



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:20 PM UTC

PDB ID : 9QC9 / pdb_00009qc9
Title : Yeast 20S proteasome double mutant: beta5_F(-46)S / beta5_G128V
Authors : Huber, E.M.; Heinemeyer, W.; Groll, M.
Deposited on : 2025-03-04
Resolution : 2.60 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:

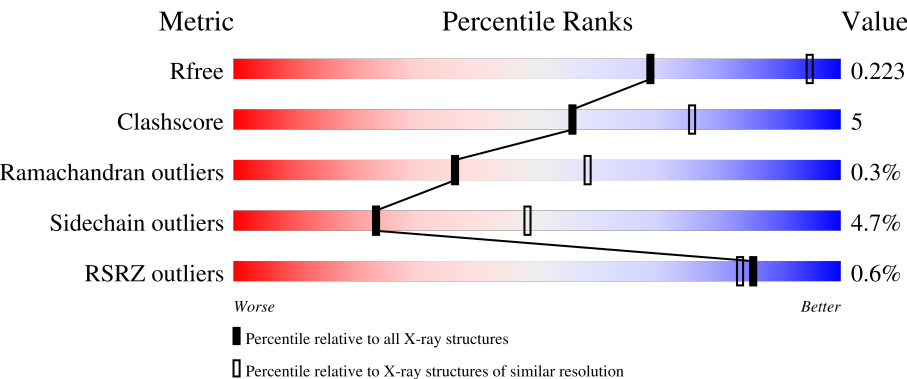
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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.



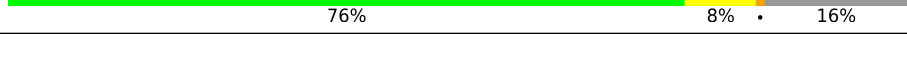
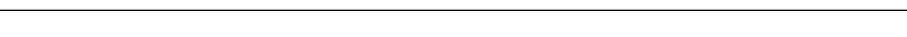
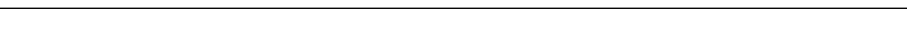
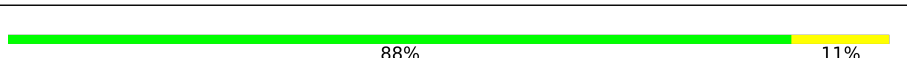
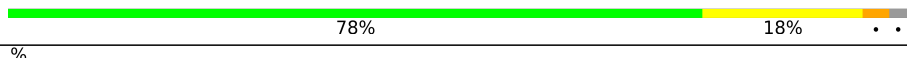
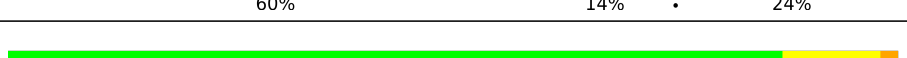
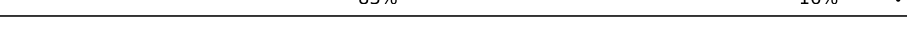
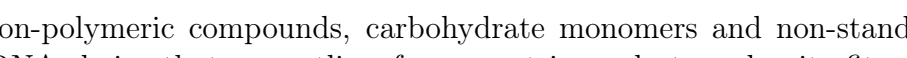
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	250	% 92%5% ..
1	O	250	% 94%6% .
2	B	258	% 83%10% • 5%
2	P	258	2% 85%9% 5%
3	C	254	% 85%7% • 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	287	
11	Y	287	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	

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
15	MG	W	301	-	-	-	X
17	MES	b	201	-	-	X	-

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 50416 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	248	Total	C	N	O	S	0	0	0
			1900	1210	313	374	3			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

- Molecule 2 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			
2	P	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	240	Total	C	N	O	S	0	0	0
			1881	1176	329	372	4			
3	Q	240	Total	C	N	O	S	0	0	0
			1881	1176	329	372	4			

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	7			
4	R	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	7			

- Molecule 5 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			
5	S	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			

- Molecule 6 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	243	Total	C	N	O	S	0	0	0
			1892	1203	329	356	4			
6	T	243	Total	C	N	O	S	0	0	0
			1892	1203	329	356	4			

- Molecule 7 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	241	Total	C	N	O	S	0	0	0
			1907	1214	320	365	8			
7	U	241	Total	C	N	O	S	0	0	0
			1907	1214	320	365	8			

- Molecule 8 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	226	Total	C	N	O	S	0	0	0
			1719	1082	298	332	7			
8	V	226	Total	C	N	O	S	0	0	0
			1719	1082	298	332	7			

- 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
			1581	1010	258	305	8			
9	W	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

- Molecule 10 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	6			

- Molecule 11 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	219	Total	C	N	O	S	0	0	0
			1700	1083	291	319	7			
11	Y	219	Total	C	N	O	S	0	0	0
			1700	1083	291	319	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	130	VAL	GLY	engineered mutation	UNP P30656
Y	130	VAL	GLY	engineered mutation	UNP P30656

- Molecule 12 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

- Molecule 13 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	a	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 14 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
14	b	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

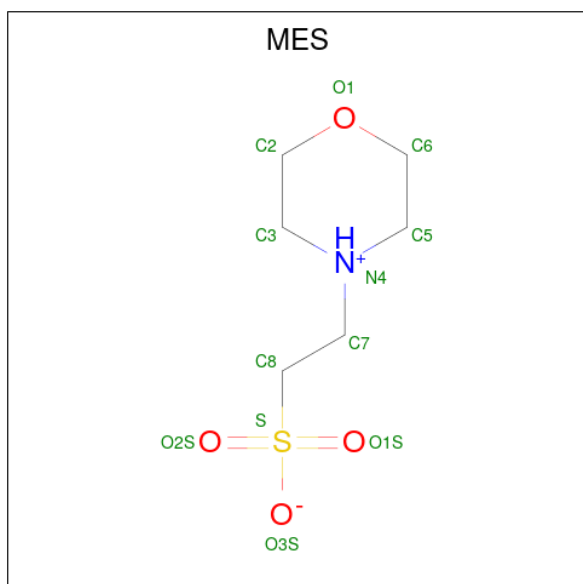
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	G	1	Total	Mg	0	0
			1	1		
15	I	1	Total	Mg	0	0
			1	1		
15	N	1	Total	Mg	0	0
			1	1		
15	V	1	Total	Mg	0	0
			1	1		
15	W	1	Total	Mg	0	0
			1	1		
15	Z	1	Total	Mg	0	0
			1	1		

- Molecule 16 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	G	1	Total	Cl	0	0
			1	1		
16	U	1	Total	Cl	0	0
			1	1		

- Molecule 17 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



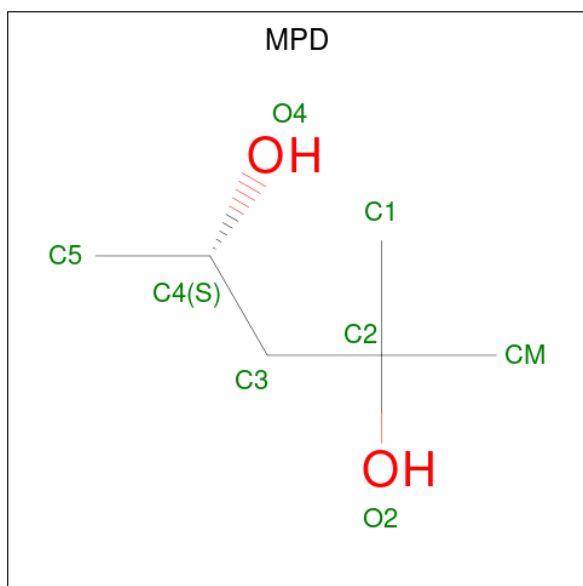
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
17	M	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
17	N	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
17	U	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
17	V	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
17	Z	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
17	b	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 18 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	K	1	Total	C	O	0	0
			8	6	2		
18	a	1	Total	C	O	0	0
			8	6	2		

- Molecule 19 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	40	Total O 40 40	0	0
19	B	24	Total O 24 24	0	0
19	C	34	Total O 34 34	0	0
19	D	26	Total O 26 26	0	0
19	E	20	Total O 20 20	0	0
19	F	30	Total O 30 30	0	0
19	G	44	Total O 44 44	0	0
19	H	40	Total O 40 40	0	0
19	I	40	Total O 40 40	0	0
19	J	18	Total O 18 18	0	0
19	K	22	Total O 22 22	0	0
19	L	29	Total O 29 29	0	0
19	M	47	Total O 47 47	0	0
19	N	41	Total O 41 41	0	0
19	O	31	Total O 31 31	0	0
19	P	21	Total O 21 21	0	0
19	Q	19	Total O 19 19	0	0
19	R	22	Total O 22 22	0	0
19	S	23	Total O 23 23	0	0
19	T	27	Total O 27 27	0	0
19	U	45	Total O 45 45	0	0
19	V	29	Total O 29 29	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	W	26	Total 26	O 26	0	0
19	X	10	Total 10	O 10	0	0
19	Y	19	Total 19	O 19	0	0
19	Z	22	Total 22	O 22	0	0
19	a	43	Total 43	O 43	0	0
19	b	41	Total 41	O 41	0	0

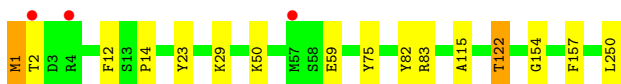
3 Residue-property plots [i](#)

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.

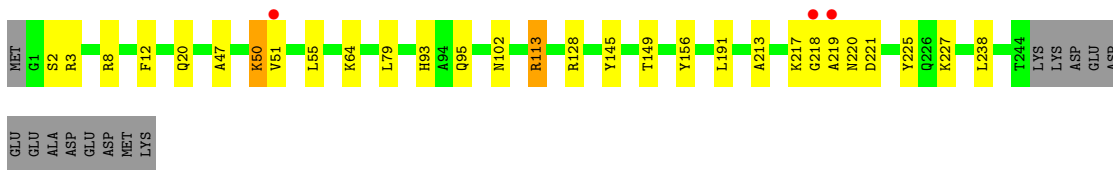
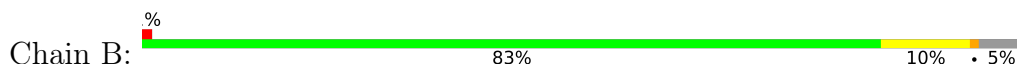
- Molecule 1: Proteasome subunit alpha type-2



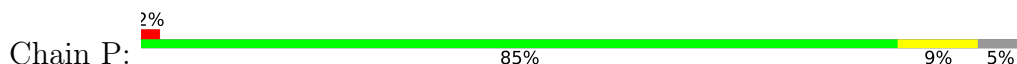
- Molecule 1: Proteasome subunit alpha type-2



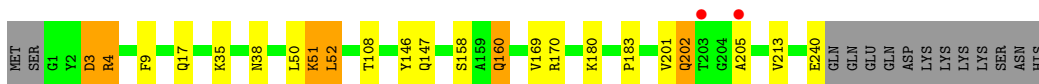
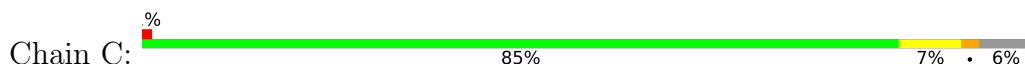
- Molecule 2: Proteasome subunit alpha type-3



- Molecule 2: Proteasome subunit alpha type-3

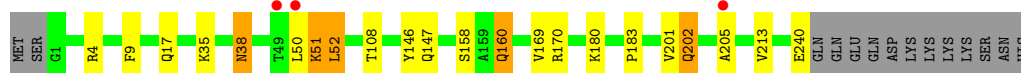


- Molecule 3: Proteasome subunit alpha type-4



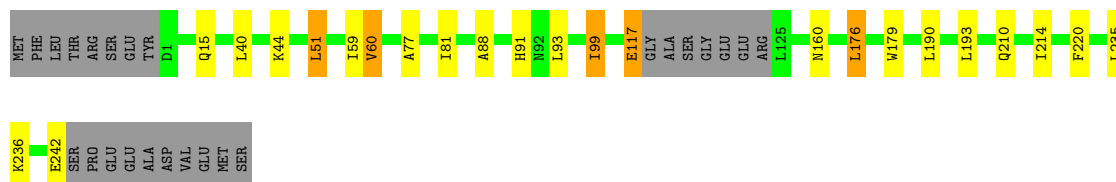
- Molecule 3: Proteasome subunit alpha type-4

Chain Q:  86% 7% 6%



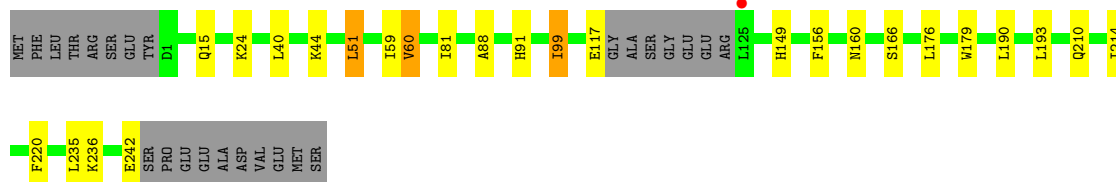
- Molecule 4: Proteasome subunit alpha type-5

Chain D:  81% 7% 10%



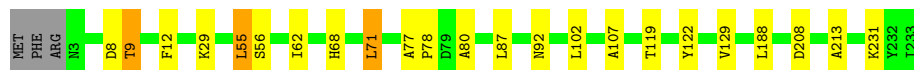
- Molecule 4: Proteasome subunit alpha type-5

Chain R:  80% 9% 10%



- Molecule 5: Proteasome subunit alpha type-6

Chain E:  89% 9% ..



- Molecule 5: Proteasome subunit alpha type-6

Chain S:  89% 9% ..



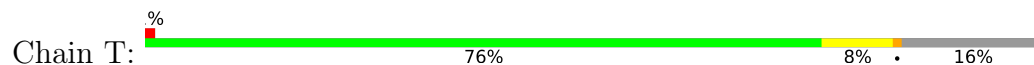
- Molecule 6: Probable proteasome subunit alpha type-7

Chain F:  77% 7% 16%



VAL MET SER SER ILE ASP ASP GLU ASN ALA ALA PRO VAL THR ALA ASN ALA THR THR THR ASP GLN GLY GLY ASP ASP ILE HIS LEU GLU

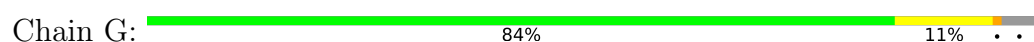
- Molecule 6: Probable proteasome subunit alpha type-7



MET THR SER ILE GLY T2 D14 Q19 I34 L77 S94 F95 K96 D110 Q114 Q117 Y122 N123 S124 M146 T161 E171 L172 E181 I195 L198 E201 E205 S216 E219 T220 N221 Q240 I243 Y244 GLY ASP ASP ASP

GLU ASP GLU ASP ASP ASP ASN VAL MET SER SER ASP ASP GLU ASN ALA ALA VAL THR ASN ALA THR THR THR ASP ASP ASP

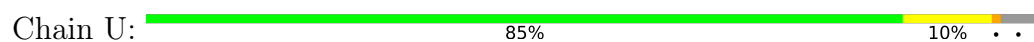
- Molecule 7: Proteasome subunit alpha type-1



MET SER GLY ALA ALA ALA SER ALA ALA G2 E13 F23 T26 L34 V43 S61 R68 M72 V73 V74 N75 G76 P77 I78 P79 N83 N114 L115 R122 M125 T133 K165 Q166 Q167 T171 V194 L205 E215 K223

R235 L236 Q242 ASP

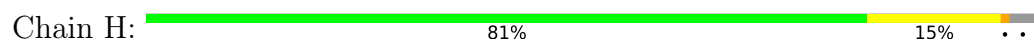
- Molecule 7: Proteasome subunit alpha type-1



MET SER GLY ALA ALA ALA SER ALA ALA G2 P12 E13 F23 T26 L34 V43 S61 R68 V73 V74 N75 G76 P77 I78 P79 N83 N114 L115 R122 M125 T133 K165 Q166 Q167 T171 V194 L205 E215 K223

R235 L236 Q242 ASP

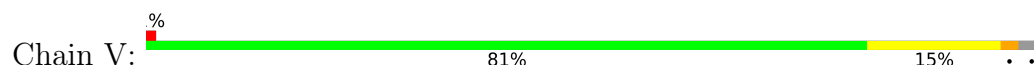
- Molecule 8: Proteasome subunit beta type-2



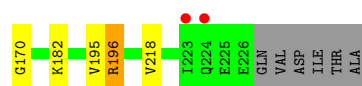
T1 T2 I3 V4 I14 R19 S20 T21 Q22 A27 D28 K29 N30 K33 L34 K40 C43 A44 E53 A54 V55 T56 Q57 I63 L68 P74 L80 K84 L98 I99 D104 P105 I113 L127 G128 I163 W164 N165 D166 L167 G170

K182 V196 R196 E226 GLN VAL ASP ILE THR ALA

- Molecule 8: Proteasome subunit beta type-2



T1 T2 I3 I14 R19 S20 T21 Q22 A27 N30 K33 L34 K40 C43 A44 E53 A54 V55 T56 Q57 I63 L68 P74 L80 K84 L98 I99 D104 P105 F111 S112 I113 T119 L127 G128 Q144 I163 L167



• Molecule 9: Proteasome subunit beta type-3

Chain I: 88% 11%



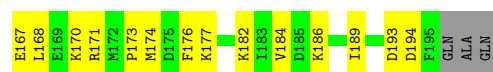
• Molecule 9: Proteasome subunit beta type-3

Chain W: 87% 12%



• Molecule 10: Proteasome subunit beta type-4

Chain J: 74% 21% . .



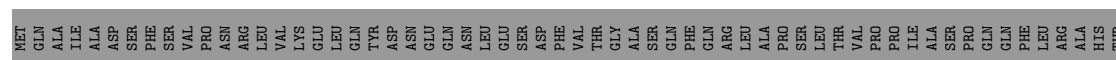
• Molecule 10: Proteasome subunit beta type-4

Chain X: 78% 18% . .



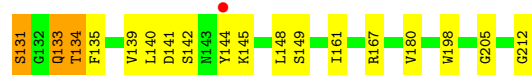
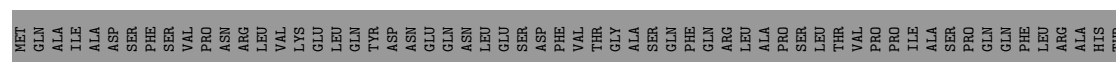
• Molecule 11: Proteasome subunit beta type-5

Chain K: 59% 15% 24%

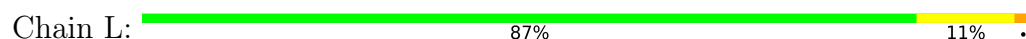




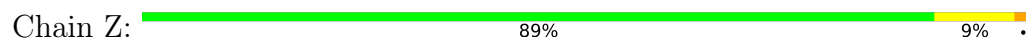
• Molecule 11: Proteasome subunit beta type-5



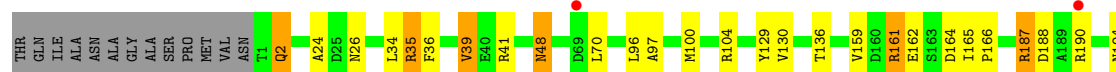
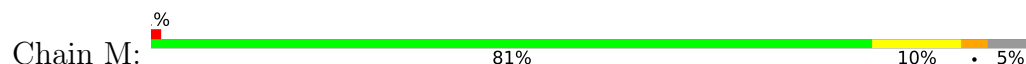
• Molecule 12: Proteasome subunit beta type-6



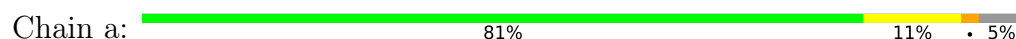
• Molecule 12: Proteasome subunit beta type-6



• Molecule 13: Proteasome subunit beta type-7

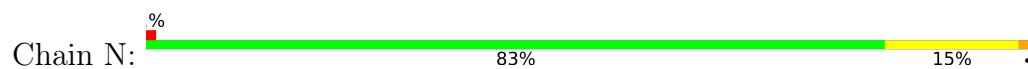


• Molecule 13: Proteasome subunit beta type-7

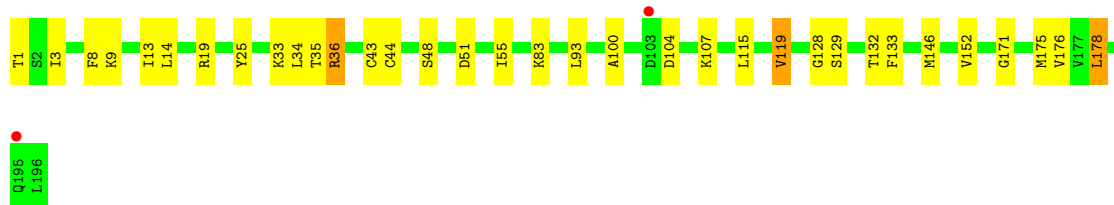
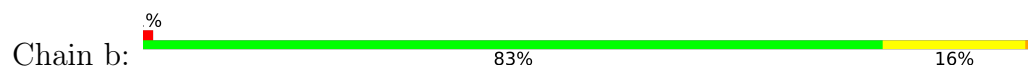




- Molecule 14: Proteasome subunit beta type-1



- Molecule 14: Proteasome subunit beta type-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	134.72Å 300.35Å 144.55Å 90.00° 112.80° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60 15.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.4 (15.00-2.60) 97.4 (15.00-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.186 , 0.224 0.185 , 0.223	Depositor DCC
R_{free} test set	15744 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	35.0	Xtriage
Anisotropy	1.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	50416	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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: CL, MG, MES, MPD

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	1.02	0/1937	1.42	0/2622
1	O	1.02	0/1952	1.41	0/2642
2	B	1.01	0/1934	1.44	0/2618
2	P	1.02	0/1934	1.45	0/2618
3	C	1.02	0/1910	1.46	1/2586 (0.0%)
3	Q	1.02	0/1910	1.46	0/2586
4	D	1.02	0/1837	1.46	0/2475
4	R	1.02	0/1837	1.47	0/2475
5	E	1.02	0/1800	1.41	0/2433
5	S	1.02	0/1800	1.42	0/2433
6	F	1.01	0/1932	1.44	4/2609 (0.2%)
6	T	1.01	0/1932	1.46	4/2609 (0.2%)
7	G	1.00	0/1945	1.44	2/2634 (0.1%)
7	U	1.01	0/1945	1.42	2/2634 (0.1%)
8	H	1.01	0/1750	1.42	2/2373 (0.1%)
8	V	1.02	0/1750	1.41	0/2373
9	I	1.00	0/1611	1.40	1/2174 (0.0%)
9	W	1.01	0/1611	1.41	3/2174 (0.1%)
10	J	0.96	0/1589	1.40	0/2142
10	X	0.97	0/1589	1.40	2/2142 (0.1%)
11	K	0.99	1/1738 (0.1%)	1.46	2/2350 (0.1%)
11	Y	0.99	1/1738 (0.1%)	1.46	3/2350 (0.1%)
12	L	0.99	0/1795	1.38	0/2420
12	Z	0.99	0/1795	1.39	0/2420
13	M	1.02	0/1855	1.41	5/2514 (0.2%)
13	a	1.01	0/1855	1.39	3/2514 (0.1%)
14	N	1.00	0/1541	1.42	0/2087
14	b	1.00	0/1541	1.41	0/2087
All	All	1.01	2/50363 (0.0%)	1.43	34/68094 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Y	140	LEU	N-CA	5.58	1.49	1.46
11	K	140	LEU	N-CA	5.53	1.49	1.46

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	T	77	LEU	CA-C-N	7.35	124.87	120.24
6	T	77	LEU	C-N-CA	7.35	124.87	120.24
7	G	77	PRO	CA-C-N	6.50	124.33	120.24
7	G	77	PRO	C-N-CA	6.50	124.33	120.24
11	Y	2	THR	CB-CA-C	6.42	123.20	110.42
7	U	77	PRO	CA-C-N	6.12	124.09	120.24
7	U	77	PRO	C-N-CA	6.12	124.09	120.24
9	W	183	GLY	CA-C-O	-5.93	118.36	122.22
13	a	188	ASP	CA-CB-CG	5.84	118.44	112.60
3	C	3	ASP	N-CA-CB	-5.80	102.60	110.67
9	I	183	GLY	CA-C-O	-5.80	118.45	122.22
6	F	34	ILE	CA-C-N	5.73	125.55	121.65
6	F	34	ILE	C-N-CA	5.73	125.55	121.65
6	T	34	ILE	CA-C-N	5.52	125.41	121.65
6	T	34	ILE	C-N-CA	5.52	125.41	121.65
13	M	188	ASP	CA-CB-CG	5.41	118.01	112.60
10	X	2	ASP	CA-C-N	-5.41	116.09	123.12
10	X	2	ASP	C-N-CA	-5.41	116.09	123.12
6	F	77	LEU	CA-C-N	5.27	124.54	120.33
6	F	77	LEU	C-N-CA	5.27	124.54	120.33
11	Y	1	THR	CA-C-N	5.18	131.44	121.54
11	Y	1	THR	C-N-CA	5.18	131.44	121.54
13	a	34	LEU	CA-C-N	5.13	127.41	120.44
13	a	34	LEU	C-N-CA	5.13	127.41	120.44
11	K	1	THR	CA-C-N	5.12	131.32	121.54
11	K	1	THR	C-N-CA	5.12	131.32	121.54
13	M	34	LEU	CA-C-N	5.10	127.07	120.44
13	M	34	LEU	C-N-CA	5.10	127.07	120.44
13	M	164	ASP	CA-C-N	5.08	124.39	120.33
13	M	164	ASP	C-N-CA	5.08	124.39	120.33
8	H	4	VAL	CA-C-N	5.08	125.11	121.65
8	H	4	VAL	C-N-CA	5.08	125.11	121.65
9	W	67	ARG	CA-C-N	5.06	127.38	120.54
9	W	67	ARG	C-N-CA	5.06	127.38	120.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1900	0	1910	19	0
1	O	1915	0	1929	10	0
2	B	1904	0	1904	26	0
2	P	1904	0	1904	13	0
3	C	1881	0	1895	14	0
3	Q	1881	0	1895	10	0
4	D	1813	0	1797	15	0
4	R	1813	0	1797	12	0
5	E	1773	0	1775	18	0
5	S	1773	0	1775	14	0
6	F	1892	0	1883	8	0
6	T	1892	0	1883	13	0
7	G	1907	0	1901	15	0
7	U	1907	0	1901	14	0
8	H	1719	0	1719	18	0
8	V	1719	0	1719	20	0
9	I	1581	0	1574	17	0
9	W	1581	0	1574	17	0
10	J	1561	0	1569	35	0
10	X	1561	0	1569	32	0
11	K	1700	0	1664	45	0
11	Y	1700	0	1664	28	0
12	L	1757	0	1711	21	0
12	Z	1757	0	1711	19	0
13	M	1824	0	1832	22	0
13	a	1824	0	1832	20	0
14	N	1512	0	1481	24	0
14	b	1512	0	1481	28	0
15	G	1	0	0	0	0
15	I	1	0	0	0	0
15	N	1	0	0	0	0
15	V	1	0	0	0	0
15	W	1	0	0	0	0
15	Z	1	0	0	0	0
16	G	1	0	0	0	0
16	U	1	0	0	0	0
17	G	12	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	H	12	0	13	1	0
17	M	12	0	13	1	0
17	N	12	0	13	4	0
17	U	12	0	13	0	0
17	V	12	0	13	1	0
17	Z	12	0	13	0	0
17	b	12	0	13	6	0
18	K	8	0	14	2	0
18	a	8	0	14	0	0
19	A	40	0	0	0	0
19	B	24	0	0	2	0
19	C	34	0	0	0	0
19	D	26	0	0	0	0
19	E	20	0	0	0	0
19	F	30	0	0	0	0
19	G	44	0	0	0	0
19	H	40	0	0	0	0
19	I	40	0	0	0	0
19	J	18	0	0	0	0
19	K	22	0	0	1	0
19	L	29	0	0	0	0
19	M	47	0	0	2	0
19	N	41	0	0	0	0
19	O	31	0	0	1	0
19	P	21	0	0	2	0
19	Q	19	0	0	0	0
19	R	22	0	0	0	0
19	S	23	0	0	0	0
19	T	27	0	0	0	0
19	U	45	0	0	0	0
19	V	29	0	0	0	0
19	W	26	0	0	0	0
19	X	10	0	0	0	0
19	Y	19	0	0	0	0
19	Z	22	0	0	0	0
19	a	43	0	0	3	0
19	b	41	0	0	0	0
All	All	50416	0	49381	468	0

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

All (468) 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)
11:K:133:GLN:HB3	11:K:135:PHE:CE1	1.75	1.19
11:K:133:GLN:HB3	11:K:135:PHE:CZ	1.91	1.05
14:b:128:GLY:HA2	17:b:201:MES:H82	1.38	1.04
11:K:73:ARG:HH21	11:K:105:THR:HG22	1.20	1.02
1:A:4:ARG:HB2	2:B:2:SER:OG	1.65	0.94
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.11	0.90
11:K:73:ARG:NH2	11:K:105:THR:HG22	1.87	0.89
11:Y:129:VAL:HG22	11:Y:134:THR:HG23	1.51	0.89
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.21	0.89
11:K:6:PHE:HB3	11:K:126:ILE:HD12	1.53	0.89
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.38	0.88
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.39	0.88
11:K:120:THR:CG2	11:K:122:LEU:CD2	2.51	0.88
11:K:6:PHE:HB3	11:K:126:ILE:CD1	2.04	0.88
1:A:4:ARG:HB2	2:B:2:SER:CB	2.06	0.85
13:M:233:ILE:HD11	14:b:36:ARG:HD2	1.59	0.85
1:A:4:ARG:CB	2:B:2:SER:OG	2.28	0.81
14:N:115:LEU:HD11	17:N:202:MES:H51	1.65	0.79
11:K:133:GLN:CB	11:K:135:PHE:CE1	2.62	0.78
6:F:123:ASN:C	6:F:123:ASN:HD22	1.92	0.78
11:K:120:THR:HG23	11:K:122:LEU:CD2	2.14	0.77
5:E:92:ASN:ND2	12:L:70:ASN:HD21	1.82	0.76
6:T:123:ASN:C	6:T:123:ASN:HD22	1.94	0.76
2:B:12:PHE:H	3:C:17:GLN:HE22	1.34	0.75
14:b:128:GLY:HA2	17:b:201:MES:C8	2.15	0.75
5:E:92:ASN:HD21	12:L:70:ASN:ND2	1.83	0.74
10:X:3:ILE:HD13	10:X:176:PHE:CD2	2.23	0.74
8:H:3:ILE:HG22	8:H:99:ILE:HD12	1.70	0.73
10:X:3:ILE:HD13	10:X:176:PHE:CG	2.24	0.73
8:H:43:CYS:SG	8:H:56:THR:CG2	2.76	0.73
1:A:4:ARG:HD3	5:E:122:TYR:CD2	2.23	0.73
2:B:8:ARG:HD2	3:C:4:ARG:NH1	2.03	0.72
8:V:43:CYS:SG	8:V:56:THR:CG2	2.78	0.72
7:G:23:PHE:O	7:G:26:THR:HB	1.89	0.72
14:N:152:VAL:HA	14:N:175:MET:HE1	1.71	0.72
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.54	0.72
11:K:120:THR:CG2	11:K:122:LEU:HD23	2.19	0.72
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.37	0.72
7:U:23:PHE:O	7:U:26:THR:HB	1.89	0.72
14:b:152:VAL:HA	14:b:175:MET:HE1	1.70	0.72
1:A:128:ARG:HH11	1:A:128:ARG:HG3	1.55	0.71
8:V:3:ILE:HG22	8:V:99:ILE:HD12	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ARG:HD3	5:E:122:TYR:HD2	1.56	0.70
3:C:9:PHE:H	4:D:15:GLN:HE22	1.41	0.69
5:S:92:ASN:HD21	12:Z:70:ASN:ND2	1.91	0.69
10:J:3:ILE:HD13	10:J:176:PHE:CD2	2.28	0.68
1:A:128:ARG:HH11	1:A:128:ARG:CG	2.05	0.68
13:M:2:GLN:NE2	19:M:401:HOH:O	2.26	0.68
13:a:2:GLN:NE2	19:a:401:HOH:O	2.26	0.68
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.59	0.67
9:W:37:ASN:HD22	9:W:37:ASN:H	1.40	0.67
5:S:92:ASN:ND2	12:Z:70:ASN:HD21	1.90	0.67
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.43	0.66
17:N:202:MES:H22	17:N:202:MES:H81	1.76	0.66
2:B:93:HIS:HB3	19:B:301:HOH:O	1.96	0.66
1:A:4:ARG:HB2	2:B:2:SER:HB3	1.77	0.66
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.44	0.65
10:J:35:THR:HG23	10:J:43:LEU:HD11	1.77	0.65
13:M:232:LYS:NZ	19:M:402:HOH:O	2.29	0.65
12:Z:31:THR:CG2	12:Z:36:ASN:HD21	2.08	0.65
12:L:31:THR:CG2	12:L:36:ASN:HD21	2.10	0.65
10:X:3:ILE:CD1	10:X:176:PHE:CD2	2.80	0.65
9:I:37:ASN:H	9:I:37:ASN:HD22	1.43	0.64
5:S:12:PHE:H	6:T:19:GLN:HE22	1.43	0.64
11:Y:2:THR:HG22	11:Y:161:ILE:HD12	1.80	0.64
10:X:35:THR:HG23	10:X:43:LEU:HD11	1.79	0.64
8:H:43:CYS:SG	8:H:56:THR:HG21	2.37	0.64
2:P:217:LYS:C	2:P:219:ALA:H	2.06	0.64
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.80	0.64
2:B:217:LYS:C	2:B:219:ALA:H	2.06	0.63
11:Y:73:ARG:HH21	11:Y:105:THR:HG22	1.64	0.63
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.63	0.62
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.63	0.62
14:N:13:ILE:HG21	14:N:175:MET:HE2	1.81	0.62
8:V:43:CYS:SG	8:V:56:THR:HG21	2.40	0.62
5:E:12:PHE:H	6:F:19:GLN:HE22	1.48	0.61
1:O:12:PHE:H	2:P:20:GLN:HE22	1.46	0.61
11:K:133:GLN:CB	11:K:135:PHE:CZ	2.76	0.61
10:J:3:ILE:HD13	10:J:176:PHE:CG	2.36	0.61
13:a:27:LEU:HD21	13:a:34:LEU:HD22	1.83	0.61
10:J:177:LYS:NZ	10:X:170:LYS:O	2.32	0.61
11:K:76:VAL:N	11:K:108:GLU:OE2	2.34	0.60
1:O:1:MET:HG3	6:T:122:TYR:CZ	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:33:ASP:OD2	10:X:182:LYS:NZ	2.34	0.60
3:C:3:ASP:OD1	4:D:117:GLU:C	2.44	0.60
12:L:8:ASN:HA	12:L:30:ILE:O	2.02	0.60
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.83	0.60
12:Z:49:ASN:HD21	12:Z:211:GLY:HA2	1.67	0.59
10:J:170:LYS:O	10:X:177:LYS:NZ	2.34	0.59
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.84	0.59
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.50	0.59
13:M:159:VAL:HG23	13:M:159:VAL:O	2.03	0.59
14:b:13:ILE:HG21	14:b:175:MET:HE2	1.84	0.59
11:K:90:TYR:OH	18:K:301:MPD:O2	2.20	0.59
10:X:41:HIS:CD2	10:X:109:LYS:HD3	2.38	0.59
11:K:6:PHE:HB3	11:K:126:ILE:HD13	1.82	0.59
11:K:2:THR:HG22	11:K:161:ILE:HD12	1.84	0.59
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.02	0.59
14:N:1:THR:OG1	14:N:33:LYS:NZ	2.36	0.58
13:M:228:TYR:HE2	14:b:35:THR:HG21	1.68	0.58
10:J:25:ILE:HA	10:X:173:PRO:HG2	1.85	0.57
10:J:41:HIS:CD2	10:J:109:LYS:HD3	2.39	0.57
10:X:49:GLU:OE2	10:X:99:GLN:NE2	2.37	0.57
1:A:4:ARG:CD	5:E:122:TYR:HD2	2.17	0.57
7:G:61:SER:OG	7:G:215:GLU:OE2	2.21	0.57
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.34	0.57
11:Y:1:THR:HB	11:Y:131:SER:H	1.68	0.57
13:a:159:VAL:HG23	13:a:159:VAL:O	2.03	0.57
8:V:19:ARG:NH1	8:V:167:LEU:O	2.37	0.57
12:L:49:ASN:HD21	12:L:211:GLY:HA2	1.69	0.57
9:I:101:PRO:O	10:J:93:ARG:NH1	2.38	0.56
8:H:19:ARG:NH1	8:H:167:LEU:O	2.38	0.56
10:J:35:THR:CG2	10:J:43:LEU:HD11	2.35	0.56
14:b:83:LYS:HG3	14:b:119:VAL:CG2	2.36	0.56
9:I:58:ASP:OD2	10:J:93:ARG:NH2	2.39	0.56
3:C:35:LYS:HG2	3:C:158:SER:O	2.06	0.56
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.88	0.56
11:K:145:LYS:HB2	11:K:148:LEU:HD13	1.87	0.56
6:T:123:ASN:HD22	6:T:124:SER:N	2.03	0.56
2:B:3:ARG:HG3	3:C:4:ARG:HH21	1.71	0.56
6:F:123:ASN:HD22	6:F:124:SER:N	2.03	0.56
2:B:8:ARG:CD	3:C:4:ARG:NH1	2.69	0.55
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.87	0.55
9:W:101:PRO:O	10:X:93:ARG:NH1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:3:ILE:H	10:X:18:SER:HB3	1.71	0.55
10:J:33:ASP:OD2	10:J:182:LYS:NZ	2.36	0.55
13:M:233:ILE:HD11	14:b:36:ARG:CD	2.33	0.55
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.42	0.55
9:W:58:ASP:OD2	10:X:93:ARG:NH2	2.40	0.55
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	1.87	0.55
4:D:176:LEU:HD22	5:E:55:LEU:CD2	2.36	0.54
10:X:35:THR:CG2	10:X:43:LEU:HD11	2.37	0.54
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.89	0.54
1:A:12:PHE:H	2:B:20:GLN:HE22	1.54	0.54
10:J:149:ARG:NH1	11:Y:205:GLY:C	2.65	0.54
14:b:128:GLY:CA	17:b:201:MES:H82	2.25	0.54
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.90	0.54
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.43	0.54
2:B:95:GLN:NE2	9:I:71:ASN:HD22	2.06	0.54
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.90	0.54
10:J:49:GLU:OE2	10:J:99:GLN:NE2	2.40	0.54
8:H:3:ILE:HG12	8:H:44:ALA:HB1	1.91	0.53
7:G:167:GLN:HE21	7:G:171:THR:HG23	1.74	0.53
8:H:128:GLY:HA2	17:H:301:MES:H82	1.90	0.53
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.91	0.53
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.43	0.53
11:K:1:THR:CB	11:K:131:SER:H	2.21	0.53
11:K:2:THR:HG22	11:K:161:ILE:CD1	2.38	0.53
11:K:4:LEU:HD11	11:K:126:ILE:HD11	1.90	0.53
2:P:93:HIS:HB3	19:P:302:HOH:O	2.08	0.53
11:K:129:VAL:HG22	11:K:134:THR:HG23	1.91	0.53
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.08	0.53
12:L:113:GLY:HA2	12:L:207:VAL:HG11	1.91	0.53
7:G:68:ARG:HH12	14:N:36:ARG:HH22	1.56	0.53
8:V:3:ILE:HG12	8:V:44:ALA:HB1	1.90	0.53
11:Y:7:ARG:HH11	11:Y:7:ARG:HG2	1.74	0.53
11:Y:46:ALA:HB3	11:Y:98:GLY:O	2.09	0.52
12:Z:42:LYS:HD2	12:Z:55:ASN:HD22	1.74	0.52
11:K:46:ALA:HB3	11:K:98:GLY:O	2.10	0.52
6:T:123:ASN:C	6:T:123:ASN:ND2	2.66	0.52
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.09	0.52
3:C:51:LYS:O	3:C:52:LEU:HB2	2.08	0.52
8:H:53:GLU:OE1	8:H:57:GLN:NE2	2.43	0.52
11:K:120:THR:HG23	11:K:122:LEU:HD22	1.89	0.52
11:K:205:GLY:C	10:X:149:ARG:NH1	2.68	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:71:LEU:HD22	5:S:71:LEU:C	2.35	0.52
12:Z:113:GLY:HA2	12:Z:207:VAL:HG11	1.92	0.52
11:K:120:THR:HG22	11:K:122:LEU:HD23	1.92	0.52
14:b:1:THR:OG1	14:b:33:LYS:NZ	2.40	0.52
12:L:189:THR:HG22	8:V:196:ARG:NH1	2.25	0.51
11:Y:133:GLN:HB3	11:Y:135:PHE:CE1	2.45	0.51
10:J:18:SER:HB2	10:J:176:PHE:HB2	1.93	0.51
10:J:167:GLU:OE1	10:J:171:ARG:NH2	2.43	0.51
10:J:3:ILE:CD1	10:J:176:PHE:CD2	2.93	0.51
12:L:141:ALA:HB1	12:L:195:HIS:NE2	2.25	0.51
9:W:37:ASN:H	9:W:37:ASN:ND2	2.08	0.51
12:Z:141:ALA:HB1	12:Z:195:HIS:NE2	2.26	0.51
14:N:55:ILE:HD11	14:N:93:LEU:HD13	1.93	0.50
1:O:1:MET:HG3	6:T:122:TYR:CE1	2.46	0.50
13:M:97:ALA:HA	13:M:130:VAL:HG21	1.93	0.50
10:J:173:PRO:HG2	10:X:25:ILE:HA	1.92	0.50
10:X:18:SER:HB2	10:X:176:PHE:HB2	1.93	0.50
5:E:71:LEU:C	5:E:71:LEU:HD22	2.36	0.50
10:X:167:GLU:OE1	10:X:171:ARG:NH2	2.44	0.50
5:S:62:ILE:HG21	5:S:213:ALA:HB2	1.94	0.50
11:Y:133:GLN:HB3	11:Y:135:PHE:CZ	2.47	0.50
13:M:96:LEU:O	13:M:100:MET:HG2	2.12	0.50
12:L:42:LYS:HD2	12:L:55:ASN:HD22	1.76	0.49
9:I:37:ASN:H	9:I:37:ASN:ND2	2.10	0.49
12:L:100:LYS:HD3	12:L:105:TYR:CZ	2.48	0.49
14:N:35:THR:OG1	14:N:43:CYS:SG	2.70	0.49
12:Z:1:GLN:HG2	13:a:1:THR:HG21	1.93	0.49
5:E:62:ILE:HG21	5:E:213:ALA:HB2	1.94	0.49
1:A:83:ARG:HE	7:G:114:ASN:HD21	1.61	0.49
10:J:161:LEU:O	10:J:165:VAL:HG23	2.13	0.49
14:N:133:PHE:HA	14:b:132:THR:O	2.12	0.49
1:A:128:ARG:CG	1:A:128:ARG:NH1	2.72	0.49
5:S:98:PHE:O	13:a:91:TYR:HA	2.12	0.49
7:U:167:GLN:HE21	7:U:171:THR:HG23	1.78	0.49
10:X:109:LYS:NZ	10:X:186:LYS:O	2.44	0.49
12:Z:100:LYS:HD3	12:Z:105:TYR:CZ	2.48	0.49
1:A:4:ARG:HB3	2:B:2:SER:OG	2.12	0.49
7:U:61:SER:OG	7:U:215:GLU:OE2	2.28	0.49
7:U:78:ILE:N	7:U:79:PRO:CD	2.76	0.49
13:a:150:MET:HE1	13:a:187:ARG:HG2	1.94	0.49
14:b:55:ILE:HD11	14:b:93:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:100:LYS:HD3	12:Z:105:TYR:CE2	2.47	0.48
14:b:14:LEU:HB3	14:b:34:LEU:HD22	1.95	0.48
11:K:131:SER:HB2	11:K:168:ASP:OD2	2.13	0.48
11:Y:114:TYR:CE1	11:Y:134:THR:HG21	2.48	0.48
8:H:1:THR:OG1	8:H:33:LYS:NZ	2.44	0.48
9:I:141:ALA:HB2	9:I:177:ASP:HB2	1.95	0.48
11:K:120:THR:HG22	11:K:122:LEU:CD2	2.41	0.48
13:M:187:ARG:HG3	14:b:25:TYR:CE1	2.48	0.48
5:S:71:LEU:C	5:S:71:LEU:CD2	2.86	0.48
14:b:19:ARG:O	14:b:33:LYS:NZ	2.46	0.48
7:U:73:VAL:HG12	7:U:133:THR:HB	1.95	0.48
7:G:78:ILE:N	7:G:79:PRO:CD	2.76	0.48
10:J:25:ILE:HG12	10:J:25:ILE:O	2.11	0.48
12:L:100:LYS:HD3	12:L:105:TYR:CE2	2.48	0.48
14:N:35:THR:HG21	13:a:228:TYR:HE2	1.78	0.48
10:J:4:ILE:HG13	10:J:4:ILE:O	2.13	0.48
13:a:96:LEU:O	13:a:100:MET:HG2	2.12	0.48
11:Y:-1:HIS:HE1	11:Y:31:VAL:HG21	1.79	0.48
8:V:1:THR:OG1	8:V:33:LYS:NZ	2.44	0.48
10:X:28:LEU:HD21	11:Y:134:THR:HB	1.96	0.48
6:T:198:LEU:HD12	6:T:243:ILE:HG22	1.96	0.48
10:X:29:LYS:HE3	11:Y:123:LYS:O	2.14	0.47
10:X:161:LEU:O	10:X:165:VAL:HG23	2.14	0.47
13:a:97:ALA:HA	13:a:130:VAL:HG21	1.96	0.47
10:J:92:ILE:HG21	10:J:122:LEU:HA	1.96	0.47
8:V:53:GLU:OE1	8:V:57:GLN:NE2	2.47	0.47
10:X:4:ILE:HG13	10:X:4:ILE:O	2.13	0.47
11:Y:128:CYS:SG	11:Y:139:VAL:CG2	3.03	0.47
14:N:47:GLY:HA2	17:N:202:MES:H71	1.97	0.47
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.96	0.47
11:Y:128:CYS:SG	11:Y:139:VAL:HG22	2.55	0.47
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.45	0.47
6:F:198:LEU:HD12	6:F:243:ILE:HG22	1.96	0.47
11:Y:-5:ILE:HB	12:Z:127:PRO:HG2	1.97	0.47
11:Y:97:MET:N	11:Y:117:SER:OG	2.45	0.47
5:E:71:LEU:C	5:E:71:LEU:CD2	2.88	0.47
10:J:29:LYS:HE3	11:K:123:LYS:O	2.14	0.47
10:J:109:LYS:NZ	10:J:186:LYS:O	2.44	0.47
8:V:80:LEU:HD13	8:V:119:THR:HG21	1.96	0.47
10:X:25:ILE:O	10:X:25:ILE:HG12	2.11	0.47
10:X:81:SER:OG	10:X:125:LYS:NZ	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:176:LEU:HA	5:E:55:LEU:HD21	1.96	0.47
7:G:68:ARG:O	7:G:223:LYS:HA	2.15	0.47
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.96	0.47
14:b:176:VAL:HG12	14:b:178:LEU:HD13	1.96	0.47
1:A:28:VAL:HG11	1:A:133:SER:HB2	1.97	0.47
1:A:83:ARG:HE	7:G:114:ASN:ND2	2.13	0.47
8:V:40:LYS:HE2	8:V:182:LYS:O	2.15	0.47
5:E:68:HIS:HE1	5:E:102:LEU:O	1.98	0.47
14:N:14:LEU:HB3	14:N:34:LEU:HD22	1.96	0.47
7:G:73:VAL:HG12	7:G:133:THR:HB	1.96	0.46
2:P:95:GLN:HE21	9:W:68:TYR:HA	1.80	0.46
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.63	0.46
8:V:218:VAL:CG2	9:W:196:LYS:HB2	2.45	0.46
10:X:92:ILE:HG21	10:X:122:LEU:HA	1.96	0.46
10:X:160:LEU:HD12	10:X:160:LEU:O	2.14	0.46
5:S:68:HIS:HE1	5:S:102:LEU:O	1.98	0.46
7:U:83:ASN:C	7:U:83:ASN:HD22	2.22	0.46
3:C:201:VAL:O	3:C:202:GLN:CB	2.63	0.46
10:J:160:LEU:HD12	10:J:160:LEU:O	2.14	0.46
13:M:194:ASN:ND2	13:M:213:GLN:HG2	2.30	0.46
10:X:161:LEU:HD12	10:X:161:LEU:HA	1.81	0.46
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.97	0.46
7:G:83:ASN:C	7:G:83:ASN:HD22	2.24	0.46
8:H:63:ILE:HG23	8:H:74:PRO:HB3	1.97	0.46
9:I:94:LEU:HD11	9:I:106:PRO:HG2	1.97	0.46
17:b:201:MES:H51	17:b:201:MES:S	2.56	0.46
8:H:40:LYS:HE2	8:H:182:LYS:O	2.16	0.46
14:N:3:ILE:HB	14:N:44:CYS:HB3	1.97	0.46
11:K:133:GLN:CB	11:K:135:PHE:HE1	2.24	0.46
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.45	0.46
14:b:3:ILE:HB	14:b:44:CYS:HB3	1.98	0.46
9:W:94:LEU:HD11	9:W:106:PRO:HG2	1.97	0.46
8:H:84:LYS:HA	8:H:113:ILE:HD11	1.98	0.46
11:K:128:CYS:SG	11:K:139:VAL:HG22	2.55	0.46
8:V:80:LEU:HD21	8:V:111:PHE:HB2	1.98	0.46
13:a:232:LYS:NZ	19:a:402:HOH:O	2.31	0.46
2:B:217:LYS:C	2:B:219:ALA:N	2.73	0.46
4:D:44:LYS:HE3	4:D:210:GLN:HB2	1.98	0.46
8:V:63:ILE:HG23	8:V:74:PRO:HB3	1.99	0.46
2:B:145:TYR:OH	2:B:217:LYS:N	2.49	0.45
13:M:165:ILE:HB	13:M:166:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:68:ARG:O	7:U:223:LYS:HA	2.16	0.45
11:Y:2:THR:HG22	11:Y:161:ILE:CD1	2.44	0.45
14:b:35:THR:OG1	14:b:43:CYS:SG	2.74	0.45
14:N:13:ILE:HG21	14:N:175:MET:CE	2.47	0.45
9:W:170:LEU:C	9:W:170:LEU:HD23	2.40	0.45
13:M:35:ARG:HD2	13:M:36:PHE:CZ	2.51	0.45
2:B:50:LYS:HD3	2:B:50:LYS:HA	1.83	0.45
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.47	0.45
12:Z:31:THR:HG23	12:Z:36:ASN:ND2	2.26	0.45
11:K:-5:ILE:HB	12:L:127:PRO:HG2	1.98	0.45
4:R:44:LYS:HE3	4:R:210:GLN:HB2	1.98	0.45
1:A:97:TYR:OH	9:I:77:GLU:OE2	2.31	0.45
9:I:56:ALA:HB3	10:J:124:THR:HG23	1.98	0.45
10:J:29:LYS:HD2	11:K:122:LEU:HD12	1.99	0.45
12:L:31:THR:HG23	12:L:36:ASN:ND2	2.30	0.45
2:P:145:TYR:OH	2:P:217:LYS:N	2.49	0.45
10:J:161:LEU:HD12	10:J:161:LEU:HA	1.81	0.45
11:K:128:CYS:SG	11:K:139:VAL:CG2	3.05	0.45
13:M:233:ILE:CD1	14:b:36:ARG:HD2	2.40	0.45
8:V:128:GLY:HA2	17:V:302:MES:H81	1.99	0.45
9:W:141:ALA:HB2	9:W:177:ASP:HB2	1.98	0.45
4:D:91:HIS:HB3	4:D:99:ILE:HG22	2.00	0.44
9:I:7:ASN:HA	9:I:29:GLY:O	2.17	0.44
4:R:91:HIS:CD2	4:R:99:ILE:HG22	2.51	0.44
9:I:170:LEU:C	9:I:170:LEU:HD23	2.41	0.44
4:R:91:HIS:HB3	4:R:99:ILE:HG22	1.99	0.44
8:V:43:CYS:SG	8:V:56:THR:HG22	2.56	0.44
7:G:34:LEU:C	7:G:34:LEU:HD23	2.43	0.44
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.83	0.44
6:T:110:ASP:O	6:T:114:GLN:HG2	2.17	0.44
14:N:14:LEU:HD11	14:N:100:ALA:HB3	2.00	0.44
9:W:7:ASN:HA	9:W:29:GLY:O	2.17	0.44
13:a:165:ILE:HB	13:a:166:PRO:HD3	1.99	0.44
10:J:81:SER:OG	10:J:125:LYS:NZ	2.35	0.44
11:K:120:THR:CG2	11:K:122:LEU:HD22	2.41	0.44
14:b:14:LEU:HD11	14:b:100:ALA:HB3	1.99	0.44
4:D:91:HIS:CD2	4:D:99:ILE:HG22	2.53	0.44
5:E:9:THR:HG21	5:E:119:THR:HA	2.00	0.44
5:S:71:LEU:HD22	5:S:71:LEU:O	2.18	0.44
14:b:129:SER:N	17:b:201:MES:H81	2.33	0.44
3:Q:108:THR:HG21	3:Q:146:TYR:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:84:LYS:HA	8:V:113:ILE:HD11	1.99	0.44
8:H:165:ASN:HD22	13:a:156:ARG:HH11	1.65	0.44
9:W:26:LEU:HD21	9:W:185:VAL:HG23	2.00	0.44
17:b:201:MES:H51	17:b:201:MES:O1S	2.18	0.44
5:S:77:ALA:N	5:S:78:PRO:CD	2.81	0.43
11:K:3:THR:HA	11:K:16:VAL:HG12	2.00	0.43
14:N:48:SER:HB3	14:N:51:ASP:HB2	2.00	0.43
12:Z:28:ARG:HG2	12:Z:30:ILE:HG23	2.00	0.43
2:B:8:ARG:HD2	3:C:4:ARG:HH12	1.82	0.43
9:I:26:LEU:HD21	9:I:185:VAL:HG23	2.00	0.43
2:P:113:ARG:NE	19:P:302:HOH:O	2.41	0.43
11:Y:73:ARG:NH2	11:Y:104:TYR:O	2.41	0.43
9:W:56:ALA:HB3	10:X:124:THR:HG23	2.00	0.43
5:E:77:ALA:N	5:E:78:PRO:CD	2.82	0.43
6:F:110:ASP:O	6:F:114:GLN:HG2	2.18	0.43
13:a:184:LEU:O	13:a:188:ASP:HB3	2.19	0.43
11:K:65:LEU:O	11:K:69:ARG:HG3	2.19	0.43
12:L:28:ARG:HG2	12:L:30:ILE:HG23	2.01	0.43
13:M:161:ARG:HE	13:M:161:ARG:HB3	1.70	0.43
14:N:19:ARG:O	14:N:33:LYS:NZ	2.48	0.43
11:Y:12:ILE:HB	11:Y:180:VAL:HB	2.00	0.43
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.99	0.43
5:S:9:THR:HG21	5:S:119:THR:HA	2.01	0.43
13:a:26:ASN:HA	13:a:39:VAL:O	2.19	0.43
1:A:115:ALA:HB1	1:A:154:GLY:O	2.19	0.43
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.84	0.43
17:N:202:MES:H61	17:N:202:MES:H82	2.01	0.43
6:T:171:GLU:HB3	6:T:195:ILE:HG12	2.00	0.43
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.00	0.43
11:Y:65:LEU:O	11:Y:69:ARG:HG3	2.19	0.43
14:b:48:SER:HB3	14:b:51:ASP:HB2	2.01	0.43
4:D:60:VAL:HG11	4:D:81:ILE:HG21	2.01	0.42
1:O:50:LYS:HB3	19:O:327:HOH:O	2.19	0.42
1:O:115:ALA:HB1	1:O:154:GLY:O	2.19	0.42
3:Q:160:GLN:HE21	3:Q:160:GLN:CA	2.16	0.42
3:C:108:THR:HG21	3:C:146:TYR:HB3	2.01	0.42
4:D:77:ALA:O	4:D:81:ILE:HG12	2.18	0.42
11:K:12:ILE:HB	11:K:180:VAL:HB	2.01	0.42
11:Y:1:THR:OG1	11:Y:2:THR:OG1	2.30	0.42
2:B:113:ARG:NE	19:B:301:HOH:O	2.37	0.42
18:K:301:MPD:O2	18:K:301:MPD:H52	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:29:LYS:HE2	12:Z:194:ARG:NH2	2.34	0.42
8:H:196:ARG:NH2	9:I:150:GLU:HG3	2.34	0.42
11:K:43:GLY:HA3	11:K:56:GLU:OE1	2.20	0.42
7:U:165:LYS:HD2	7:U:205:LEU:HD22	2.02	0.42
8:V:22:GLN:HG3	8:V:27:ALA:HB2	2.00	0.42
2:B:93:HIS:CE1	2:B:113:ARG:HG2	2.55	0.42
4:R:60:VAL:HG11	4:R:81:ILE:HG21	2.02	0.42
8:V:104:ASP:HB2	8:V:105:PRO:HD2	2.01	0.42
10:X:45:SER:OG	10:X:103:LEU:HB2	2.19	0.42
7:G:72:MET:HE3	7:G:74:VAL:CG2	2.50	0.42
14:N:14:LEU:O	14:N:175:MET:HA	2.19	0.42
6:T:96:LYS:NZ	19:a:404:HOH:O	2.52	0.42
7:U:34:LEU:C	7:U:34:LEU:HD23	2.44	0.42
14:N:171:GLY:HA2	13:a:219:TRP:CH2	2.54	0.42
14:b:14:LEU:O	14:b:175:MET:HA	2.20	0.42
6:F:171:GLU:HB3	6:F:195:ILE:HG12	2.00	0.42
7:G:165:LYS:HD2	7:G:205:LEU:HD22	2.02	0.42
8:H:22:GLN:HG3	8:H:27:ALA:HB2	2.00	0.42
13:M:48:ASN:C	13:M:48:ASN:HD22	2.28	0.42
13:M:159:VAL:O	13:M:159:VAL:CG2	2.67	0.42
3:Q:160:GLN:HE22	3:Q:170:ARG:HE	1.67	0.42
8:H:98:LEU:HB2	8:H:113:ILE:HG23	2.00	0.42
10:J:46:PHE:HD1	10:J:53:THR:HB	1.85	0.42
12:L:152:ASN:O	12:L:156:PHE:HA	2.19	0.42
4:R:59:ILE:HG22	4:R:220:PHE:HZ	1.85	0.42
5:S:80:ALA:HB2	5:S:129:VAL:HG21	2.02	0.41
7:U:78:ILE:HG22	7:U:79:PRO:HD3	2.02	0.41
8:V:98:LEU:HB2	8:V:113:ILE:HG23	2.01	0.41
3:C:160:GLN:HE22	3:C:170:ARG:HE	1.68	0.41
4:D:51:LEU:HD12	4:D:51:LEU:C	2.45	0.41
7:G:43:VAL:HG11	7:G:194:VAL:HA	2.02	0.41
1:O:14:PRO:HA	2:P:23:TYR:CD1	2.56	0.41
7:U:68:ARG:HH12	14:b:36:ARG:HH22	1.68	0.41
13:a:139:SER:HB3	13:a:141:THR:O	2.20	0.41
5:E:80:ALA:HB2	5:E:129:VAL:HG21	2.01	0.41
8:H:104:ASP:HB2	8:H:105:PRO:HD2	2.02	0.41
10:J:143:LEU:HD23	10:J:164:CYS:SG	2.59	0.41
4:R:51:LEU:C	4:R:51:LEU:HD12	2.46	0.41
10:X:136:SER:HB3	10:X:168:LEU:HD22	2.02	0.41
2:B:213:ALA:HA	2:B:227:LYS:O	2.20	0.41
10:J:28:LEU:HD21	11:K:134:THR:HB	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:133:GLN:HG2	11:K:135:PHE:HZ	1.85	0.41
13:M:162:GLU:O	13:M:165:ILE:HG13	2.20	0.41
13:M:219:TRP:CH2	14:b:171:GLY:HA2	2.55	0.41
2:P:93:HIS:CE1	2:P:113:ARG:HG2	2.55	0.41
11:Y:167:ARG:HD3	11:Y:167:ARG:HA	1.84	0.41
4:D:93:LEU:HD11	19:K:418:HOH:O	2.20	0.41
2:B:149:THR:O	2:B:156:TYR:HA	2.21	0.41
8:H:163:ILE:HG23	8:H:170:GLY:HA2	2.02	0.41
6:T:240:GLN:HE21	6:T:240:GLN:HA	1.85	0.41
9:W:62:LEU:CD1	9:W:104:VAL:HG21	2.51	0.41
11:Y:198:TRP:CZ3	11:Y:212:GLY:HA3	2.56	0.41
4:D:59:ILE:HG22	4:D:220:PHE:HZ	1.86	0.41
10:J:119:ILE:HA	10:J:124:THR:O	2.21	0.41
11:K:2:THR:HG21	11:K:164:ALA:HB3	2.02	0.41
4:R:24:LYS:O	4:R:166:SER:HA	2.21	0.41
6:T:216:SER:HB3	6:T:219:GLU:HB2	2.03	0.41
8:V:163:ILE:HG23	8:V:170:GLY:HA2	2.02	0.41
10:J:45:SER:OG	10:J:103:LEU:HB2	2.21	0.41
10:J:184:VAL:HG22	10:J:189:ILE:HG12	2.03	0.41
11:K:1:THR:HB	11:K:131:SER:H	1.86	0.41
1:O:75:TYR:HB3	1:O:82:TYR:CD1	2.55	0.41
2:P:213:ALA:HA	2:P:227:LYS:O	2.21	0.41
12:Z:13:LEU:HD11	12:Z:150:LEU:HD21	2.02	0.41
14:b:8:PHE:HB2	14:b:146:MET:O	2.20	0.41
7:G:78:ILE:HG22	7:G:79:PRO:HD3	2.02	0.41
11:K:120:THR:HG23	11:K:122:LEU:HD21	1.98	0.41
12:L:13:LEU:HD11	12:L:150:LEU:HD21	2.02	0.41
14:N:8:PHE:HB2	14:N:146:MET:O	2.21	0.41
14:b:13:ILE:HG21	14:b:175:MET:CE	2.49	0.41
6:F:46:VAL:HB	6:F:73:VAL:HG21	2.03	0.40
10:J:136:SER:HB3	10:J:168:LEU:HD22	2.02	0.40
2:B:8:ARG:NE	3:C:4:ARG:NH1	2.69	0.40
11:K:114:TYR:CE1	11:K:134:THR:HG21	2.57	0.40
13:M:24:ALA:HB1	13:M:41:ARG:NH2	2.36	0.40
13:M:26:ASN:HA	13:M:39:VAL:O	2.22	0.40
13:M:35:ARG:NH2	14:N:114:PRO:HB3	2.36	0.40
14:N:132:THR:O	14:b:133:PHE:HA	2.21	0.40
2:B:219:ALA:HB2	2:B:225:TYR:HB2	2.03	0.40
6:F:240:GLN:HE21	6:F:240:GLN:HA	1.85	0.40
12:L:216:PHE:CD2	17:M:301:MES:H61	2.57	0.40
3:Q:38:ASN:HD22	3:Q:38:ASN:C	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:149:HIS:O	4:R:156:PHE:HA	2.20	0.40
6:T:146:MET:HE3	6:T:161:THR:HB	2.04	0.40
13:a:159:VAL:O	13:a:159:VAL:CG2	2.68	0.40
13:a:161:ARG:HE	13:a:161:ARG:HB3	1.67	0.40
1:A:64:VAL:HG11	1:A:212:ALA:HB3	2.03	0.40
11:K:142:SER:HB3	10:X:167:GLU:OE1	2.21	0.40
12:L:146:ILE:HG22	12:L:150:LEU:HD22	2.03	0.40
13:M:129:TYR:O	13:M:136:THR:HA	2.21	0.40
7:U:43:VAL:HG11	7:U:194:VAL:HA	2.02	0.40
5:E:71:LEU:HD22	5:E:71:LEU:O	2.22	0.40
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.57	0.40
1:O:83:ARG:HE	7:U:114:ASN:HD21	1.70	0.40
11:Y:3:THR:HA	11:Y:16:VAL:HG12	2.04	0.40
11:Y:43:GLY:HA3	11:Y:56:GLU:OE1	2.21	0.40
13:a:129:TYR:O	13:a:136:THR:HA	2.22	0.40
13:a:162:GLU:O	13:a:165:ILE:HG13	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	246/250 (98%)	239 (97%)	7 (3%)	0	100	100
1	O	248/250 (99%)	237 (96%)	10 (4%)	1 (0%)	30	51
2	B	242/258 (94%)	232 (96%)	6 (2%)	4 (2%)	7	15
2	P	242/258 (94%)	233 (96%)	5 (2%)	4 (2%)	7	15
3	C	238/254 (94%)	229 (96%)	6 (2%)	3 (1%)	9	21
3	Q	238/254 (94%)	230 (97%)	5 (2%)	3 (1%)	9	21
4	D	231/260 (89%)	226 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	R	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
5	E	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
5	S	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
6	F	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
6	T	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
7	G	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
7	U	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
8	H	224/232 (97%)	219 (98%)	5 (2%)	0	100	100
8	V	224/232 (97%)	219 (98%)	5 (2%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
10	J	193/198 (98%)	191 (99%)	2 (1%)	0	100	100
10	X	193/198 (98%)	191 (99%)	2 (1%)	0	100	100
11	K	217/287 (76%)	209 (96%)	7 (3%)	1 (0%)	24	46
11	Y	217/287 (76%)	207 (95%)	9 (4%)	1 (0%)	24	46
12	L	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
12	Z	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
13	M	231/246 (94%)	222 (96%)	8 (4%)	1 (0%)	30	51
13	a	231/246 (94%)	223 (96%)	7 (3%)	1 (0%)	30	51
14	N	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
14	b	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
All	All	6296/6764 (93%)	6123 (97%)	154 (2%)	19 (0%)	36	58

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
2	B	221	ASP
3	C	202	GLN
2	P	51	VAL
2	P	221	ASP
3	Q	202	GLN
2	B	218	GLY
2	B	220	ASN
11	K	144	TYR

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Mol	Chain	Res	Type
13	M	39	VAL
1	O	2	THR
2	P	218	GLY
2	P	220	ASN
11	Y	144	TYR
3	C	205	ALA
3	Q	205	ALA
13	a	83	ALA
3	Q	183	PRO
3	C	183	PRO

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	207/209 (99%)	198 (96%)	9 (4%)	26	51
1	O	209/209 (100%)	203 (97%)	6 (3%)	37	65
2	B	203/216 (94%)	196 (97%)	7 (3%)	32	60
2	P	203/216 (94%)	196 (97%)	7 (3%)	32	60
3	C	212/226 (94%)	201 (95%)	11 (5%)	21	44
3	Q	212/226 (94%)	201 (95%)	11 (5%)	21	44
4	D	194/215 (90%)	182 (94%)	12 (6%)	16	36
4	R	194/215 (90%)	182 (94%)	12 (6%)	16	36
5	E	190/193 (98%)	181 (95%)	9 (5%)	23	48
5	S	190/193 (98%)	182 (96%)	8 (4%)	26	52
6	F	201/239 (84%)	191 (95%)	10 (5%)	22	46
6	T	201/239 (84%)	193 (96%)	8 (4%)	28	55
7	G	206/210 (98%)	197 (96%)	9 (4%)	25	50
7	U	206/210 (98%)	197 (96%)	9 (4%)	25	50
8	H	185/190 (97%)	173 (94%)	12 (6%)	15	35
8	V	185/190 (97%)	172 (93%)	13 (7%)	14	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	172/173 (99%)	170 (99%)	2 (1%)	63	83
9	W	172/173 (99%)	170 (99%)	2 (1%)	63	83
10	J	173/175 (99%)	161 (93%)	12 (7%)	14	32
10	X	173/175 (99%)	164 (95%)	9 (5%)	21	44
11	K	175/236 (74%)	164 (94%)	11 (6%)	16	36
11	Y	175/236 (74%)	162 (93%)	13 (7%)	13	29
12	L	185/185 (100%)	179 (97%)	6 (3%)	34	62
12	Z	185/185 (100%)	178 (96%)	7 (4%)	29	56
13	M	199/208 (96%)	188 (94%)	11 (6%)	19	41
13	a	199/208 (96%)	191 (96%)	8 (4%)	28	55
14	N	162/162 (100%)	155 (96%)	7 (4%)	26	51
14	b	162/162 (100%)	155 (96%)	7 (4%)	26	51
All	All	5330/5674 (94%)	5082 (95%)	248 (5%)	23	48

All (248) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	6	SER
1	A	29	LYS
1	A	59	GLU
1	A	122	THR
1	A	128	ARG
1	A	133	SER
1	A	157	PHE
1	A	250	LEU
2	B	50	LYS
2	B	55	LEU
2	B	79	LEU
2	B	102	ASN
2	B	113	ARG
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	50	LEU
3	C	51	LYS
3	C	52	LEU

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Mol	Chain	Res	Type
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	213	VAL
3	C	240	GLU
4	D	40	LEU
4	D	51	LEU
4	D	60	VAL
4	D	99	ILE
4	D	117	GLU
4	D	176	LEU
4	D	190	LEU
4	D	193	LEU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	8	ASP
5	E	9	THR
5	E	29	LYS
5	E	55	LEU
5	E	56	SER
5	E	71	LEU
5	E	188	LEU
5	E	208	ASP
5	E	231	LYS
6	F	68	ARG
6	F	94	SER
6	F	117	GLN
6	F	123	ASN
6	F	172	LEU
6	F	181	GLU
6	F	201	GLU
6	F	202	ASP
6	F	221	ASN
6	F	240	GLN
7	G	13	GLU
7	G	26	THR
7	G	75	ASN
7	G	83	ASN
7	G	115	LEU

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Mol	Chain	Res	Type
7	G	122	ARG
7	G	125	MET
7	G	235	ARG
7	G	236	LEU
8	H	14	ILE
8	H	20	SER
8	H	30	ASN
8	H	34	LEU
8	H	55	VAL
8	H	56	THR
8	H	68	LEU
8	H	80	LEU
8	H	113	ILE
8	H	127	LEU
8	H	195	VAL
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
10	J	1	MET
10	J	3	ILE
10	J	18	SER
10	J	23	ARG
10	J	25	ILE
10	J	26	SER
10	J	35	THR
10	J	136	SER
10	J	161	LEU
10	J	174	MET
10	J	193	ASP
10	J	194	ASP
11	K	2	THR
11	K	9	GLN
11	K	84	SER
11	K	117	SER
11	K	122	LEU
11	K	126	ILE
11	K	130	VAL
11	K	131	SER
11	K	141	ASP
11	K	142	SER
11	K	149	SER
12	L	1	GLN

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Mol	Chain	Res	Type
12	L	23	LEU
12	L	31	THR
12	L	42	LYS
12	L	49	ASN
12	L	150	LEU
13	M	2	GLN
13	M	35	ARG
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
13	M	190	ARG
13	M	225	ILE
13	M	232	LYS
13	M	233	ILE
14	N	9	LYS
14	N	36	ARG
14	N	104	ASP
14	N	107	LYS
14	N	115	LEU
14	N	119	VAL
14	N	178	LEU
1	O	1	MET
1	O	29	LYS
1	O	59	GLU
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	50	LYS
2	P	55	LEU
2	P	79	LEU
2	P	102	ASN
2	P	113	ARG
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	50	LEU
3	Q	51	LYS
3	Q	52	LEU
3	Q	147	GLN

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Mol	Chain	Res	Type
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	213	VAL
3	Q	240	GLU
4	R	40	LEU
4	R	51	LEU
4	R	60	VAL
4	R	99	ILE
4	R	117	GLU
4	R	176	LEU
4	R	190	LEU
4	R	193	LEU
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	8	ASP
5	S	9	THR
5	S	29	LYS
5	S	55	LEU
5	S	56	SER
5	S	71	LEU
5	S	188	LEU
5	S	231	LYS
6	T	94	SER
6	T	117	GLN
6	T	123	ASN
6	T	172	LEU
6	T	181	GLU
6	T	201	GLU
6	T	221	ASN
6	T	240	GLN
7	U	13	GLU
7	U	26	THR
7	U	75	ASN
7	U	83	ASN
7	U	115	LEU
7	U	122	ARG
7	U	125	MET
7	U	235	ARG
7	U	236	LEU

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Mol	Chain	Res	Type
8	V	14	ILE
8	V	20	SER
8	V	30	ASN
8	V	34	LEU
8	V	55	VAL
8	V	56	THR
8	V	68	LEU
8	V	80	LEU
8	V	113	ILE
8	V	127	LEU
8	V	144	GLN
8	V	195	VAL
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
10	X	18	SER
10	X	23	ARG
10	X	25	ILE
10	X	26	SER
10	X	35	THR
10	X	136	SER
10	X	161	LEU
10	X	193	ASP
10	X	194	ASP
11	Y	2	THR
11	Y	7	ARG
11	Y	9	GLN
11	Y	84	SER
11	Y	106	ARG
11	Y	117	SER
11	Y	130	VAL
11	Y	131	SER
11	Y	133	GLN
11	Y	134	THR
11	Y	141	ASP
11	Y	142	SER
11	Y	149	SER
12	Z	1	GLN
12	Z	23	LEU
12	Z	31	THR
12	Z	42	LYS
12	Z	49	ASN

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Mol	Chain	Res	Type
12	Z	150	LEU
12	Z	172	LEU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
13	a	225	ILE
13	a	232	LYS
14	b	9	LYS
14	b	36	ARG
14	b	104	ASP
14	b	107	LYS
14	b	115	LEU
14	b	119	VAL
14	b	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (166) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	124	HIS
2	B	155	ASN
2	B	176	GLN
3	C	17	GLN
3	C	38	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
3	C	165	ASN
3	C	233	GLN
4	D	15	GLN
4	D	91	HIS
4	D	100	ASN
4	D	160	ASN

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Mol	Chain	Res	Type
4	D	225	ASN
5	E	68	HIS
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	151	ASN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	143	HIS
6	F	191	GLN
6	F	203	ASN
6	F	240	GLN
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
7	G	175	ASN
8	H	22	GLN
8	H	30	ASN
8	H	57	GLN
8	H	66	HIS
8	H	86	HIS
8	H	165	ASN
8	H	172	ASN
8	H	189	ASN
9	I	37	ASN
9	I	88	GLN
9	I	168	GLN
9	I	172	ASN
10	J	55	GLN
10	J	99	GLN
10	J	191	GLN
11	K	9	GLN
11	K	85	ASN
11	K	133	GLN

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Mol	Chain	Res	Type
11	K	176	ASN
11	K	190	ASN
11	K	191	HIS
12	L	3	ASN
12	L	49	ASN
12	L	55	ASN
12	L	70	ASN
12	L	76	HIS
12	L	79	HIS
12	L	80	ASN
12	L	153	GLN
12	L	158	ASN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	108	ASN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	161	GLN
2	P	20	GLN
2	P	58	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	124	HIS
2	P	146	GLN
2	P	176	GLN
2	P	232	GLN
3	Q	17	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	233	GLN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	160	ASN
4	R	225	ASN

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Mol	Chain	Res	Type
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	151	ASN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	203	ASN
6	T	240	GLN
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	167	GLN
7	U	172	ASN
7	U	175	ASN
8	V	22	GLN
8	V	30	ASN
8	V	57	GLN
8	V	66	HIS
8	V	165	ASN
8	V	172	ASN
8	V	189	ASN
9	W	37	ASN
9	W	44	HIS
9	W	88	GLN
9	W	168	GLN
10	X	55	GLN
10	X	99	GLN
10	X	191	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	176	ASN
11	Y	190	ASN
11	Y	209	ASN

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Mol	Chain	Res	Type
12	Z	3	ASN
12	Z	8	ASN
12	Z	29	ASN
12	Z	36	ASN
12	Z	49	ASN
12	Z	55	ASN
12	Z	70	ASN
12	Z	80	ASN
12	Z	153	GLN
13	a	18	ASN
13	a	26	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN
14	b	69	GLN
14	b	161	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 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	MES	N	202	-	12,12,12	0.76	0	15,16,16	0.81	0
17	MES	M	301	-	12,12,12	0.72	0	15,16,16	0.31	0
17	MES	H	301	-	12,12,12	0.70	0	15,16,16	0.37	0
17	MES	V	302	-	12,12,12	0.69	0	15,16,16	0.40	0
17	MES	Z	302	-	12,12,12	0.72	0	15,16,16	0.34	0
17	MES	b	201	-	12,12,12	0.68	0	15,16,16	0.42	0
18	MPD	K	301	-	7,7,7	0.16	0	9,10,10	0.46	0
17	MES	U	302	-	12,12,12	0.75	0	15,16,16	0.42	0
18	MPD	a	301	-	7,7,7	0.15	0	9,10,10	0.38	0
17	MES	G	303	-	12,12,12	0.76	0	15,16,16	0.39	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
17	MES	N	202	-	-	0/6/14/14	0/1/1/1
17	MES	M	301	-	-	3/6/14/14	0/1/1/1
17	MES	H	301	-	-	0/6/14/14	0/1/1/1
17	MES	V	302	-	-	3/6/14/14	0/1/1/1
17	MES	Z	302	-	-	1/6/14/14	0/1/1/1
17	MES	b	201	-	-	3/6/14/14	0/1/1/1
18	MPD	K	301	-	-	2/5/5/5	-
17	MES	U	302	-	-	3/6/14/14	0/1/1/1
18	MPD	a	301	-	-	0/5/5/5	-
17	MES	G	303	-	-	2/6/14/14	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	G	303	MES	C8-C7-N4-C5
17	G	303	MES	N4-C7-C8-S
17	M	301	MES	C7-C8-S-O1S

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Mol	Chain	Res	Type	Atoms
17	V	302	MES	C7-C8-S-O2S
17	Z	302	MES	C8-C7-N4-C5
18	K	301	MPD	C2-C3-C4-O4
18	K	301	MPD	C2-C3-C4-C5
17	M	301	MES	C7-C8-S-O3S
17	U	302	MES	C7-C8-S-O3S
17	V	302	MES	C7-C8-S-O3S
17	M	301	MES	C7-C8-S-O2S
17	U	302	MES	C7-C8-S-O1S
17	U	302	MES	C7-C8-S-O2S
17	V	302	MES	C7-C8-S-O1S
17	b	201	MES	C7-C8-S-O1S
17	b	201	MES	C7-C8-S-O3S
17	b	201	MES	C7-C8-S-O2S

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	N	202	MES	4	0
17	M	301	MES	1	0
17	H	301	MES	1	0
17	V	302	MES	1	0
17	b	201	MES	6	0
18	K	301	MPD	2	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	248/250 (99%)	-0.49	2 (0%) 82 80	37, 48, 77, 115	0
1	O	250/250 (100%)	-0.43	3 (1%) 76 73	42, 55, 89, 118	0
2	B	244/258 (94%)	-0.30	3 (1%) 76 73	38, 53, 87, 137	0
2	P	244/258 (94%)	-0.37	5 (2%) 65 60	41, 55, 88, 134	0
3	C	240/254 (94%)	-0.33	2 (0%) 82 80	40, 56, 109, 126	0
3	Q	240/254 (94%)	-0.20	3 (1%) 75 71	46, 63, 130, 150	0
4	D	235/260 (90%)	-0.43	0 100 100	42, 56, 78, 105	0
4	R	235/260 (90%)	-0.42	1 (0%) 88 86	44, 59, 82, 113	0
5	E	231/234 (98%)	-0.41	0 100 100	43, 57, 85, 104	0
5	S	231/234 (98%)	-0.35	0 100 100	43, 63, 90, 110	0
6	F	243/288 (84%)	-0.45	0 100 100	37, 52, 87, 119	0
6	T	243/288 (84%)	-0.46	2 (0%) 82 80	42, 59, 97, 113	0
7	G	241/252 (95%)	-0.53	0 100 100	36, 48, 72, 108	0
7	U	241/252 (95%)	-0.43	1 (0%) 88 86	41, 53, 76, 114	0
8	H	226/232 (97%)	-0.45	0 100 100	37, 46, 72, 130	0
8	V	226/232 (97%)	-0.45	2 (0%) 81 78	40, 50, 75, 136	0
9	I	204/205 (99%)	-0.69	0 100 100	36, 45, 64, 84	0
9	W	204/205 (99%)	-0.66	0 100 100	37, 47, 69, 88	0
10	J	195/198 (98%)	-0.41	1 (0%) 87 85	37, 56, 83, 117	0
10	X	195/198 (98%)	-0.52	0 100 100	40, 59, 82, 105	0
11	K	219/287 (76%)	-0.36	3 (1%) 73 69	38, 51, 84, 112	0
11	Y	219/287 (76%)	-0.40	2 (0%) 81 78	40, 51, 83, 103	0
12	L	222/222 (100%)	-0.65	0 100 100	36, 48, 69, 89	0
12	Z	222/222 (100%)	-0.63	0 100 100	37, 49, 69, 91	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.62	2 (0%) 81 78	36, 46, 63, 74	0
13	a	233/246 (94%)	-0.59	1 (0%) 88 86	36, 47, 61, 75	0
14	N	196/196 (100%)	-0.56	1 (0%) 87 85	36, 43, 61, 97	0
14	b	196/196 (100%)	-0.49	2 (1%) 79 76	36, 45, 62, 99	0
All	All	6356/6764 (93%)	-0.46	36 (0%) 85 83	36, 52, 85, 150	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	219	ALA	4.5
1	O	2	THR	4.2
10	J	1	MET	4.1
3	Q	50	LEU	3.6
8	V	223	ILE	3.3
13	a	1	THR	3.2
1	O	4	ARG	3.0
13	M	69	ASP	2.9
2	B	51	VAL	2.9
3	C	203	THR	2.9
2	B	219	ALA	2.8
11	K	-5	ILE	2.7
13	M	190	ARG	2.7
3	C	205	ALA	2.7
3	Q	205	ALA	2.6
2	B	218	GLY	2.5
2	P	218	GLY	2.5
4	R	125	LEU	2.4
14	b	103	ASP	2.4
11	K	139	VAL	2.4
2	P	1	GLY	2.3
14	b	195	GLN	2.3
11	Y	-5	ILE	2.3
1	A	3	ASP	2.3
3	Q	49	THR	2.2
14	N	195	GLN	2.2
6	T	205	GLU	2.2
6	T	14	ASP	2.2
1	O	57	MET	2.2
11	Y	144	TYR	2.2
2	P	220	ASN	2.1
1	A	4	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
2	P	51	VAL	2.1
8	V	224	GLN	2.0
7	U	68	ARG	2.0
11	K	144	TYR	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
15	MG	W	301	1/1	0.71	0.41	127,127,127,127	0
15	MG	N	201	1/1	0.78	0.16	50,50,50,50	0
17	MES	M	301	12/12	0.83	0.17	102,108,113,113	0
17	MES	V	302	12/12	0.85	0.16	74,95,99,108	0
15	MG	Z	301	1/1	0.88	0.26	127,127,127,127	0
17	MES	Z	302	12/12	0.88	0.13	74,80,95,97	0
18	MPD	a	301	8/8	0.89	0.12	69,75,77,77	0
17	MES	b	201	12/12	0.92	0.16	59,72,79,81	0
18	MPD	K	301	8/8	0.92	0.11	60,64,66,66	0
17	MES	H	301	12/12	0.92	0.12	73,88,94,95	0
17	MES	N	202	12/12	0.93	0.11	65,75,87,87	0
17	MES	G	303	12/12	0.93	0.13	70,86,104,105	0
17	MES	U	302	12/12	0.95	0.11	71,82,87,90	0
15	MG	V	301	1/1	0.96	0.17	89,89,89,89	0
15	MG	I	301	1/1	0.97	0.18	125,125,125,125	0
15	MG	G	301	1/1	0.98	0.10	63,63,63,63	0
16	CL	U	301	1/1	0.98	0.10	69,69,69,69	0
16	CL	G	302	1/1	0.99	0.06	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.