09	-	33,33,33,33	0
15	CL	M	301	1/1	0.97	0.08	-	39,39,39,39	0
15	CL	R	301	1/1	0.96	0.13	-	32,32,32,32	0
15	CL	L	301	1/1	0.99	0.05	-	32,32,32,32	0
15	CL	M	304	1/1	0.91	0.09	-	48,48,48,48	0
15	CL	A	301	1/1	0.99	0.08	-	34,34,34,34	0
15	CL	V	303	1/1	0.99	0.12	-	30,30,30,30	0
15	CL	J	301	1/1	0.92	0.06	-	35,35,35,35	0
15	CL	X	302	1/1	0.80	0.20	-	51,51,51,51	0
15	CL	X	303	1/1	0.90	0.17	-	72,72,72,72	0
18	IOD	H	302	1/1	0.99	0.07	-	49,49,49,49	0
18	IOD	K	302	1/1	1.00	0.03	-	53,53,53,53	0
16	K	M	305	1/1	0.95	0.20	-	37,37,37,37	0
15	CL	V	305	1/1	0.82	0.23	-	44,44,44,44	0
18	IOD	Y	302	1/1	0.99	0.02	-	55,55,55,55	0
18	IOD	V	302	1/1	1.00	0.13	-	17,17,17,17	0
15	CL	Q	303	1/1	0.98	0.03	-	32,32,32,32	0
15	CL	O	302	1/1	0.97	0.08	-	44,44,44,44	0
15	CL	a	301	1/1	0.97	0.10	-	33,33,33,33	0
16	K	X	304	1/1	0.90	0.23	-	70,70,70,70	0
15	CL	a	302	1/1	0.98	0.07	-	29,29,29,29	0
16	K	K	303	1/1	0.74	0.18	-	51,51,51,51	0
15	CL	D	301	1/1	0.96	0.10	-	35,35,35,35	0
15	CL	P	301	1/1	0.86	0.19	-	39,39,39,39	0
15	CL	L	302	1/1	0.90	0.15	-	24,24,24,24	0
18	IOD	b	202	1/1	0.99	0.03	-	46,46,46,46	0
15	CL	X	301	1/1	0.94	0.25	-	46,46,46,46	0
15	CL	S	302	1/1	0.82	0.13	-	45,45,45,45	0
15	CL	a	304	1/1	0.90	0.12	-	44,44,44,44	0
16	K	G	301	1/1	0.85	0.22	-	56,56,56,56	0
15	CL	a	303	1/1	0.82	0.14	-	44,44,44,44	0
16	K	Z	303	1/1	0.96	0.07	-	24,24,24,24	0
15	CL	A	303	1/1	0.89	0.13	-	45,45,45,45	0
16	K	Z	302	1/1	0.86	0.15	-	47,47,47,47	0

6.5 Other polymers

There are no such residues in this entry.