



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 1, 2025 – 10:34 am BST

PDB ID : 9QBI / pdb_00009qbi
Title : Yeast 20S proteasome mutant: beta5_G128V (b5-propeptide in trans)
Authors : Huber, E.M.; Heinemeyer, W.; Groll, M.
Deposited on : 2025-03-03
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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

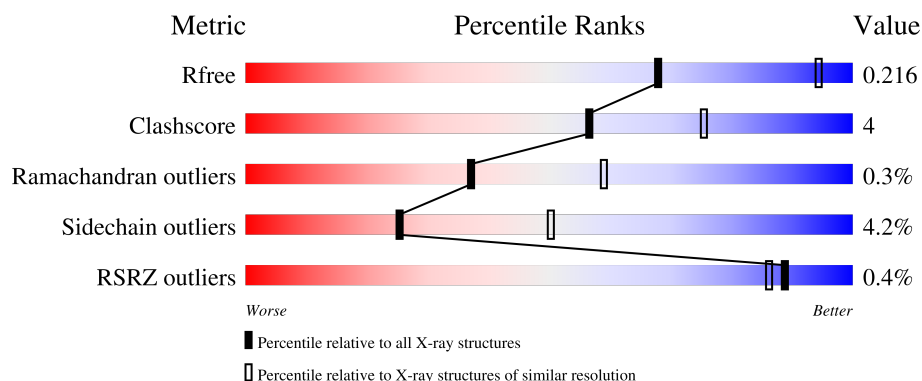
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (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	<div><div></div>96%<div></div></div>
1	O	250	<div><div></div>96%<div></div></div>
2	B	258	<div><div>2%</div><div></div>86%<div></div>8%<div></div>5%</div>
2	P	258	<div><div>2%</div><div></div>86%<div></div>9%<div></div>5%</div>
3	C	254	<div><div></div>86%<div></div>7%<div></div>6%</div>

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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	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 50157 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	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
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	237	Total	C	N	O	S	0	0	0
			1860	1163	326	367	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	210	Total	C	N	O	S	0	0	0
			1631	1037	278	309	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1647	1048	280	312	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 SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	B	1	Total	O	S	0	0
			5	4	1		
15	P	1	Total	O	S	0	0
			5	4	1		

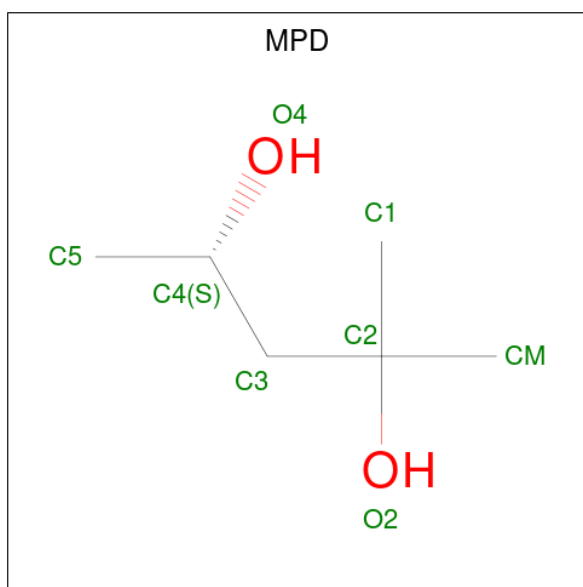
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	G	1	Total	Mg	0	0
			1	1		
16	N	1	Total	Mg	0	0
			1	1		
16	W	1	Total	Mg	0	0
			1	1		

- Molecule 17 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

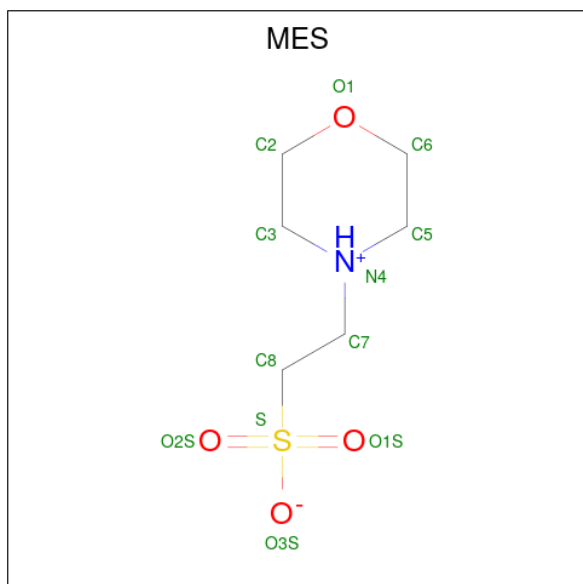
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	G	1	Total	Cl	0	0
			1	1		
17	U	1	Total	Cl	0	0
			1	1		

- 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 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	N	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
19	Z	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
19	b	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	16	Total	O	0	0
			16	16		
20	B	25	Total	O	0	0
			25	25		
20	C	21	Total	O	0	0
			21	21		
20	D	23	Total	O	0	0
			23	23		
20	E	17	Total	O	0	0
			17	17		
20	F	26	Total	O	0	0
			26	26		
20	G	37	Total	O	0	0
			37	37		
20	H	40	Total	O	0	0
			40	40		
20	I	35	Total	O	0	0
			35	35		
20	J	26	Total	O	0	0
			26	26		
20	K	23	Total	O	0	0
			23	23		
20	L	31	Total	O	0	0
			31	31		
20	M	47	Total	O	0	0
			47	47		
20	N	25	Total	O	0	0
			25	25		
20	O	23	Total	O	0	0
			23	23		
20	P	13	Total	O	0	0
			13	13		

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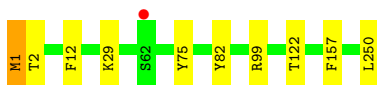
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	Q	15	Total 15	O 15	0	0
20	R	19	Total 19	O 19	0	0
20	S	11	Total 11	O 11	0	0
20	T	20	Total 20	O 20	0	0
20	U	37	Total 37	O 37	0	0
20	V	37	Total 37	O 37	0	0
20	W	28	Total 28	O 28	0	0
20	X	19	Total 19	O 19	0	0
20	Y	27	Total 27	O 27	0	0
20	Z	25	Total 25	O 25	0	0
20	a	41	Total 41	O 41	0	0
20	b	36	Total 36	O 36	0	0

3 Residue-property plots

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

Chain A: 




- Molecule 1: Proteasome subunit alpha type-2

Chain O: 




- Molecule 2: Proteasome subunit alpha type-3

Chain B: 




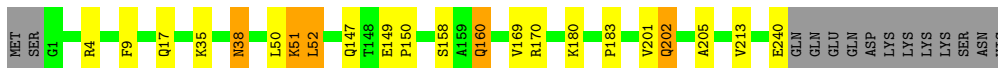
- Molecule 2: Proteasome subunit alpha type-3

Chain P: 

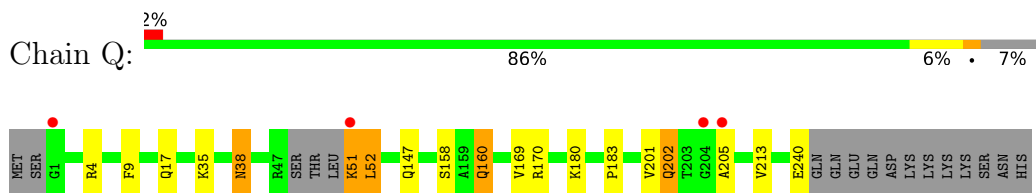


- Molecule 3: Proteasome subunit alpha type-4

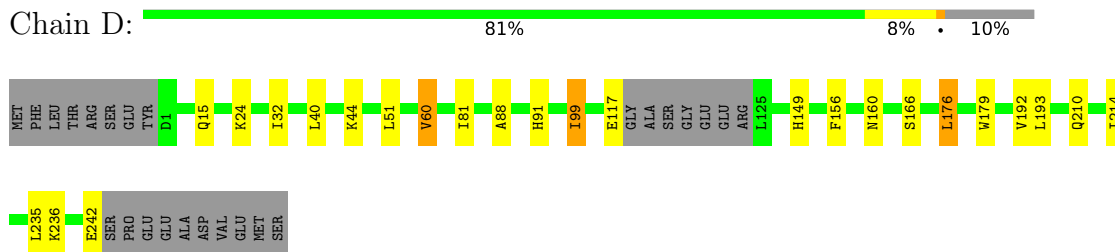
Chain C: 



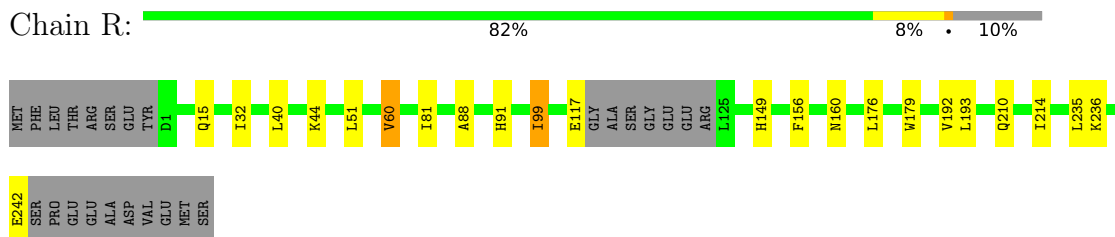
- Molecule 3: Proteasome subunit alpha type-4



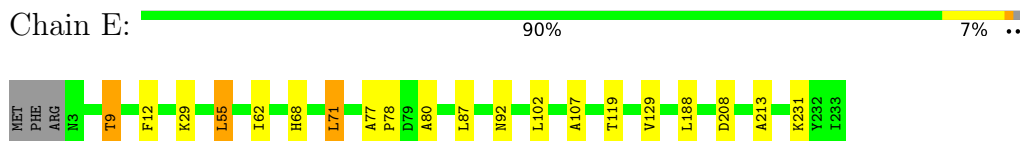
- Molecule 4: Proteasome subunit alpha type-5



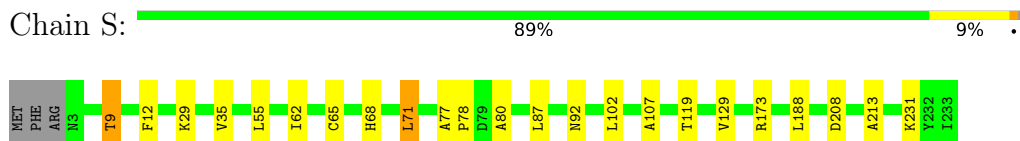
- Molecule 4: Proteasome subunit alpha type-5



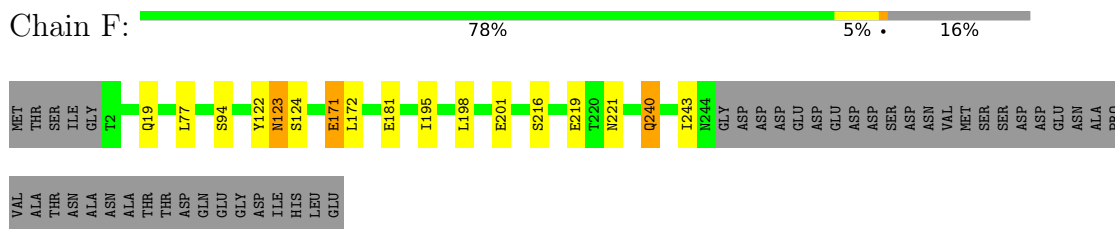
- Molecule 5: Proteasome subunit alpha type-6



- Molecule 5: Proteasome subunit alpha type-6



- Molecule 6: Probable proteasome subunit alpha type-7

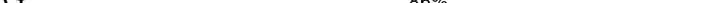


- Molecule 6: Probable proteasome subunit alpha type-7

Chain T: 78% 5% • 16%



- Molecule 7: Proteasome subunit alpha type-1

Chain G:  86% 9% . .




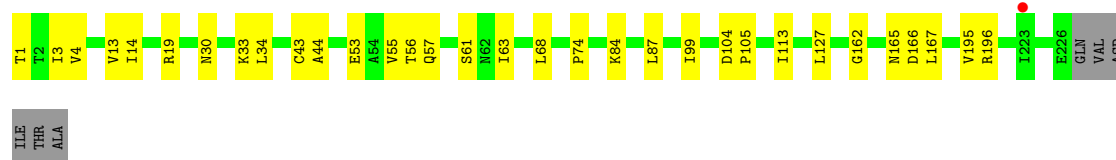
- Molecule 7: Proteasome subunit alpha type-1

Chain U: 87% 8% . .

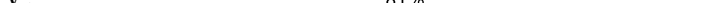


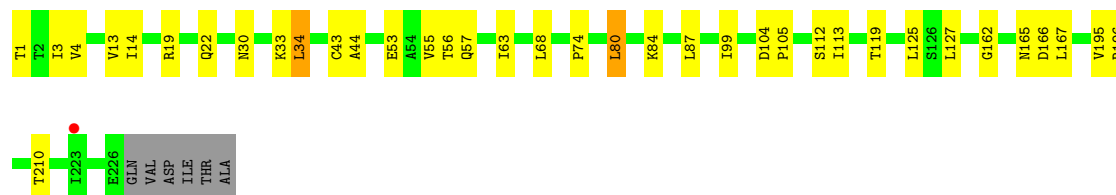
- Molecule 8: Proteasome subunit beta type-2

Chain H:  84% 14%



- Molecule 8: Proteasome subunit beta type-2

Chain V:  81% 15% . .



- Molecule 9: Proteasome subunit beta type-3

Chain I: 91% 8%



- Molecule 9: Proteasome subunit beta type-3

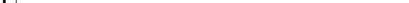
Residue Class	Number of Amino Acids
MET	1
S1	1
G9	2
I10	2
V20	2
L26	2
G34	2
N37	4
K41	2
D58	2
N71	2
L94	2
P101	2
P106	2
A141	2
S167	2
L170	2
L171	2
G183	2
A184	3
V185	2
I189	2
K200	2
D204	2

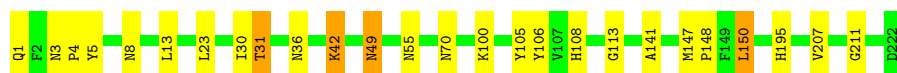
- | |
|------|
| M1 |
| D2 |
| I3 |
| L4 |
| L5 |
| G6 |
| I7 |
| S8 |
| V21 |
| T22 |
| T25 |
| S26 |
| V27 |
| L28 |
| K29 |
| D33 |
| R34 |
| T35 |
| R36 |
| Q37 |
| H41 |
| M44 |
| S45 |
| A50 |
| I92 |
| R93 |
| L103 |
| T104 |
| K109 |
| L119 |
| L122 |
| G123 |
| T124 |
| H132 |
| H133 |
| G134 |
| Y135 |
| S136 |
| T140 |
| F141 |
| S142 |
| L143 |
| R149 |
| T150 |

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|------|------|------|------|------|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| R149 | L161 | K162 | L163 | E167 | M1 | D2 | I3 | I4 | L5 | G6 | I7 | A16 | S17 | S18 | V21 | T22 | T25 | S26 | V27 | L28 | D33 | K34 | T35 | R36 | Q37 | H41 | M44 | S45 | A50 | E58 | I92 | R93 | L103 | I104 | K109 | I119 | L122 | G123 | T124 | A132 | H133 | G134 | Y135 | S136 | T140 | F141 | S142 | L143 |
|------|------|------|------|------|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

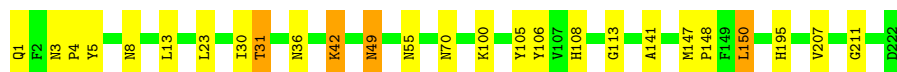
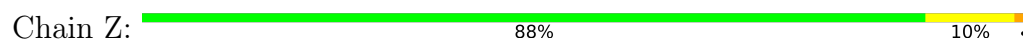
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|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| L148 | S149 | L156 | G157 | K158 | T161 | R167 | V175 | Y178 | H179 | V180 | T181 | E182 | L196 | V200 | E204 | G205 | S206 | G212 | T1 | Q9 | I12 | A20 | V31 | K32 | K33 | V34 | F40 | L41 | L42 | A46 | C63 | E67 | R73 | S84 | K91 | M97 | G98 | Y104 | T105 | R106 | D116 | S117 | T120 | R121 | L122 | V129 | V130 | Q133 | T134 | F135 | A136 | Y137 | G138 | V139 | L140 | D141 | S142 | N143 | Y144 | K145 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

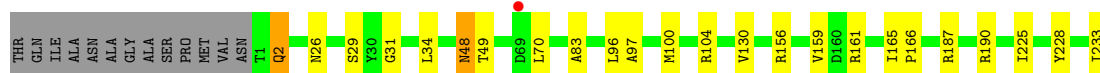
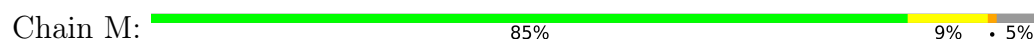
- Chain L:  88% 10%



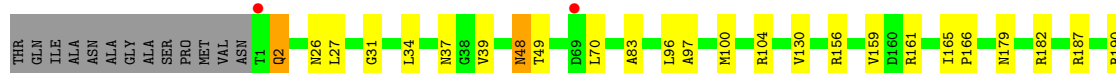
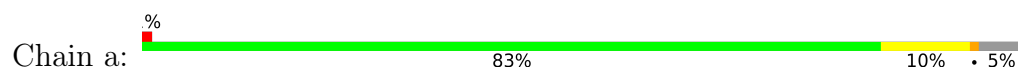
- Molecule 12: Proteasome subunit beta type-6



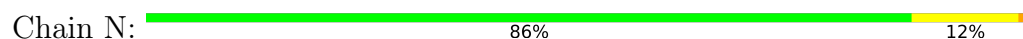
- Molecule 13: Proteasome subunit beta type-7



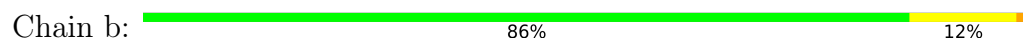
- Molecule 13: Proteasome subunit beta type-7



- 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	134.62Å 301.12Å 144.57Å 90.00° 112.72° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60 15.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.6 (15.00-2.60) 98.6 (15.00-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.177 , 0.215 0.178 , 0.216	Depositor DCC
R_{free} test set	15984 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	1.336	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 57.4	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	50157	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% 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: SO4, MES, CL, MG, 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	0/1952	1.41	0/2642
1	O	1.02	0/1952	1.42	0/2642
2	B	1.02	0/1934	1.43	0/2618
2	P	1.02	0/1934	1.44	0/2618
3	C	1.02	0/1910	1.45	0/2586
3	Q	1.02	0/1888	1.46	0/2554
4	D	1.03	0/1837	1.47	0/2475
4	R	1.03	0/1837	1.48	0/2475
5	E	1.03	0/1800	1.43	0/2433
5	S	1.03	0/1800	1.44	2/2433 (0.1%)
6	F	1.02	0/1932	1.45	2/2609 (0.1%)
6	T	1.02	0/1932	1.46	2/2609 (0.1%)
7	G	1.00	0/1945	1.42	0/2634
7	U	1.01	0/1945	1.42	0/2634
8	H	1.01	0/1750	1.41	2/2373 (0.1%)
8	V	1.02	0/1750	1.41	2/2373 (0.1%)
9	I	1.01	0/1611	1.39	1/2174 (0.0%)
9	W	1.02	0/1611	1.40	1/2174 (0.0%)
10	J	0.96	0/1589	1.39	0/2142
10	X	0.96	0/1589	1.39	0/2142
11	K	0.97	0/1666	1.39	0/2253
11	Y	0.97	0/1684	1.40	0/2279
12	L	1.00	0/1795	1.38	0/2420
12	Z	0.99	0/1795	1.38	0/2420
13	M	1.03	1/1855 (0.1%)	1.39	0/2514
13	a	1.01	0/1855	1.39	1/2514 (0.0%)
14	N	1.00	0/1541	1.42	0/2087
14	b	1.00	0/1541	1.41	0/2087
All	All	1.01	1/50230 (0.0%)	1.42	13/67914 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	26	ASN	C-O	-5.40	1.17	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	T	77	LEU	CA-C-N	7.64	125.05	120.24
6	T	77	LEU	C-N-CA	7.64	125.05	120.24
6	F	77	LEU	CA-C-N	7.51	124.97	120.24
6	F	77	LEU	C-N-CA	7.51	124.97	120.24
9	W	183	GLY	CA-C-O	-5.97	118.34	122.22
13	a	37	ASN	CA-CB-CG	-5.96	106.64	112.60
9	I	183	GLY	CA-C-O	-5.91	118.38	122.22
8	H	4	VAL	CA-C-N	5.71	125.53	121.65
8	H	4	VAL	C-N-CA	5.71	125.53	121.65
5	S	35	VAL	CA-C-N	5.29	125.25	121.65
5	S	35	VAL	C-N-CA	5.29	125.25	121.65
8	V	4	VAL	CA-C-N	5.16	125.16	121.65
8	V	4	VAL	C-N-CA	5.16	125.16	121.65

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	1915	0	1929	4	0
1	O	1915	0	1929	4	0
2	B	1904	0	1904	12	0
2	P	1904	0	1904	10	0
3	C	1881	0	1895	10	0
3	Q	1860	0	1871	9	0
4	D	1813	0	1797	12	0
4	R	1813	0	1797	10	0
5	E	1773	0	1775	13	0
5	S	1773	0	1775	14	0
6	F	1892	0	1883	9	0
6	T	1892	0	1883	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	1907	0	1901	13	0
7	U	1907	0	1901	12	0
8	H	1719	0	1719	15	0
8	V	1719	0	1719	18	0
9	I	1581	0	1574	15	0
9	W	1581	0	1574	16	0
10	J	1561	0	1569	57	0
10	X	1561	0	1569	60	0
11	K	1631	0	1588	53	0
11	Y	1647	0	1601	60	0
12	L	1757	0	1711	17	0
12	Z	1757	0	1711	16	0
13	M	1824	0	1832	12	0
13	a	1824	0	1832	14	0
14	N	1512	0	1481	18	0
14	b	1512	0	1481	19	0
15	B	5	0	0	0	0
15	P	5	0	0	0	0
16	G	1	0	0	0	0
16	N	1	0	0	0	0
16	W	1	0	0	0	0
17	G	1	0	0	0	0
17	U	1	0	0	0	0
18	K	8	0	14	1	0
18	a	8	0	14	0	0
19	M	12	0	13	0	0
19	N	12	0	13	2	0
19	Z	12	0	13	0	0
19	b	12	0	13	3	0
20	A	16	0	0	0	0
20	B	25	0	0	0	0
20	C	21	0	0	0	0
20	D	23	0	0	0	0
20	E	17	0	0	0	0
20	F	26	0	0	0	0
20	G	37	0	0	0	0
20	H	40	0	0	0	0
20	I	35	0	0	1	0
20	J	26	0	0	0	0
20	K	23	0	0	1	0
20	L	31	0	0	0	0
20	M	47	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	N	25	0	0	0	0
20	O	23	0	0	0	0
20	P	13	0	0	0	0
20	Q	15	0	0	0	0
20	R	19	0	0	0	0
20	S	11	0	0	1	0
20	T	20	0	0	0	0
20	U	37	0	0	0	0
20	V	37	0	0	0	0
20	W	28	0	0	0	0
20	X	19	0	0	1	0
20	Y	27	0	0	0	0
20	Z	25	0	0	0	0
20	a	41	0	0	1	0
20	b	36	0	0	0	0
All	All	50157	0	49185	442	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 4.

All (442) 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)
10:J:171:ARG:NH1	11:Y:141:ASP:HB3	1.55	1.21
10:J:171:ARG:HH12	11:Y:141:ASP:CB	1.70	1.04
10:J:171:ARG:NH1	11:Y:141:ASP:CB	2.21	1.02
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.02	0.99
10:J:149:ARG:NH1	11:Y:205:GLY:C	2.23	0.96
10:J:171:ARG:HH12	11:Y:141:ASP:HB3	0.82	0.96
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.07	0.95
11:K:205:GLY:C	10:X:149:ARG:NH1	2.26	0.93
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.35	0.91
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.36	0.91
14:b:128:GLY:HA2	19:b:201:MES:H82	1.53	0.89
10:X:28:LEU:HD21	11:Y:134:THR:OG1	1.72	0.89
10:J:149:ARG:HH11	11:Y:205:GLY:C	1.83	0.85
11:K:129:VAL:HG12	11:K:134:THR:CG2	2.06	0.85
11:K:141:ASP:O	11:K:141:ASP:OD2	1.95	0.84
11:K:205:GLY:C	10:X:149:ARG:HH11	1.86	0.82
11:Y:130:VAL:HG12	11:Y:135:PHE:HE1	1.44	0.82
11:K:129:VAL:HG12	11:K:134:THR:HG22	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:143:ASN:OD1	11:K:143:ASN:N	2.16	0.79
11:Y:129:VAL:HG22	11:Y:134:THR:HB	1.65	0.79
11:Y:106:ARG:HH11	11:Y:106:ARG:HG2	1.48	0.78
11:K:106:ARG:HG2	11:K:106:ARG:HH11	1.50	0.77
2:B:12:PHE:H	3:C:17:GLN:HE22	1.33	0.76
11:Y:97:MET:N	11:Y:117:SER:OG	2.20	0.74
5:S:92:ASN:HD21	12:Z:70:ASN:ND2	1.83	0.74
14:N:1:THR:OG1	14:N:33:LYS:NZ	2.21	0.74
13:a:2:GLN:NE2	20:a:401:HOH:O	2.20	0.74
11:Y:73:ARG:HH21	11:Y:105:THR:HG22	1.53	0.73
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.36	0.73
3:C:9:PHE:H	4:D:15:GLN:HE22	1.37	0.73
11:Y:46:ALA:HB3	11:Y:98:GLY:O	1.89	0.73
11:K:97:MET:N	11:K:117:SER:OG	2.21	0.73
10:X:26:SER:HG	11:Y:135:PHE:HE2	1.34	0.73
2:B:93:HIS:ND1	2:B:113:ARG:HG2	2.05	0.72
11:K:141:ASP:HB3	10:X:171:ARG:HH12	1.54	0.72
14:b:1:THR:OG1	14:b:33:LYS:NZ	2.23	0.72
2:P:93:HIS:ND1	2:P:113:ARG:HG2	2.04	0.71
11:Y:145:LYS:O	11:Y:148:LEU:HB2	1.91	0.71
8:H:3:ILE:HG22	8:H:99:ILE:HD12	1.72	0.71
7:G:23:PHE:O	7:G:26:THR:HB	1.91	0.70
10:J:141:PHE:CD1	11:Y:167:ARG:NH2	2.59	0.70
11:K:46:ALA:HB3	11:K:98:GLY:O	1.91	0.70
6:T:123:ASN:C	6:T:123:ASN:HD22	1.99	0.70
8:V:1:THR:OG1	8:V:33:LYS:NZ	2.23	0.70
8:V:3:ILE:HG22	8:V:99:ILE:HD12	1.72	0.70
11:K:73:ARG:HH21	11:K:105:THR:HG22	1.56	0.70
14:N:152:VAL:HA	14:N:175:MET:HE1	1.73	0.70
5:S:12:PHE:H	6:T:19:GLN:HE22	1.40	0.69
10:X:28:LEU:CD2	11:Y:134:THR:OG1	2.40	0.69
11:K:167:ARG:NH2	10:X:141:PHE:CD1	2.60	0.69
5:E:92:ASN:ND2	12:L:70:ASN:HD21	1.88	0.69
5:E:12:PHE:H	6:F:19:GLN:HE22	1.41	0.68
6:F:123:ASN:C	6:F:123:ASN:HD22	2.01	0.68
14:b:152:VAL:HA	14:b:175:MET:HE1	1.73	0.68
5:S:92:ASN:ND2	12:Z:70:ASN:HD21	1.83	0.68
7:U:23:PHE:O	7:U:26:THR:HB	1.94	0.67
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.42	0.67
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.43	0.67
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.61	0.66
8:H:1:THR:OG1	8:H:33:LYS:NZ	2.28	0.66
10:J:171:ARG:NH1	11:Y:141:ASP:HB2	2.09	0.65
10:X:33:ASP:OD2	10:X:182:LYS:NZ	2.29	0.65
1:O:12:PHE:H	2:P:20:GLN:HE22	1.43	0.65
10:J:33:ASP:OD2	10:J:182:LYS:NZ	2.31	0.63
10:J:174:MET:SD	10:X:174:MET:HE2	2.38	0.63
11:Y:130:VAL:HG12	11:Y:135:PHE:CE1	2.31	0.63
13:M:31:GLY:C	13:M:190:ARG:HH21	2.06	0.63
5:E:92:ASN:HD21	12:L:70:ASN:ND2	1.87	0.63
11:Y:143:ASN:OD1	11:Y:143:ASN:N	2.32	0.63
8:H:165:ASN:HD22	13:a:156:ARG:HH11	1.47	0.63
12:L:49:ASN:HD21	12:L:211:GLY:HA2	1.62	0.63
10:J:35:THR:HG21	10:J:182:LYS:HZ2	1.64	0.62
10:J:35:THR:HG21	10:J:182:LYS:NZ	2.14	0.62
14:N:13:ILE:HG21	14:N:175:MET:HE2	1.82	0.62
10:X:35:THR:HG21	10:X:182:LYS:NZ	2.14	0.62
11:K:141:ASP:HB3	10:X:171:ARG:NH1	2.15	0.61
13:M:156:ARG:HH11	8:V:165:ASN:HD22	1.48	0.61
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.66	0.61
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.49	0.61
12:Z:49:ASN:HD21	12:Z:211:GLY:HA2	1.66	0.61
11:K:3:THR:OG1	11:K:129:VAL:HG22	2.02	0.60
11:K:129:VAL:HB	11:K:134:THR:HG23	1.81	0.60
12:Z:31:THR:CG2	12:Z:36:ASN:HD21	2.13	0.60
8:H:43:CYS:SG	8:H:56:THR:HG21	2.42	0.60
10:X:35:THR:HG21	10:X:182:LYS:HZ2	1.66	0.60
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.83	0.60
12:L:31:THR:CG2	12:L:36:ASN:HD21	2.15	0.59
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.66	0.59
11:K:145:LYS:HG3	11:K:148:LEU:HD13	1.84	0.59
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.83	0.59
11:Y:130:VAL:CG1	11:Y:135:PHE:CE1	2.85	0.59
6:T:123:ASN:HD22	6:T:124:SER:N	2.00	0.59
10:J:149:ARG:HH12	11:Y:205:GLY:C	2.07	0.59
10:X:28:LEU:O	11:Y:136:ALA:HB2	2.02	0.59
10:X:41:HIS:CD2	10:X:109:LYS:HD3	2.37	0.59
2:B:217:LYS:C	2:B:219:ALA:H	2.10	0.59
2:P:217:LYS:C	2:P:219:ALA:H	2.11	0.59
13:a:31:GLY:C	13:a:190:ARG:HH21	2.09	0.59
11:K:129:VAL:CG2	11:K:129:VAL:O	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:130:VAL:CG1	11:Y:135:PHE:HE1	2.15	0.58
6:F:123:ASN:HD22	6:F:124:SER:N	2.01	0.58
11:K:73:ARG:NH2	11:K:104:TYR:O	2.32	0.58
10:J:41:HIS:CD2	10:J:109:LYS:HD3	2.38	0.58
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.85	0.58
13:M:2:GLN:NE2	20:M:401:HOH:O	2.35	0.58
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.86	0.58
14:b:13:ILE:HG21	14:b:175:MET:HE2	1.86	0.56
8:V:3:ILE:HG12	8:V:44:ALA:HB1	1.87	0.56
13:a:27:LEU:HD21	13:a:34:LEU:HD22	1.88	0.56
11:K:116:ASP:HB2	11:K:120:THR:HB	1.88	0.56
13:M:159:VAL:HG23	13:M:159:VAL:O	2.06	0.56
13:a:159:VAL:HG23	13:a:159:VAL:O	2.05	0.56
11:Y:116:ASP:HB2	11:Y:120:THR:HB	1.88	0.56
11:K:106:ARG:HH11	11:K:106:ARG:CG	2.19	0.55
11:K:129:VAL:CG1	11:K:134:THR:CG2	2.84	0.55
11:Y:73:ARG:NH2	11:Y:104:TYR:O	2.36	0.55
11:Y:1:THR:OG1	11:Y:33:LYS:NZ	2.37	0.55
3:C:35:LYS:HG2	3:C:158:SER:O	2.06	0.55
2:B:95:GLN:NE2	9:I:71:ASN:HD22	2.05	0.55
9:I:58:ASP:OD2	10:J:93:ARG:NH2	2.38	0.55
8:V:43:CYS:SG	8:V:56:THR:HG21	2.45	0.55
10:X:7:ILE:CG2	10:X:161:LEU:HD13	2.36	0.55
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.36	0.55
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.89	0.55
10:J:35:THR:O	10:J:36:ARG:HD3	2.07	0.55
14:b:83:LYS:HG3	14:b:119:VAL:CG2	2.37	0.54
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.90	0.54
10:J:141:PHE:HD1	11:Y:167:ARG:NH2	2.06	0.54
10:J:7:ILE:CG2	10:J:161:LEU:HD13	2.37	0.54
10:J:18:SER:HB2	10:J:176:PHE:HB2	1.90	0.54
12:L:42:LYS:HD2	12:L:55:ASN:HD22	1.71	0.54
8:V:19:ARG:NH1	8:V:167:LEU:O	2.41	0.54
14:b:1:THR:HB	19:b:201:MES:O2S	2.07	0.54
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.08	0.54
8:H:53:GLU:OE1	8:H:57:GLN:NE2	2.41	0.53
8:H:3:ILE:HG12	8:H:44:ALA:HB1	1.89	0.53
1:A:12:PHE:H	2:B:20:GLN:HE22	1.56	0.53
10:J:167:GLU:OE1	10:J:171:ARG:NH2	2.41	0.53
11:K:129:VAL:CB	11:K:134:THR:HG23	2.38	0.53
11:K:205:GLY:C	10:X:149:ARG:HH12	2.11	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.90	0.53
9:W:58:ASP:OD2	10:X:93:ARG:NH2	2.40	0.53
12:Z:42:LYS:HD2	12:Z:55:ASN:HD22	1.73	0.53
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.91	0.53
8:V:53:GLU:OE1	8:V:57:GLN:NE2	2.42	0.53
8:H:19:ARG:NH1	8:H:167:LEU:O	2.42	0.53
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.90	0.53
11:Y:129:VAL:CG2	11:Y:134:THR:HB	2.36	0.52
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.92	0.52
12:L:8:ASN:HA	12:L:30:ILE:O	2.10	0.52
2:P:95:GLN:NE2	9:W:71:ASN:HD22	2.06	0.52
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.44	0.52
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.44	0.52
7:U:83:ASN:C	7:U:83:ASN:HD22	2.17	0.52
11:K:1:THR:OG1	11:K:33:LYS:NZ	2.39	0.52
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.09	0.52
10:X:18:SER:HB2	10:X:176:PHE:HB2	1.91	0.52
8:H:43:CYS:SG	8:H:56:THR:CG2	2.98	0.51
10:J:35:THR:CG2	10:J:182:LYS:HZ2	2.23	0.51
10:X:5:LEU:HD23	10:X:132:ALA:HB2	1.91	0.51
11:Y:106:ARG:HH11	11:Y:106:ARG:CG	2.18	0.51
14:N:136:GLY:HA2	14:b:161:GLN:HE21	1.75	0.51
10:X:28:LEU:O	11:Y:136:ALA:CB	2.58	0.51
13:M:97:ALA:HA	13:M:130:VAL:HG21	1.93	0.51
5:S:71:LEU:HD22	5:S:71:LEU:C	2.35	0.51
11:Y:143:ASN:HB2	11:Y:156:LEU:HD13	1.93	0.51
11:Y:34:VAL:HG11	11:Y:178:TYR:CE1	2.46	0.51
3:C:51:LYS:O	3:C:52:LEU:HB2	2.10	0.51
10:J:5:LEU:HD23	10:J:132:ALA:HB2	1.91	0.51
11:K:34:VAL:HG11	11:K:178:TYR:CE1	2.46	0.51
7:G:83:ASN:C	7:G:83:ASN:HD22	2.20	0.50
11:K:40:PHE:CD1	11:K:73:ARG:NH1	2.79	0.50
14:N:115:LEU:HD11	19:N:202:MES:H51	1.94	0.50
14:b:128:GLY:HA2	19:b:201:MES:C8	2.34	0.50
10:X:5:LEU:HD21	10:X:140:THR:HG21	1.93	0.50
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.11	0.50
13:a:97:ALA:HA	13:a:130:VAL:HG21	1.93	0.50
10:J:25:ILE:HD13	11:K:133:GLN:HG2	1.93	0.50
10:J:50:ALA:O	11:K:91:LYS:NZ	2.45	0.50
10:J:141:PHE:CD1	11:Y:167:ARG:CZ	2.94	0.50
10:J:149:ARG:NH1	11:Y:206:SER:N	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:1:MET:N	10:X:174:MET:HG3	2.26	0.50
11:Y:40:PHE:CD1	11:Y:73:ARG:NH1	2.80	0.50
10:J:5:LEU:HD21	10:J:140:THR:HG21	1.94	0.49
11:Y:130:VAL:HG13	11:Y:135:PHE:CZ	2.47	0.49
11:K:63:CYS:O	11:K:67:GLU:HG3	2.11	0.49
1:A:1:MET:HG3	6:F:122:TYR:CZ	2.47	0.49
10:J:3:ILE:HG13	10:J:136:SER:HB3	1.94	0.49
8:V:43:CYS:SG	8:V:56:THR:CG2	3.01	0.49
7:U:78:ILE:N	7:U:79:PRO:CD	2.75	0.49
10:X:3:ILE:HG13	10:X:136:SER:HB3	1.94	0.49
11:Y:106:ARG:HB2	11:Y:182:GLU:OE1	2.13	0.49
9:W:37:ASN:HD22	9:W:37:ASN:H	1.61	0.49
11:K:90:TYR:OH	18:K:301:MPD:O2	2.23	0.49
9:I:37:ASN:H	9:I:37:ASN:HD22	1.61	0.49
10:X:35:THR:CG2	10:X:182:LYS:HZ2	2.25	0.49
11:K:106:ARG:HB2	11:K:182:GLU:OE1	2.13	0.48
14:N:48:SER:HB3	14:N:51:ASP:HB2	1.95	0.48
5:S:62:ILE:HG21	5:S:213:ALA:HB2	1.95	0.48
10:J:1:MET:HE1	10:J:135:TYR:H	1.78	0.48
5:E:71:LEU:C	5:E:71:LEU:HD22	2.37	0.48
12:L:100:LYS:HD3	12:L:105:TYR:CZ	2.49	0.48
11:Y:63:CYS:O	11:Y:67:GLU:HG3	2.13	0.48
14:b:48:SER:HB3	14:b:51:ASP:HB2	1.95	0.48
7:G:78:ILE:N	7:G:79:PRO:CD	2.76	0.48
5:E:62:ILE:HG21	5:E:213:ALA:HB2	1.95	0.48
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.96	0.48
14:N:133:PHE:HA	14:b:132:THR:O	2.14	0.48
10:X:92:ILE:HG21	10:X:122:LEU:HA	1.96	0.48
11:K:167:ARG:NH2	10:X:141:PHE:HD1	2.07	0.47
11:K:167:ARG:CZ	10:X:141:PHE:CD1	2.97	0.47
14:N:132:THR:O	14:b:133:PHE:HA	2.14	0.47
10:X:35:THR:CG2	10:X:182:LYS:NZ	2.76	0.47
12:Z:100:LYS:HD3	12:Z:105:TYR:CZ	2.49	0.47
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.96	0.47
3:Q:38:ASN:C	3:Q:38:ASN:HD22	2.22	0.47
12:L:113:GLY:HA2	12:L:207:VAL:HG11	1.97	0.47
7:U:61:SER:OG	7:U:215:GLU:OE2	2.31	0.47
3:C:160:GLN:HE21	3:C:160:GLN:CA	2.13	0.47
14:N:161:GLN:HE21	14:b:136:GLY:HA2	1.78	0.47
5:E:68:HIS:HE1	5:E:102:LEU:O	1.97	0.47
10:J:35:THR:CG2	10:J:182:LYS:NZ	2.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:149:ARG:HH12	11:Y:206:SER:N	2.11	0.47
11:K:12:ILE:HB	11:K:180:VAL:HB	1.96	0.47
5:S:71:LEU:C	5:S:71:LEU:CD2	2.87	0.47
9:W:94:LEU:HD11	9:W:106:PRO:HG2	1.96	0.47
10:X:1:MET:HE1	10:X:135:TYR:H	1.80	0.47
12:Z:113:GLY:HA2	12:Z:207:VAL:HG11	1.97	0.47
9:I:94:LEU:HD11	9:I:106:PRO:HG2	1.96	0.47
4:D:91:HIS:CD2	4:D:99:ILE:HG22	2.50	0.47
11:Y:133:GLN:HB3	11:Y:135:PHE:CE2	2.50	0.47
3:C:201:VAL:O	3:C:202:GLN:CB	2.63	0.47
11:K:128:CYS:HB3	11:K:135:PHE:CE2	2.49	0.47
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.96	0.47
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.44	0.47
11:Y:12:ILE:HB	11:Y:180:VAL:HB	1.95	0.46
3:C:38:ASN:C	3:C:38:ASN:HD22	2.22	0.46
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.45	0.46
10:J:173:PRO:CG	10:X:25:ILE:O	2.63	0.46
10:X:25:ILE:HD13	11:Y:133:GLN:HG2	1.97	0.46
14:N:35:THR:HG21	13:a:228:TYR:HE2	1.81	0.46
4:R:91:HIS:CD2	4:R:99:ILE:HG22	2.50	0.46
10:X:93:ARG:NH1	20:X:201:HOH:O	2.48	0.46
5:E:71:LEU:C	5:E:71:LEU:CD2	2.89	0.46
7:G:68:ARG:O	7:G:223:LYS:HA	2.16	0.46
9:I:58:ASP:CG	10:J:93:ARG:NH2	2.74	0.46
13:M:228:TYR:HE2	14:b:35:THR:HG21	1.80	0.46
3:Q:160:GLN:HE21	3:Q:160:GLN:CA	2.14	0.46
11:Y:140:LEU:H	11:Y:140:LEU:HG	1.53	0.46
10:J:25:ILE:O	10:X:173:PRO:CG	2.64	0.46
6:T:198:LEU:HD12	6:T:243:ILE:HG22	1.98	0.46
11:Y:139:VAL:HB	11:Y:140:LEU:H	1.58	0.46
10:J:92:ILE:HG21	10:J:122:LEU:HA	1.96	0.46
11:K:206:SER:N	10:X:149:ARG:HH12	2.13	0.46
8:H:162:GLY:O	8:H:166:ASP:HB3	2.16	0.46
11:K:206:SER:N	10:X:149:ARG:NH1	2.62	0.46
11:Y:145:LYS:HB3	11:Y:148:LEU:HD13	1.97	0.46
10:J:7:ILE:HG21	10:J:161:LEU:HD13	1.98	0.46
5:S:68:HIS:HE1	5:S:102:LEU:O	1.99	0.46
14:b:176:VAL:HG12	14:b:178:LEU:HD13	1.97	0.45
12:L:141:ALA:HB1	12:L:195:HIS:NE2	2.31	0.45
13:M:96:LEU:O	13:M:100:MET:HG2	2.16	0.45
10:X:1:MET:HE3	10:X:2:ASP:O	2.16	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:200:VAL:O	11:Y:204:GLU:HB2	2.16	0.45
6:F:198:LEU:HD12	6:F:243:ILE:HG22	1.98	0.45
10:J:4:ILE:HD11	10:J:133:HIS:CD2	2.52	0.45
10:J:119:ILE:HA	10:J:124:THR:O	2.17	0.45
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.64	0.45
10:X:7:ILE:HG21	10:X:161:LEU:HD13	1.97	0.45
11:Y:9:GLN:NE2	11:Y:148:LEU:O	2.50	0.45
10:J:4:ILE:HG13	10:J:4:ILE:O	2.17	0.45
10:J:7:ILE:HG22	10:J:161:LEU:HD13	1.99	0.45
10:J:37:GLN:HG3	10:J:189:ILE:CD1	2.46	0.45
10:J:173:PRO:HB2	10:X:174:MET:HE1	1.99	0.45
2:B:145:TYR:OH	2:B:217:LYS:N	2.50	0.45
7:U:73:VAL:HG12	7:U:133:THR:HB	1.98	0.45
9:W:58:ASP:CG	10:X:93:ARG:NH2	2.75	0.45
10:X:37:GLN:HG3	10:X:189:ILE:CD1	2.47	0.45
9:I:58:ASP:OD1	10:J:93:ARG:NH2	2.50	0.45
2:P:145:TYR:OH	2:P:217:LYS:N	2.49	0.45
10:X:45:SER:OG	10:X:103:LEU:HB2	2.17	0.44
13:a:48:ASN:C	13:a:48:ASN:HD22	2.25	0.44
14:b:163:ILE:HG23	14:b:170:GLY:HA2	1.99	0.44
7:G:73:VAL:HG12	7:G:133:THR:HB	1.99	0.44
9:I:101:PRO:O	10:J:93:ARG:NH1	2.50	0.44
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.99	0.44
13:M:48:ASN:C	13:M:48:ASN:HD22	2.25	0.44
1:O:1:MET:HG3	6:T:122:TYR:CZ	2.53	0.44
10:X:4:ILE:HD11	10:X:133:HIS:CD2	2.52	0.44
10:X:7:ILE:HG22	10:X:161:LEU:HD13	1.98	0.44
7:G:30:ASN:HD22	7:G:164:PRO:HG2	1.83	0.44
10:J:22:THR:HG22	10:J:27:VAL:HG22	2.00	0.44
10:J:163:LEU:O	10:J:167:GLU:HG2	2.18	0.44
11:K:200:VAL:O	11:K:204:GLU:HB2	2.17	0.44
10:X:4:ILE:HG13	10:X:4:ILE:O	2.18	0.44
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.52	0.44
10:X:1:MET:HE2	10:X:1:MET:HB3	1.70	0.44
13:a:96:LEU:O	13:a:100:MET:HG2	2.16	0.44
4:D:44:LYS:HE3	4:D:210:GLN:HB2	2.00	0.44
3:Q:160:GLN:HE22	3:Q:170:ARG:HE	1.66	0.44
11:Y:140:LEU:HD12	11:Y:141:ASP:H	1.81	0.44
7:G:83:ASN:C	7:G:83:ASN:ND2	2.76	0.44
8:V:162:GLY:O	8:V:166:ASP:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:34:LEU:C	7:G:34:LEU:HD23	2.43	0.44
9:I:34:GLY:O	11:Y:167:ARG:NH1	2.50	0.44
12:L:100:LYS:HD3	12:L:105:TYR:CE2	2.52	0.44
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.99	0.44
4:R:44:LYS:HE3	4:R:210:GLN:HB2	2.00	0.44
5:S:80:ALA:HB2	5:S:129:VAL:HG21	2.00	0.44
12:Z:100:LYS:HD3	12:Z:105:TYR:CE2	2.53	0.44
13:a:26:ASN:HA	13:a:39:VAL:O	2.18	0.44
5:E:77:ALA:N	5:E:78:PRO:CD	2.82	0.43
11:K:107:LYS:NZ	20:K:401:HOH:O	2.46	0.43
5:S:173:ARG:NH1	20:S:301:HOH:O	2.50	0.43
7:U:30:ASN:HD22	7:U:164:PRO:HG2	1.83	0.43
10:X:22:THR:HG22	10:X:27:VAL:HG22	2.00	0.43
13:a:165:ILE:HB	13:a:166:PRO:HD3	2.00	0.43
10:J:44:MET:HG3	10:J:104:ILE:HG12	2.00	0.43
10:J:45:SER:OG	10:J:103:LEU:HB2	2.18	0.43
5:E:9:THR:HG21	5:E:119:THR:HA	2.01	0.43
11:K:129:VAL:HG22	11:K:129:VAL:O	2.17	0.43
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.01	0.43
5:S:77:ALA:N	5:S:78:PRO:CD	2.81	0.43
8:V:104:ASP:HB2	8:V:105:PRO:HD2	2.00	0.43
10:X:143:LEU:HD21	10:X:163:LEU:HG	1.99	0.43
2:B:50:LYS:HD3	2:B:50:LYS:HA	1.80	0.43
5:E:80:ALA:HB2	5:E:129:VAL:HG21	2.00	0.43
10:X:26:SER:HB3	11:Y:135:PHE:CD2	2.54	0.43
10:X:167:GLU:HB3	10:X:171:ARG:NH2	2.33	0.43
10:J:1:MET:HE3	10:J:2:ASP:O	2.18	0.43
8:V:87:LEU:HD12	8:V:113:ILE:CD1	2.49	0.43
10:J:143:LEU:HD21	10:J:163:LEU:HG	2.00	0.43
7:U:34:LEU:C	7:U:34:LEU:HD23	2.43	0.43
7:U:78:ILE:HG22	7:U:79:PRO:HD3	2.01	0.43
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	2.01	0.43
10:X:119:ILE:HA	10:X:124:THR:O	2.18	0.43
14:N:139:ASP:OD2	14:b:164:LYS:NZ	2.45	0.43
10:J:25:ILE:O	10:J:25:ILE:HG12	2.09	0.43
19:N:202:MES:H61	19:N:202:MES:C8	2.49	0.43
2:B:217:LYS:C	2:B:219:ALA:N	2.77	0.42
11:K:198:TRP:CE2	9:W:200:LYS:HE3	2.54	0.42
9:W:58:ASP:OD1	10:X:93:ARG:NH2	2.50	0.42
12:Z:141:ALA:HB1	12:Z:195:HIS:NE2	2.34	0.42
8:H:63:ILE:HG23	8:H:74:PRO:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:158:LYS:HD3	11:K:196:LEU:HD11	2.01	0.42
6:F:240:GLN:HE21	6:F:240:GLN:HA	1.83	0.42
7:G:61:SER:OG	7:G:215:GLU:OE2	2.32	0.42
8:H:87:LEU:HD12	8:H:113:ILE:CD1	2.49	0.42
8:H:104:ASP:HB2	8:H:105:PRO:HD2	2.01	0.42
9:I:43:PHE:HB3	20:I:313:HOH:O	2.19	0.42
7:U:83:ASN:C	7:U:83:ASN:ND2	2.75	0.42
11:K:176:ASN:HD21	11:K:190:ASN:HD22	1.66	0.42
12:L:31:THR:HG23	12:L:36:ASN:ND2	2.31	0.42
10:X:25:ILE:CD1	11:Y:133:GLN:HG2	2.50	0.42
10:X:44:MET:HG3	10:X:104:ILE:HG12	2.00	0.42
10:X:50:ALA:O	11:Y:91:LYS:NZ	2.51	0.42
11:Y:42:LEU:HD12	11:Y:180:VAL:CG2	2.49	0.42
7:G:78:ILE:HG22	7:G:79:PRO:HD3	2.01	0.42
10:J:172:MET:HE3	10:J:172:MET:HB3	1.82	0.42
14:N:8:PHE:HB2	14:N:146:MET:O	2.20	0.42
6:F:123:ASN:C	6:F:123:ASN:ND2	2.73	0.42
9:I:141:ALA:HB2	9:I:177:ASP:HB2	2.01	0.42
5:S:9:THR:HG21	5:S:119:THR:HA	2.02	0.42
10:X:25:ILE:O	10:X:25:ILE:HG12	2.09	0.42
11:Y:158:LYS:HD3	11:Y:196:LEU:HD11	2.02	0.42
8:V:210:THR:HG21	9:W:167:SER:HB3	2.02	0.42
9:W:170:LEU:C	9:W:170:LEU:HD23	2.44	0.42
4:D:91:HIS:HB3	4:D:99:ILE:HG22	2.02	0.42
11:K:42:LEU:HD12	11:K:180:VAL:CG2	2.49	0.42
4:R:91:HIS:HB3	4:R:99:ILE:HG22	2.01	0.42
10:J:1:MET:HE2	10:J:1:MET:HB3	1.70	0.41
10:J:171:ARG:NH1	11:Y:140:LEU:O	2.53	0.41
14:N:164:LYS:NZ	14:b:139:ASP:OD2	2.43	0.41
1:O:75:TYR:HB3	1:O:82:TYR:CD1	2.54	0.41
2:P:114:LEU:HD23	2:P:114:LEU:HA	1.94	0.41
8:V:80:LEU:HD13	8:V:119:THR:HG21	2.02	0.41
8:H:84:LYS:HA	8:H:113:ILE:HD11	2.03	0.41
7:U:165:LYS:HD2	7:U:205:LEU:HD22	2.02	0.41
10:X:36:ARG:NH1	10:X:58:GLU:CG	2.83	0.41
3:C:160:GLN:HE22	3:C:170:ARG:HE	1.68	0.41
2:B:149:THR:O	2:B:156:TYR:HA	2.20	0.41
8:V:84:LYS:HA	8:V:113:ILE:HD11	2.02	0.41
12:Z:13:LEU:HD11	12:Z:150:LEU:HD21	2.02	0.41
1:A:75:TYR:HB3	1:A:82:TYR:CD1	2.56	0.41
13:M:48:ASN:HD22	13:M:49:THR:N	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:171:GLU:HB3	6:T:195:ILE:HG12	2.03	0.41
8:V:63:ILE:HG23	8:V:74:PRO:HB3	2.03	0.41
1:A:99:ARG:HE	8:H:61:SER:HG	1.69	0.41
4:D:149:HIS:O	4:D:156:PHE:HA	2.20	0.41
11:K:167:ARG:NH1	9:W:34:GLY:O	2.48	0.41
6:T:240:GLN:HE21	6:T:240:GLN:HA	1.84	0.41
8:H:87:LEU:HD12	8:H:113:ILE:HD11	2.02	0.41
11:K:3:THR:OG1	11:K:129:VAL:CG2	2.69	0.41
11:K:130:VAL:HG23	11:K:135:PHE:HE1	1.85	0.41
13:a:179:ASN:HD22	13:a:182:ARG:HH11	1.68	0.41
7:G:72:MET:HE3	7:G:74:VAL:CG2	2.51	0.41
11:K:140:LEU:H	11:K:140:LEU:HG	1.56	0.41
2:B:95:GLN:HE21	9:I:68:TYR:HA	1.86	0.41
4:D:176:LEU:HD22	5:E:55:LEU:CD2	2.51	0.41
10:J:3:ILE:HD13	10:J:176:PHE:CD2	2.55	0.41
11:K:176:ASN:ND2	11:K:190:ASN:HD22	2.19	0.41
6:T:216:SER:HB3	6:T:219:GLU:HB2	2.03	0.41
8:V:34:LEU:HD12	8:V:34:LEU:HA	1.93	0.41
8:V:112:SER:HB3	8:V:125:LEU:HD13	2.02	0.41
9:W:101:PRO:O	10:X:93:ARG:NH1	2.54	0.41
12:Z:5:TYR:CE1	12:Z:106:TYR:HB2	2.56	0.41
4:D:60:VAL:HG11	4:D:81:ILE:HG21	2.03	0.41
9:I:26:LEU:HD21	9:I:185:VAL:HG23	2.02	0.41
9:W:26:LEU:HD21	9:W:185:VAL:HG23	2.03	0.41
10:X:16:ALA:HB2	10:X:161:LEU:HD21	2.03	0.41
13:a:233:ILE:HD12	13:a:233:ILE:HG21	1.87	0.41
7:G:165:LYS:HD2	7:G:205:LEU:HD22	2.03	0.40
10:J:29:LYS:HE3	11:K:123:LYS:O	2.21	0.40
13:M:190:ARG:NH1	20:M:404:HOH:O	2.54	0.40
2:P:213:ALA:HA	2:P:227:LYS:O	2.21	0.40
10:X:3:ILE:HD13	10:X:176:PHE:CD2	2.56	0.40
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.02	0.40
12:L:5:TYR:CE1	12:L:106:TYR:HB2	2.57	0.40
14:N:14:LEU:O	14:N:175:MET:HA	2.21	0.40
5:S:65:CYS:SG	5:S:71:LEU:CD1	3.09	0.40
4:R:32:ILE:HD12	4:R:192:VAL:HG23	2.02	0.40
4:R:149:HIS:O	4:R:156:PHE:HA	2.21	0.40
11:Y:167:ARG:HA	11:Y:167:ARG:HD3	1.89	0.40
13:a:48:ASN:HD22	13:a:49:THR:N	2.19	0.40
4:D:24:LYS:O	4:D:166:SER:HA	2.22	0.40
4:D:32:ILE:HD12	4:D:192:VAL:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:216:SER:HB3	6:F:219:GLU:HB2	2.03	0.40
7:G:68:ARG:HH12	14:N:36:ARG:HH22	1.68	0.40
12:L:13:LEU:HD11	12:L:150:LEU:HD21	2.02	0.40
12:L:147:MET:N	12:L:148:PRO:CD	2.85	0.40
9:W:20:VAL:HG23	9:W:189:ILE:HB	2.03	0.40
11:Y:161:ILE:CG2	11:Y:175:VAL:HG22	2.52	0.40
12:Z:147:MET:N	12:Z:148:PRO:CD	2.84	0.40
14:b:3:ILE:HB	14:b:44:CYS:HB3	2.03	0.40
6:F:171:GLU:HB3	6:F:195:ILE:HG12	2.03	0.40
11:K:161:ILE:CG2	11:K:175:VAL:HG22	2.52	0.40
13:M:34:LEU:HD12	14:b:164:LYS:O	2.20	0.40
4:R:60:VAL:HG11	4:R:81:ILE:HG21	2.04	0.40
6:T:123:ASN:C	6:T:123:ASN:ND2	2.71	0.40
8:V:87:LEU:HD12	8:V:113:ILE:HD11	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	30	52
1	O	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	30	52
2	B	242/258 (94%)	233 (96%)	5 (2%)	4 (2%)	7	16
2	P	242/258 (94%)	233 (96%)	5 (2%)	4 (2%)	7	16
3	C	238/254 (94%)	232 (98%)	3 (1%)	3 (1%)	10	21
3	Q	233/254 (92%)	227 (97%)	3 (1%)	3 (1%)	10	21
4	D	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
4	R	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
5	E	229/234 (98%)	220 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	S	229/234 (98%)	221 (96%)	8 (4%)	0	100	100
6	F	241/288 (84%)	237 (98%)	4 (2%)	0	100	100
6	T	241/288 (84%)	237 (98%)	4 (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%)	218 (97%)	6 (3%)	0	100	100
8	V	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
9	I	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	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	206/212 (97%)	202 (98%)	4 (2%)	0	100	100
11	Y	210/212 (99%)	202 (96%)	7 (3%)	1 (0%)	25	47
12	L	220/222 (99%)	216 (98%)	4 (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	52
13	a	231/246 (94%)	222 (96%)	8 (4%)	1 (0%)	30	52
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	6275/6614 (95%)	6111 (97%)	145 (2%)	19 (0%)	37	59

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
2	B	51	VAL
2	B	221	ASP
3	C	202	GLN
1	O	2	THR
2	P	51	VAL
2	P	221	ASP
3	Q	202	GLN
2	B	218	GLY
2	B	220	ASN
2	P	218	GLY

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Mol	Chain	Res	Type
2	P	220	ASN
3	C	205	ALA
3	Q	205	ALA
11	Y	139	VAL
13	a	83	ALA
13	M	83	ALA
3	Q	183	PRO
3	C	183	PRO

5.3.2 Protein sidechains [i](#)

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	209/209 (100%)	204 (98%)	5 (2%)	44	70
1	O	209/209 (100%)	204 (98%)	5 (2%)	44	70
2	B	203/216 (94%)	197 (97%)	6 (3%)	36	63
2	P	203/216 (94%)	197 (97%)	6 (3%)	36	63
3	C	212/226 (94%)	201 (95%)	11 (5%)	19	41
3	Q	209/226 (92%)	199 (95%)	10 (5%)	21	44
4	D	194/215 (90%)	183 (94%)	11 (6%)	17	37
4	R	194/215 (90%)	183 (94%)	11 (6%)	17	37
5	E	190/193 (98%)	183 (96%)	7 (4%)	29	55
5	S	190/193 (98%)	183 (96%)	7 (4%)	29	55
6	F	201/239 (84%)	193 (96%)	8 (4%)	27	52
6	T	201/239 (84%)	193 (96%)	8 (4%)	27	52
7	G	206/210 (98%)	198 (96%)	8 (4%)	27	53
7	U	206/210 (98%)	198 (96%)	8 (4%)	27	53
8	H	185/190 (97%)	176 (95%)	9 (5%)	21	43
8	V	185/190 (97%)	174 (94%)	11 (6%)	16	35
9	I	172/173 (99%)	170 (99%)	2 (1%)	67	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	W	172/173 (99%)	170 (99%)	2 (1%)	67	85
10	J	173/175 (99%)	164 (95%)	9 (5%)	19	41
10	X	173/175 (99%)	166 (96%)	7 (4%)	27	52
11	K	169/170 (99%)	156 (92%)	13 (8%)	10	22
11	Y	170/170 (100%)	156 (92%)	14 (8%)	9	20
12	L	185/185 (100%)	178 (96%)	7 (4%)	28	54
12	Z	185/185 (100%)	178 (96%)	7 (4%)	28	54
13	M	199/208 (96%)	190 (96%)	9 (4%)	23	47
13	a	199/208 (96%)	191 (96%)	8 (4%)	27	52
14	N	162/162 (100%)	155 (96%)	7 (4%)	25	49
14	b	162/162 (100%)	155 (96%)	7 (4%)	25	49
All	All	5318/5542 (96%)	5095 (96%)	223 (4%)	25	50

All (223) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	29	LYS
1	A	122	THR
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	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
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	213	VAL
3	C	240	GLU

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Mol	Chain	Res	Type
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	193	LEU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	55	LEU
5	E	71	LEU
5	E	188	LEU
5	E	208	ASP
5	E	231	LYS
6	F	94	SER
6	F	123	ASN
6	F	171	GLU
6	F	172	LEU
6	F	181	GLU
6	F	201	GLU
6	F	221	ASN
6	F	240	GLN
7	G	13	GLU
7	G	26	THR
7	G	83	ASN
7	G	115	LEU
7	G	122	ARG
7	G	125	MET
7	G	235	ARG
7	G	236	LEU
8	H	13	VAL
8	H	14	ILE
8	H	30	ASN
8	H	34	LEU
8	H	55	VAL
8	H	68	LEU
8	H	127	LEU
8	H	195	VAL

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Mol	Chain	Res	Type
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
10	J	1	MET
10	J	25	ILE
10	J	35	THR
10	J	36	ARG
10	J	92	ILE
10	J	149	ARG
10	J	174	MET
10	J	193	ASP
10	J	194	ASP
11	K	1	THR
11	K	9	GLN
11	K	84	SER
11	K	106	ARG
11	K	117	SER
11	K	129	VAL
11	K	130	VAL
11	K	134	THR
11	K	140	LEU
11	K	142	SER
11	K	143	ASN
11	K	145	LYS
11	K	149	SER
12	L	1	GLN
12	L	23	LEU
12	L	31	THR
12	L	42	LYS
12	L	49	ASN
12	L	108	HIS
12	L	150	LEU
13	M	2	GLN
13	M	29	SER
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
13	M	225	ILE
13	M	233	ILE
14	N	1	THR

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Mol	Chain	Res	Type
14	N	9	LYS
14	N	36	ARG
14	N	104	ASP
14	N	107	LYS
14	N	119	VAL
14	N	178	LEU
1	O	1	MET
1	O	29	LYS
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	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	51	LYS
3	Q	52	LEU
3	Q	147	GLN
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	193	LEU
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	55	LEU
5	S	71	LEU

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Mol	Chain	Res	Type
5	S	188	LEU
5	S	208	ASP
5	S	231	LYS
6	T	94	SER
6	T	123	ASN
6	T	171	GLU
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	83	ASN
7	U	115	LEU
7	U	122	ARG
7	U	125	MET
7	U	235	ARG
7	U	236	LEU
8	V	13	VAL
8	V	14	ILE
8	V	22	GLN
8	V	30	ASN
8	V	34	LEU
8	V	55	VAL
8	V	68	LEU
8	V	80	LEU
8	V	127	LEU
8	V	195	VAL
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
10	X	1	MET
10	X	25	ILE
10	X	35	THR
10	X	92	ILE
10	X	149	ARG
10	X	193	ASP
10	X	194	ASP
11	Y	1	THR
11	Y	9	GLN
11	Y	84	SER

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Mol	Chain	Res	Type
11	Y	106	ARG
11	Y	117	SER
11	Y	130	VAL
11	Y	133	GLN
11	Y	134	THR
11	Y	135	PHE
11	Y	139	VAL
11	Y	140	LEU
11	Y	143	ASN
11	Y	145	LYS
11	Y	149	SER
12	Z	1	GLN
12	Z	23	LEU
12	Z	31	THR
12	Z	42	LYS
12	Z	49	ASN
12	Z	108	HIS
12	Z	150	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	233	ILE
14	b	1	THR
14	b	9	LYS
14	b	36	ARG
14	b	104	ASP
14	b	107	LYS
14	b	119	VAL
14	b	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (159) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	20	GLN
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN

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Mol	Chain	Res	Type
2	B	124	HIS
2	B	155	ASN
2	B	176	GLN
3	C	17	GLN
3	C	38	ASN
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
4	D	100	ASN
4	D	106	GLN
4	D	160	ASN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
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	66	HIS
8	H	165	ASN
8	H	172	ASN
8	H	189	ASN

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Mol	Chain	Res	Type
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	24	ASN
11	K	85	ASN
11	K	176	ASN
12	L	3	ASN
12	L	8	ASN
12	L	29	ASN
12	L	36	ASN
12	L	49	ASN
12	L	55	ASN
12	L	76	HIS
12	L	80	ASN
12	L	92	ASN
12	L	153	GLN
13	M	18	ASN
13	M	26	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	69	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	155	ASN
2	P	176	GLN
2	P	232	GLN
3	Q	17	GLN
3	Q	38	ASN

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Mol	Chain	Res	Type
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	106	GLN
4	R	160	ASN
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
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	88	GLN

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Mol	Chain	Res	Type
9	W	168	GLN
9	W	172	ASN
10	X	55	GLN
10	X	99	GLN
10	X	191	GLN
11	Y	9	GLN
11	Y	24	ASN
11	Y	85	ASN
11	Y	176	ASN
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	76	HIS
12	Z	79	HIS
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	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 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 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	$\# Z > 2$
19	MES	b	201	-	12,12,12	0.70	0	14,16,16	0.44	0
19	MES	N	202	-	12,12,12	0.80	0	14,16,16	0.81	0
19	MES	M	301	-	12,12,12	0.73	0	14,16,16	0.43	0
18	MPD	K	301	-	7,7,7	0.14	0	9,10,10	0.47	0
15	SO4	P	301	-	4,4,4	0.38	0	6,6,6	0.05	0
19	MES	Z	301	-	12,12,12	0.74	0	14,16,16	0.45	0
18	MPD	a	301	-	7,7,7	0.11	0	9,10,10	0.37	0
15	SO4	B	301	-	4,4,4	0.39	0	6,6,6	0.05	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
19	MES	b	201	-	-	4/6/14/14	0/1/1/1
19	MES	N	202	-	-	2/6/14/14	0/1/1/1
18	MPD	K	301	-	-	1/5/5/5	-
19	MES	M	301	-	-	3/6/14/14	0/1/1/1
19	MES	Z	301	-	-	1/6/14/14	0/1/1/1
18	MPD	a	301	-	-	0/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	K	301	MPD	C2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
19	N	202	MES	C8-C7-N4-C5
19	Z	301	MES	C8-C7-N4-C5
19	M	301	MES	C7-C8-S-O3S
19	b	201	MES	N4-C7-C8-S
19	N	202	MES	C8-C7-N4-C3
19	b	201	MES	C8-C7-N4-C3
19	b	201	MES	C8-C7-N4-C5
19	b	201	MES	C7-C8-S-O3S
19	M	301	MES	C7-C8-S-O1S
19	M	301	MES	C7-C8-S-O2S

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	b	201	MES	3	0
19	N	202	MES	2	0
18	K	301	MPD	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/250 (100%)	-0.64	1 (0%) 89 86	40, 50, 85, 118	0
1	O	250/250 (100%)	-0.65	1 (0%) 89 86	43, 57, 95, 125	0
2	B	244/258 (94%)	-0.55	4 (1%) 70 65	39, 55, 91, 148	0
2	P	244/258 (94%)	-0.57	4 (1%) 70 65	42, 58, 94, 136	0
3	C	240/254 (94%)	-0.62	0 100 100	41, 58, 108, 129	0
3	Q	237/254 (93%)	-0.48	4 (1%) 69 64	47, 67, 124, 145	0
4	D	235/260 (90%)	-0.70	0 100 100	41, 59, 84, 112	0
4	R	235/260 (90%)	-0.65	0 100 100	42, 63, 89, 117	0
5	E	231/234 (98%)	-0.63	0 100 100	43, 62, 91, 119	0
5	S	231/234 (98%)	-0.51	0 100 100	44, 68, 98, 120	0
6	F	243/288 (84%)	-0.69	0 100 100	39, 55, 89, 110	0
6	T	243/288 (84%)	-0.63	0 100 100	42, 62, 101, 120	0
7	G	241/252 (95%)	-0.74	0 100 100	37, 51, 80, 115	0
7	U	241/252 (95%)	-0.64	0 100 100	42, 55, 80, 121	0
8	H	226/232 (97%)	-0.73	1 (0%) 89 86	38, 48, 71, 134	0
8	V	226/232 (97%)	-0.70	1 (0%) 89 86	41, 51, 73, 136	0
9	I	204/205 (99%)	-0.88	0 100 100	35, 47, 68, 90	0
9	W	204/205 (99%)	-0.86	1 (0%) 87 84	36, 48, 71, 95	0
10	J	195/198 (98%)	-0.60	0 100 100	37, 55, 89, 112	0
10	X	195/198 (98%)	-0.69	0 100 100	39, 56, 87, 118	0
11	K	210/212 (99%)	-0.57	4 (1%) 66 61	39, 52, 91, 114	0
11	Y	212/212 (100%)	-0.57	3 (1%) 73 68	40, 53, 91, 113	0
12	L	222/222 (100%)	-0.84	0 100 100	36, 48, 70, 96	0
12	Z	222/222 (100%)	-0.85	0 100 100	37, 49, 70, 95	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.85	1 (0%) 89 86	37, 47, 65, 72	0
13	a	233/246 (94%)	-0.84	2 (0%) 81 77	36, 47, 63, 75	0
14	N	196/196 (100%)	-0.82	0 100 100	36, 44, 68, 95	0
14	b	196/196 (100%)	-0.80	0 100 100	36, 45, 68, 93	0
All	All	6339/6614 (95%)	-0.69	27 (0%) 89 86	35, 53, 90, 148	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	Y	137	TYR	3.8
8	V	223	ILE	3.6
11	K	139	VAL	3.5
1	O	249	ALA	3.4
2	P	219	ALA	3.3
13	a	69	ASP	3.3
3	Q	204	GLY	3.3
2	P	51	VAL	3.3
13	M	69	ASP	3.1
11	Y	134	THR	3.0
2	B	219	ALA	2.9
2	P	222	GLY	2.7
11	K	140	LEU	2.6
11	K	135	PHE	2.6
3	Q	205	ALA	2.4
2	B	51	VAL	2.4
13	a	1	THR	2.3
1	A	62	SER	2.3
11	K	136	ALA	2.2
3	Q	1	GLY	2.2
8	H	223	ILE	2.2
11	Y	130	VAL	2.2
2	B	220	ASN	2.1
2	B	222	GLY	2.1
3	Q	51	LYS	2.0
9	W	1	SER	2.0
2	P	218	GLY	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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
16	MG	N	201	1/1	0.85	0.12	145,145,145,145	0
16	MG	G	301	1/1	0.87	0.14	87,87,87,87	0
19	MES	M	301	12/12	0.87	0.18	120,131,141,142	0
18	MPD	a	301	8/8	0.89	0.15	88,96,102,104	0
19	MES	N	202	12/12	0.89	0.14	75,93,106,107	0
19	MES	Z	301	12/12	0.90	0.14	108,115,121,122	0
19	MES	b	201	12/12	0.90	0.13	77,92,102,104	0
17	CL	U	301	1/1	0.91	0.23	94,94,94,94	0
18	MPD	K	301	8/8	0.93	0.14	79,82,85,87	0
16	MG	W	301	1/1	0.93	0.41	161,161,161,161	0
17	CL	G	302	1/1	0.94	0.09	63,63,63,63	0
15	SO4	B	301	5/5	0.94	0.14	95,102,111,114	0
15	SO4	P	301	5/5	0.96	0.11	93,96,105,106	0

6.5 Other polymers [i](#)

There are no such residues in this entry.