



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 3, 2024 – 08:17 pm BST

PDB ID : 9FT1
Title : Yeast 20S proteasome in complex with epoxyketone inhibitor 13
Authors : Maurits, E.; Huber, E.M.; Dekker, P.M.; Wang, X.; Heinemeyer, W.; Florea, B.I.; Groll, M.; Overkleeft, H.S.
Deposited on : 2024-06-23
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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

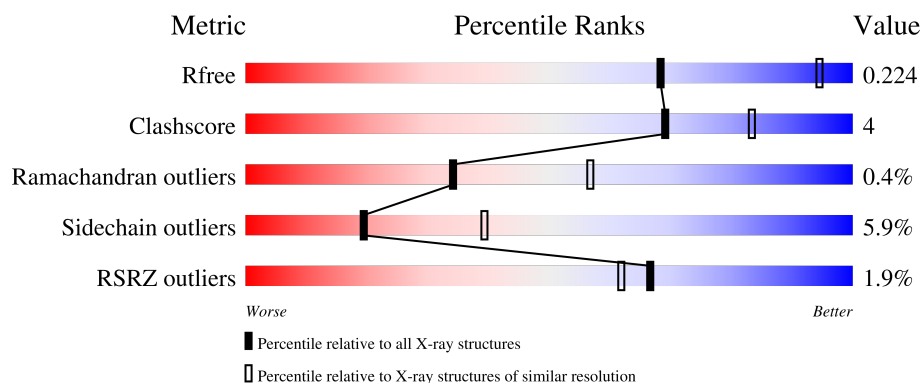
1 Overall quality at a glance

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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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>2%</div> <div> <div></div> <div>92%</div> <div>7%</div> <div>.</div> </div> </div>
1	O	250	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>8%</div> <div>.</div> </div> </div>
2	B	258	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>• 5%</div> </div> </div>
2	P	258	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>• 5%</div> </div> </div>
3	C	254	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>• 6%</div> </div> </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	231	
8	V	231	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	211	
11	Y	211	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	
15	e	4	
15	f	4	

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Mol	Chain	Length	Quality of chain
15	g	4	 50%50%
15	h	4	 50%50%

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 49970 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	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 endopeptidase complex.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	221	Total	C	N	O	S	0	0	0
			1677	1057	292	321	7			
8	V	221	Total	C	N	O	S	0	0	0
			1677	1057	292	321	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 endopeptidase complex.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	211	Total	C	N	O	S	0	0	0
			1637	1041	279	310	7			
11	Y	211	Total	C	N	O	S	0	0	0
			1637	1041	279	310	7			

- 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 a protein called 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-C]PYRAZOLE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	e	4	Total	C	N	O	0	0	0
			64	47	6	11			

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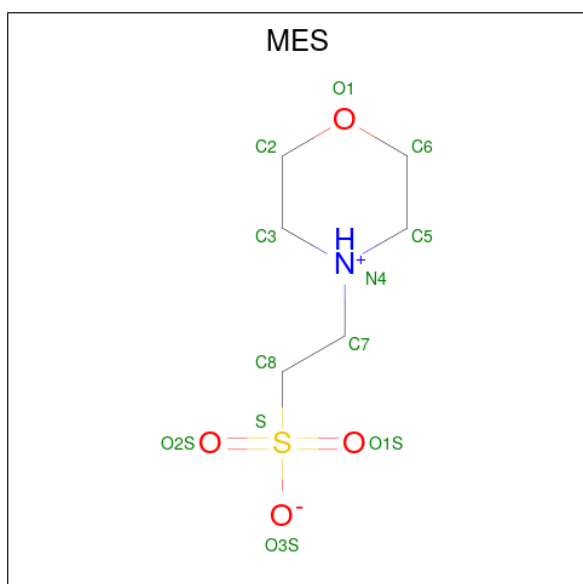
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	f	4	Total	C	N	O	0	0	0
			64	47	6	11			
15	g	4	Total	C	N	O	0	0	0
			64	47	6	11			
15	h	4	Total	C	N	O	0	0	0
			64	47	6	11			

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	G	1	Total	Mg	0	0
			1	1		
16	H	1	Total	Mg	0	0
			1	1		
16	I	1	Total	Mg	0	0
			1	1		
16	K	1	Total	Mg	0	0
			1	1		
16	N	1	Total	Mg	0	0
			1	1		
16	Y	1	Total	Mg	0	0
			1	1		
16	Z	1	Total	Mg	0	0
			1	1		

- Molecule 17 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	14	Total	O	0	0
			14	14		
18	B	14	Total	O	0	0
			14	14		
18	C	11	Total	O	0	0
			11	11		
18	D	11	Total	O	0	0
			11	11		
18	E	5	Total	O	0	0
			5	5		
18	F	11	Total	O	0	0
			11	11		
18	G	13	Total	O	0	0
			13	13		
18	H	18	Total	O	0	0
			18	18		
18	I	17	Total	O	0	0
			17	17		
18	J	19	Total	O	0	0
			19	19		
18	K	18	Total	O	0	0
			18	18		
18	L	22	Total	O	0	0
			22	22		
18	M	16	Total	O	0	0
			16	16		
18	N	14	Total	O	0	0
			14	14		
18	O	15	Total	O	0	0
			15	15		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	P	11	Total 11	O 11	0	0
18	Q	8	Total 8	O 8	0	0
18	R	7	Total 7	O 7	0	0
18	S	5	Total 5	O 5	0	0
18	T	7	Total 7	O 7	0	0
18	U	20	Total 20	O 20	0	0
18	V	10	Total 10	O 10	0	0
18	W	16	Total 16	O 16	0	0
18	X	15	Total 15	O 15	0	0
18	Y	15	Total 15	O 15	0	0
18	Z	14	Total 14	O 14	0	0
18	a	15	Total 15	O 15	0	0
18	b	18	Total 18	O 18	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.

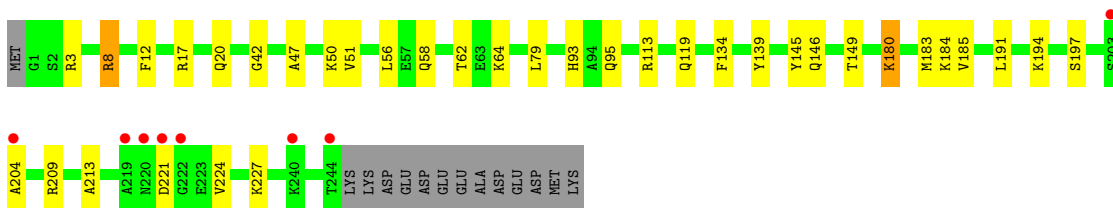
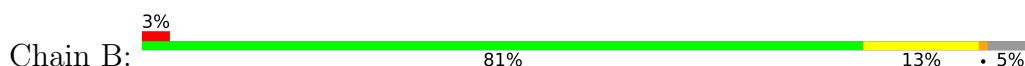
- Molecule 1: Proteasome subunit alpha type-2



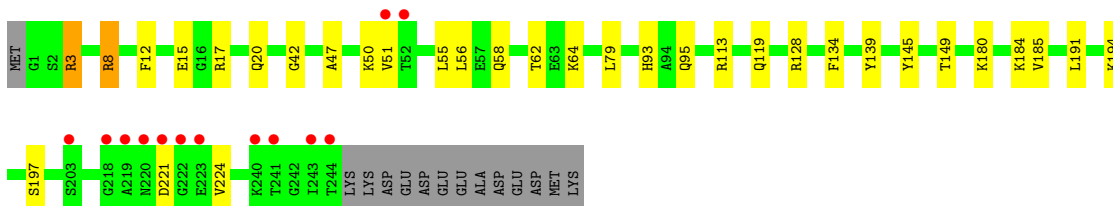
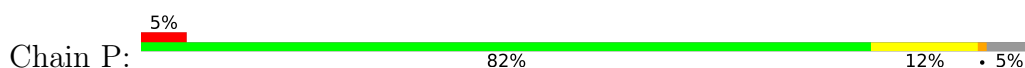
- Molecule 1: Proteasome subunit alpha type-2



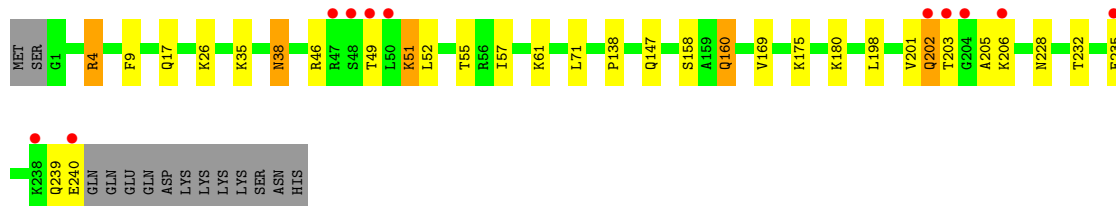
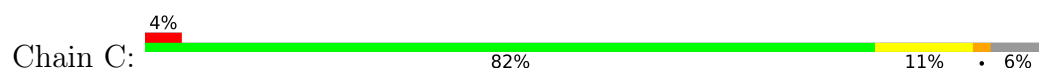
- Molecule 2: Proteasome subunit alpha type-3



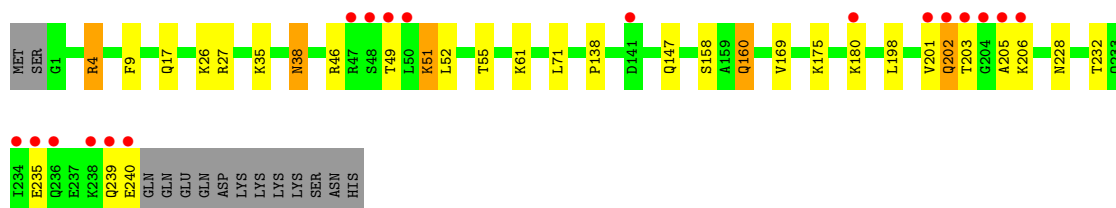
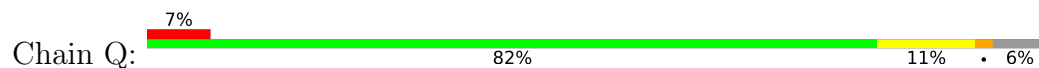
- Molecule 2: Proteasome subunit alpha type-3



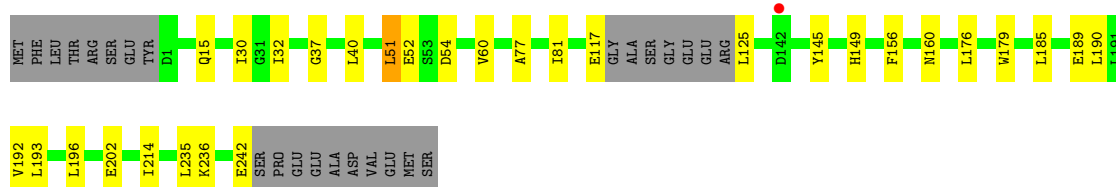
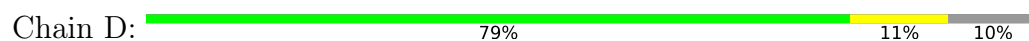
- Molecule 3: Proteasome subunit alpha type-4



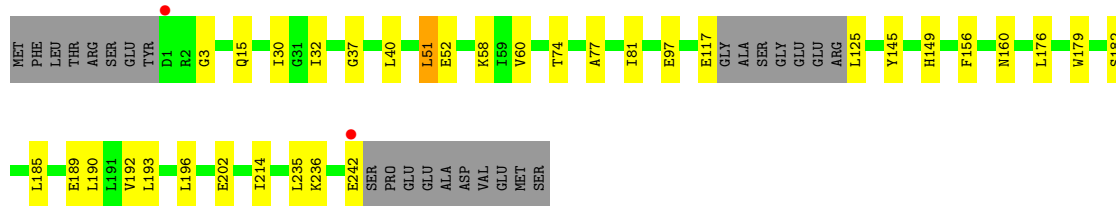
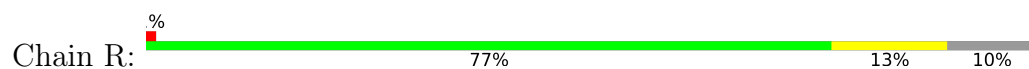
- Molecule 3: Proteasome subunit alpha type-4



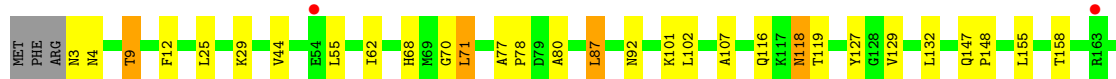
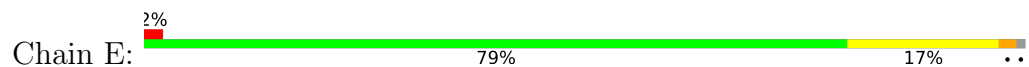
- Molecule 4: Proteasome subunit alpha type-5



- Molecule 4: Proteasome subunit alpha type-5

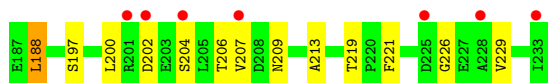
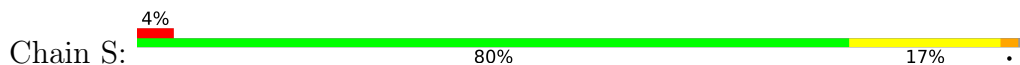


- Molecule 5: Proteasome subunit alpha type-6

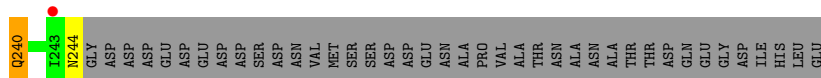
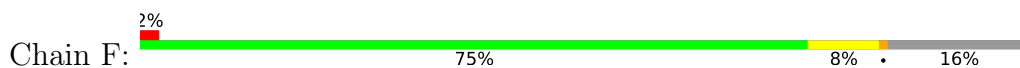




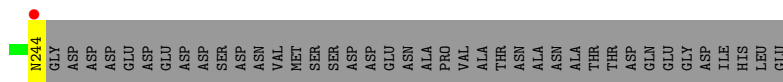
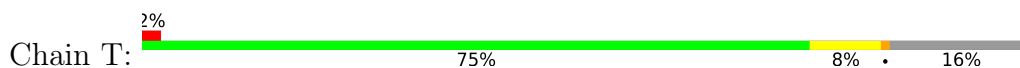
- Molecule 5: Proteasome subunit alpha type-6



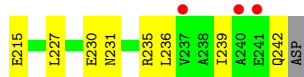
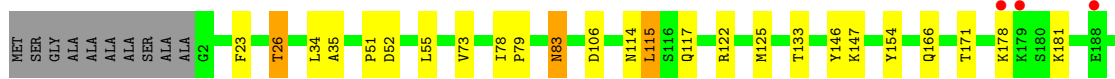
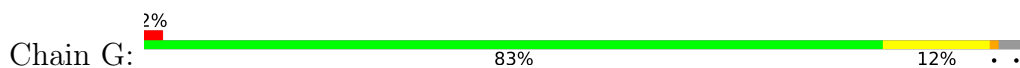
- Molecule 6: Probable proteasome subunit alpha type-7



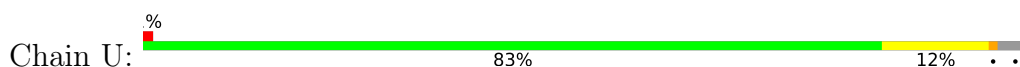
- Molecule 6: Probable proteasome subunit alpha type-7

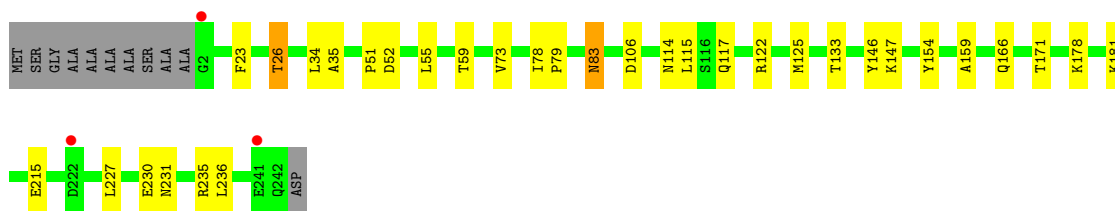


- Molecule 7: Proteasome subunit alpha type-1

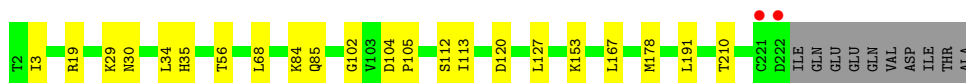
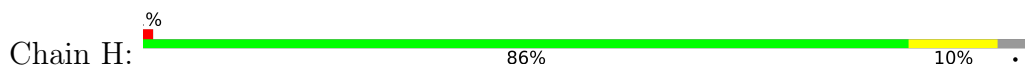


- Molecule 7: Proteasome subunit alpha type-1

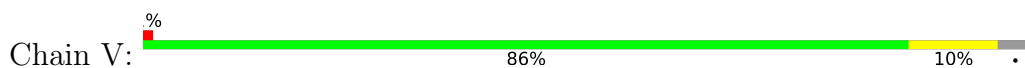




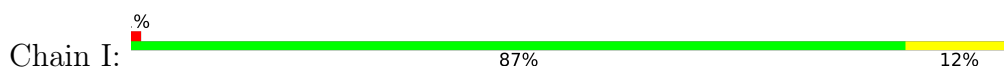
- Molecule 8: proteasome endopeptidase complex



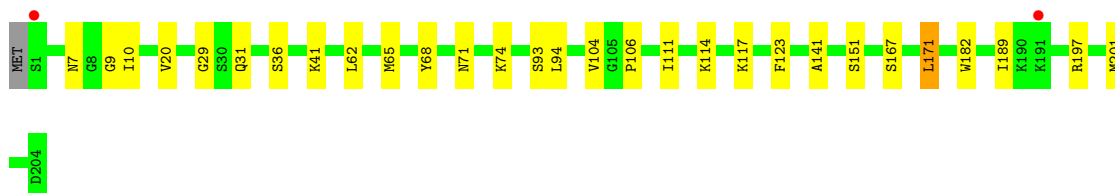
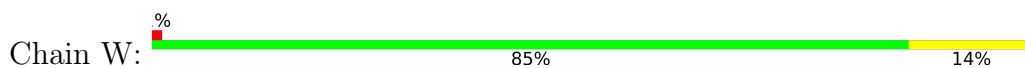
- Molecule 8: proteasome endopeptidase complex



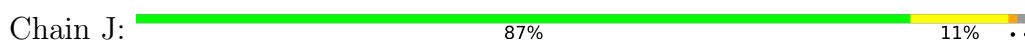
- Molecule 9: Proteasome subunit beta type-3



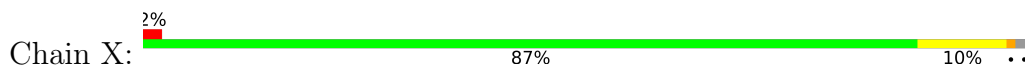
- Molecule 9: Proteasome subunit beta type-3



- Molecule 10: Proteasome subunit beta type-4

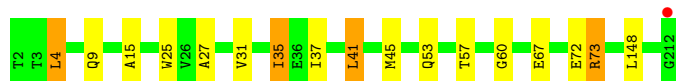


- Molecule 10: Proteasome subunit beta type-4

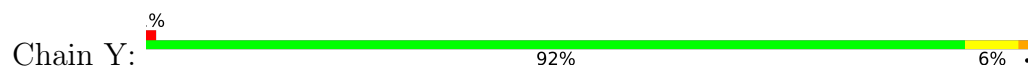




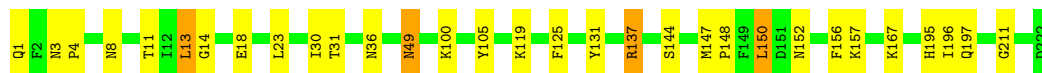
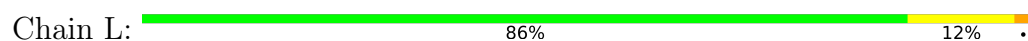
- Molecule 11: proteasome endopeptidase complex



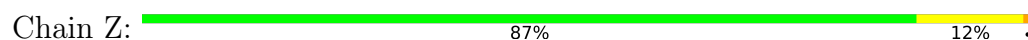
- Molecule 11: proteasome endopeptidase complex



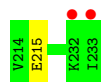
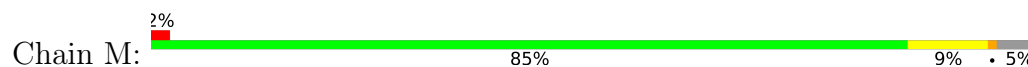
- Molecule 12: Proteasome subunit beta type-6



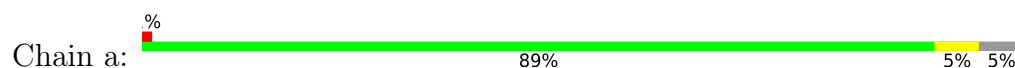
- Molecule 12: Proteasome subunit beta type-6



- 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



- Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-.C.]PYRAZOLE



- Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-.C.]PYRAZOLE



- Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-.C.]PYRAZOLE



- Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-.C.]PYRAZOLE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.00Å 300.67Å 144.54Å 90.00° 113.09° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 29.98 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.4 (30.00-2.60) 97.5 (29.98-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.182 , 0.222 0.176 , 0.224	Depositor DCC
R_{free} test set	15884 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	1.388	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	49970	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1IFL, 0A1, SEM, A1IFK, MG, MES

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.67	0/1952	0.73	0/2642
1	O	0.67	0/1952	0.72	0/2642
2	B	0.66	0/1934	0.75	0/2618
2	P	0.66	0/1934	0.75	0/2618
3	C	0.67	0/1910	0.75	0/2586
3	Q	0.68	0/1910	0.76	0/2586
4	D	0.67	0/1837	0.74	0/2475
4	R	0.67	0/1837	0.74	0/2475
5	E	0.67	0/1800	0.74	0/2433
5	S	0.67	0/1800	0.74	0/2433
6	F	0.67	0/1932	0.72	0/2609
6	T	0.67	0/1932	0.73	0/2609
7	G	0.66	0/1945	0.75	0/2634
7	U	0.66	0/1945	0.75	0/2634
8	H	0.66	0/1708	0.75	0/2316
8	V	0.66	0/1708	0.75	0/2316
9	I	0.67	0/1611	0.75	0/2174
9	W	0.66	0/1611	0.74	0/2174
10	J	0.65	0/1589	0.74	0/2142
10	X	0.65	0/1589	0.74	0/2142
11	K	0.66	0/1674	0.76	0/2264
11	Y	0.66	0/1674	0.75	0/2264
12	L	0.66	0/1795	0.73	0/2420
12	Z	0.66	0/1795	0.73	0/2420
13	M	0.67	0/1855	0.76	0/2514
13	a	0.67	0/1855	0.76	0/2514
14	N	0.66	0/1541	0.73	0/2087
14	b	0.67	0/1541	0.73	0/2087
All	All	0.66	0/50166	0.74	0/67828

There are no bond length outliers.

There are no bond angle outliers.

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	7	0
1	O	1915	0	1929	10	0
2	B	1904	0	1904	14	0
2	P	1904	0	1904	15	0
3	C	1881	0	1895	19	0
3	Q	1881	0	1895	22	0
4	D	1813	0	1797	10	0
4	R	1813	0	1797	13	0
5	E	1773	0	1775	21	0
5	S	1773	0	1775	21	0
6	F	1892	0	1883	10	0
6	T	1892	0	1883	11	0
7	G	1907	0	1901	15	0
7	U	1907	0	1901	17	0
8	H	1677	0	1678	9	0
8	V	1677	0	1678	10	0
9	I	1581	0	1574	13	0
9	W	1581	0	1574	17	0
10	J	1561	0	1569	9	0
10	X	1561	0	1569	10	0
11	K	1637	0	1585	14	0
11	Y	1637	0	1585	17	0
12	L	1757	0	1711	16	0
12	Z	1757	0	1711	15	0
13	M	1824	0	1832	9	0
13	a	1824	0	1832	0	0
14	N	1512	0	1481	3	0
14	b	1512	0	1481	0	0
15	e	64	0	20	0	0
15	f	64	0	20	0	0
15	g	64	0	20	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	h	64	0	20	0	0
16	G	1	0	0	0	0
16	H	1	0	0	0	0
16	I	1	0	0	0	0
16	K	1	0	0	0	0
16	N	1	0	0	0	0
16	Y	1	0	0	0	0
16	Z	1	0	0	0	0
17	H	12	0	13	0	0
17	V	12	0	13	0	0
17	X	12	0	13	1	0
17	b	12	0	13	0	0
17	f	12	0	13	0	0
18	A	14	0	0	0	0
18	B	14	0	0	0	0
18	C	11	0	0	0	0
18	D	11	0	0	0	0
18	E	5	0	0	0	0
18	F	11	0	0	0	0
18	G	13	0	0	0	0
18	H	18	0	0	0	0
18	I	17	0	0	0	0
18	J	19	0	0	0	0
18	K	18	0	0	0	0
18	L	22	0	0	0	0
18	M	16	0	0	0	0
18	N	14	0	0	0	0
18	O	15	0	0	0	0
18	P	11	0	0	0	0
18	Q	8	0	0	1	0
18	R	7	0	0	0	0
18	S	5	0	0	0	0
18	T	7	0	0	0	0
18	U	20	0	0	0	0
18	V	10	0	0	0	0
18	W	16	0	0	0	0
18	X	15	0	0	0	0
18	Y	15	0	0	0	0
18	Z	14	0	0	0	0
18	a	15	0	0	0	0
18	b	18	0	0	0	0
All	All	49970	0	49173	304	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 (304) 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:73:ARG:HH21	11:K:73:ARG:HG3	1.12	1.12
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.40	0.85
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.41	0.84
7:G:23:PHE:O	7:G:26:THR:HB	1.85	0.75
6:F:123:ASN:C	6:F:123:ASN:HD22	1.90	0.75
11:Y:4:LEU:HD23	11:Y:4:LEU:C	2.06	0.75
7:U:23:PHE:O	7:U:26:THR:HB	1.87	0.74
11:K:4:LEU:C	11:K:4:LEU:HD23	2.08	0.73
6:T:123:ASN:C	6:T:123:ASN:HD22	1.95	0.69
11:K:73:ARG:HG3	11:K:73:ARG:NH2	1.91	0.69
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.76	0.68
2:B:93:HIS:HB3	2:B:113:ARG:HH21	1.59	0.67
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.75	0.67
1:O:12:PHE:H	2:P:20:GLN:HE22	1.44	0.66
2:P:93:HIS:HB3	2:P:113:ARG:HH21	1.61	0.66
3:C:51:LYS:O	3:C:52:LEU:HB2	1.96	0.65
11:Y:73:ARG:HH21	11:Y:73:ARG:CG	2.10	0.65
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.61	0.65
12:L:8:ASN:HA	12:L:30:ILE:O	1.98	0.64
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.62	0.64
11:K:27:ALA:O	12:L:137:ARG:NH2	2.30	0.64
12:Z:8:ASN:HA	12:Z:30:ILE:O	1.97	0.64
11:Y:69:ARG:CG	11:Y:69:ARG:HH11	2.11	0.63
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.81	0.63
3:C:35:LYS:HG2	3:C:158:SER:O	1.99	0.62
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.81	0.62
3:Q:202:GLN:HG3	3:Q:203:THR:N	2.15	0.61
3:C:202:GLN:HG3	3:C:203:THR:N	2.15	0.61
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.00	0.61
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.48	0.60
11:Y:53:GLN:O	11:Y:57:THR:HG23	2.02	0.60
3:C:202:GLN:HG3	3:C:203:THR:H	1.67	0.60
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.83	0.60
11:K:53:GLN:O	11:K:57:THR:HG23	2.02	0.59
5:E:12:PHE:H	6:F:19:GLN:HE22	1.51	0.59
6:F:123:ASN:HD22	6:F:124:SER:N	2.01	0.59
11:Y:4:LEU:C	11:Y:4:LEU:CD2	2.72	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:202:GLN:HG3	3:Q:203:THR:H	1.68	0.58
1:A:12:PHE:H	2:B:20:GLN:HE22	1.52	0.58
6:T:123:ASN:HD22	6:T:124:SER:N	2.02	0.58
2:B:12:PHE:H	3:C:17:GLN:HE22	1.52	0.58
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.51	0.57
11:K:4:LEU:C	11:K:4:LEU:CD2	2.73	0.57
6:F:240:GLN:HE21	6:F:240:GLN:HA	1.68	0.57
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.52	0.57
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.41	0.56
5:E:71:LEU:C	5:E:71:LEU:HD23	2.25	0.56
5:S:71:LEU:C	5:S:71:LEU:HD23	2.25	0.56
11:K:4:LEU:HD22	11:K:15:ALA:HB3	1.88	0.56
5:S:12:PHE:H	6:T:19:GLN:HE22	1.54	0.56
8:H:35:HIS:CB	8:H:56:THR:HG21	2.36	0.56
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.87	0.55
5:E:9:THR:HG21	5:E:119:THR:HA	1.88	0.55
3:C:9:PHE:H	4:D:15:GLN:HE22	1.53	0.55
14:N:152:VAL:HA	14:N:175:MET:HE1	1.87	0.55
6:T:240:GLN:HE21	6:T:240:GLN:HA	1.70	0.55
8:V:35:HIS:CB	8:V:56:THR:HG21	2.36	0.55
3:Q:198:LEU:HA	3:Q:201:VAL:HG12	1.88	0.55
5:E:68:HIS:HE1	5:E:102:LEU:O	1.90	0.54
3:C:198:LEU:HA	3:C:201:VAL:HG12	1.88	0.54
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.88	0.54
6:F:172:LEU:CD1	6:F:195:ILE:HD13	2.37	0.54
2:P:15:GLU:O	3:Q:27:ARG:NH1	2.40	0.54
10:J:174:MET:HA	10:X:174:MET:HA	1.89	0.54
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.42	0.54
5:S:68:HIS:HE1	5:S:102:LEU:O	1.91	0.54
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.89	0.54
3:C:38:ASN:H	3:C:38:ASN:HD22	1.56	0.53
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.91	0.53
8:V:210:THR:HG21	9:W:167:SER:HB3	1.90	0.53
10:X:1:MET:HA	10:X:34:LYS:CE	2.39	0.53
10:J:1:MET:HA	10:J:34:LYS:CE	2.38	0.53
5:S:9:THR:HG21	5:S:119:THR:HA	1.91	0.53
5:S:71:LEU:HD23	5:S:71:LEU:O	2.09	0.53
12:L:49:ASN:HD21	12:L:211:GLY:HA2	1.74	0.53
3:Q:46:ARG:NH1	3:Q:55:THR:HG21	2.24	0.52
6:T:172:LEU:CD1	6:T:195:ILE:HD13	2.38	0.52
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:1:MET:HA	10:X:34:LYS:HE3	1.92	0.52
3:C:46:ARG:NH1	3:C:55:THR:HG21	2.25	0.52
3:Q:38:ASN:HD22	3:Q:38:ASN:H	1.57	0.52
10:J:1:MET:HA	10:J:34:LYS:HE3	1.92	0.52
11:Y:4:LEU:HD22	11:Y:15:ALA:HB3	1.92	0.51
8:V:222:ASP:OD1	9:W:74:LYS:NZ	2.42	0.51
11:Y:73:ARG:CG	11:Y:73:ARG:NH2	2.71	0.51
5:E:71:LEU:HD23	5:E:71:LEU:O	2.11	0.51
7:G:73:VAL:HG12	7:G:133:THR:HB	1.91	0.51
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.92	0.51
11:K:35:ILE:HB	11:K:45:MET:CE	2.41	0.51
6:F:216:SER:HB3	6:F:219:GLU:HB2	1.93	0.50
6:T:216:SER:HB3	6:T:219:GLU:HB2	1.93	0.50
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.92	0.50
11:Y:73:ARG:NH2	11:Y:73:ARG:HG3	2.26	0.50
12:Z:49:ASN:HD21	12:Z:211:GLY:HA2	1.75	0.50
7:G:34:LEU:C	7:G:34:LEU:HD23	2.32	0.50
11:K:67:GLU:CB	11:K:72:GLU:O	2.60	0.50
7:U:73:VAL:HG12	7:U:133:THR:HB	1.93	0.50
13:M:43:ILE:HG12	13:M:43:ILE:O	2.11	0.50
13:M:97:ALA:HA	13:M:130:VAL:HG21	1.94	0.50
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.27	0.50
4:D:51:LEU:HD12	4:D:52:GLU:N	2.27	0.49
8:H:29:LYS:HE2	12:Z:194:ARG:NH2	2.27	0.49
7:U:83:ASN:C	7:U:83:ASN:HD22	2.14	0.49
3:C:202:GLN:CG	3:C:203:THR:H	2.25	0.49
4:R:185:LEU:O	4:R:189:GLU:HG3	2.13	0.49
1:O:119:GLN:O	1:O:122:THR:HB	2.13	0.49
7:G:78:ILE:N	7:G:79:PRO:CD	2.76	0.49
3:C:201:VAL:HG13	3:C:202:GLN:N	2.27	0.48
3:Q:202:GLN:CG	3:Q:203:THR:H	2.26	0.48
11:K:67:GLU:HA	11:K:72:GLU:O	2.13	0.48
11:Y:35:ILE:HB	11:Y:45:MET:CE	2.44	0.48
3:Q:38:ASN:HD22	3:Q:38:ASN:N	2.12	0.48
7:U:34:LEU:C	7:U:34:LEU:HD23	2.34	0.48
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.79	0.48
5:E:68:HIS:CD2	5:E:101:LYS:HE2	2.49	0.48
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.96	0.48
1:A:83:ARG:HE	7:G:114:ASN:ND2	2.12	0.48
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.95	0.48
4:D:77:ALA:O	4:D:81:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:83:ARG:HE	7:U:114:ASN:ND2	2.12	0.48
7:U:78:ILE:N	7:U:79:PRO:CD	2.76	0.47
1:A:83:ARG:HE	7:G:114:ASN:HD21	1.62	0.47
4:R:51:LEU:HD12	4:R:52:GLU:N	2.29	0.47
6:T:123:ASN:C	6:T:123:ASN:ND2	2.67	0.47
5:S:70:GLY:HA3	5:S:221:PHE:CE2	2.49	0.47
3:C:38:ASN:HD22	3:C:38:ASN:N	2.11	0.47
10:J:3:ILE:HD12	10:J:176:PHE:CG	2.50	0.47
3:Q:160:GLN:HE21	3:Q:160:GLN:CA	2.16	0.47
11:Y:69:ARG:CG	11:Y:69:ARG:NH1	2.73	0.47
1:A:119:GLN:O	1:A:122:THR:HB	2.14	0.47
2:B:95:GLN:NE2	9:I:71:ASN:HD22	2.11	0.47
6:F:123:ASN:C	6:F:123:ASN:ND2	2.63	0.47
6:T:155:GLY:HA3	7:U:59:THR:HG21	1.97	0.47
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.63	0.47
3:C:202:GLN:CG	3:C:203:THR:N	2.78	0.47
8:V:84:LYS:HG3	8:V:85:GLN:N	2.29	0.47
9:W:36:SER:HB2	10:X:126:VAL:HG11	1.96	0.47
1:A:149:GLN:O	1:A:156:TYR:HA	2.15	0.47
1:O:149:GLN:O	1:O:156:TYR:HA	2.15	0.47
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.30	0.47
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.97	0.46
8:H:210:THR:HG21	9:I:167:SER:HB3	1.96	0.46
4:R:77:ALA:O	4:R:81:ILE:HG12	2.15	0.46
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.81	0.46
12:L:147:MET:N	12:L:148:PRO:HD2	2.30	0.46
2:P:42:GLY:HA2	2:P:145:TYR:CE1	2.50	0.46
10:X:91:SER:HA	10:X:94:SER:OG	2.16	0.46
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.96	0.46
1:O:55:LEU:HB3	7:U:159:ALA:O	2.16	0.46
1:O:115:ALA:HB1	1:O:154:GLY:O	2.16	0.46
5:S:155:LEU:HD13	5:S:158:THR:HB	1.98	0.46
6:T:156:TYR:CE2	7:U:55:LEU:HD23	2.51	0.46
5:E:70:GLY:HA3	5:E:221:PHE:CE2	2.51	0.46
12:L:18:GLU:O	12:L:119:LYS:HA	2.16	0.46
4:D:185:LEU:O	4:D:189:GLU:HG3	2.15	0.46
13:M:156:ARG:HH11	8:V:165:ASN:HD22	1.62	0.46
4:D:30:ILE:HD12	4:D:196:LEU:HG	1.97	0.46
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.63	0.46
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.98	0.46
10:X:3:ILE:HD12	10:X:176:PHE:CG	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:25:ILE:HD11	11:Y:134:THR:HG21	1.97	0.46
2:B:42:GLY:HA2	2:B:145:TYR:CE1	2.51	0.46
4:D:32:ILE:HD12	4:D:192:VAL:HG23	1.98	0.46
7:G:83:ASN:C	7:G:83:ASN:HD22	2.20	0.46
5:S:68:HIS:CD2	5:S:101:LYS:HE2	2.52	0.45
5:S:118:ASN:N	5:S:118:ASN:HD22	2.13	0.45
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.51	0.45
5:S:109:HIS:HB3	6:T:82:ARG:NH2	2.31	0.45
4:R:30:ILE:HD12	4:R:196:LEU:HG	1.98	0.45
4:R:32:ILE:HD12	4:R:192:VAL:HG23	1.98	0.45
8:H:19:ARG:NH1	8:H:167:LEU:O	2.49	0.45
8:H:84:LYS:HG3	8:H:85:GLN:N	2.30	0.45
17:X:201:MES:H62	11:Y:98:GLY:HA3	1.98	0.45
5:E:155:LEU:HD13	5:E:158:THR:HB	1.99	0.45
2:P:95:GLN:NE2	9:W:71:ASN:HD22	2.14	0.45
4:R:51:LEU:HD12	4:R:51:LEU:C	2.37	0.45
7:U:106:ASP:HB3	7:U:146:TYR:CZ	2.51	0.45
4:D:51:LEU:HD12	4:D:51:LEU:C	2.37	0.45
5:E:118:ASN:N	5:E:118:ASN:HD22	2.14	0.45
9:I:7:ASN:HA	9:I:29:GLY:O	2.17	0.45
9:I:94:LEU:HD11	9:I:106:PRO:HG2	1.98	0.45
12:L:13:LEU:HD12	12:L:14:GLY:N	2.32	0.45
4:R:149:HIS:O	4:R:156:PHE:HA	2.17	0.45
5:S:206:THR:OG1	5:S:209:ASN:HB2	2.17	0.45
13:M:96:LEU:O	13:M:100:MET:HG2	2.18	0.44
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.99	0.44
3:Q:202:GLN:CG	3:Q:203:THR:N	2.79	0.44
9:W:65:MET:CE	9:W:93:SER:HB3	2.47	0.44
2:B:8:ARG:HD2	3:C:4:ARG:NH2	2.32	0.44
10:J:36:ARG:NH1	10:J:58:GLU:OE2	2.51	0.44
9:I:171:LEU:HD11	9:I:201:MET:HB3	1.99	0.44
13:M:27:LEU:HB2	13:M:192:SER:HB3	2.00	0.44
5:S:62:ILE:HG21	5:S:213:ALA:HB2	1.99	0.44
11:Y:25:TRP:CZ3	12:Z:144:SER:HA	2.53	0.44
1:A:44:VAL:HG23	1:A:211:LEU:HD21	1.99	0.44
5:E:226:GLY:O	5:E:229:VAL:HG22	2.18	0.44
1:O:44:VAL:HG23	1:O:211:LEU:HD21	1.98	0.44
9:W:7:ASN:HA	9:W:29:GLY:O	2.17	0.44
10:X:60:ILE:O	10:X:64:ILE:HG12	2.17	0.44
11:Y:73:ARG:HH21	11:Y:73:ARG:HG3	1.82	0.44
13:M:127:LEU:HG	13:M:142:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.65	0.44
2:P:3:ARG:NH2	4:R:3:GLY:HA2	2.33	0.44
5:E:62:ILE:HG21	5:E:213:ALA:HB2	2.00	0.44
5:S:226:GLY:O	5:S:229:VAL:HG22	2.18	0.44
12:Z:13:LEU:HD12	12:Z:14:GLY:N	2.32	0.44
2:B:139:TYR:CD1	2:B:224:VAL:HG21	2.54	0.43
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.98	0.43
1:A:115:ALA:HB1	1:A:154:GLY:O	2.17	0.43
9:I:65:MET:CE	9:I:93:SER:HB3	2.49	0.43
5:S:44:VAL:HG23	5:S:188:LEU:HD13	1.99	0.43
5:E:127:TYR:O	5:E:148:PRO:CB	2.67	0.43
5:E:206:THR:OG1	5:E:209:ASN:HB2	2.19	0.43
11:K:37:ILE:HG23	11:K:60:GLY:HA2	2.00	0.43
9:W:94:LEU:HD11	9:W:106:PRO:HG2	1.99	0.43
12:Z:18:GLU:O	12:Z:119:LYS:HA	2.19	0.43
4:R:37:GLY:HA2	4:R:145:TYR:CE1	2.53	0.43
8:V:112:SER:OG	8:V:120:ASP:HB2	2.19	0.43
3:C:201:VAL:O	3:C:202:GLN:CB	2.66	0.43
11:K:25:TRP:CZ3	12:L:144:SER:HA	2.54	0.43
7:G:34:LEU:HD23	7:G:35:ALA:N	2.34	0.43
2:B:146:GLN:HG2	3:C:57:ILE:HG21	2.01	0.43
5:E:9:THR:CG2	5:E:119:THR:HA	2.48	0.43
13:M:43:ILE:HG21	13:M:64:GLU:HG2	2.01	0.42
8:V:214:LYS:O	9:W:197:ARG:HA	2.19	0.42
9:W:171:LEU:HD11	9:W:201:MET:HB3	2.01	0.42
5:E:44:VAL:HG23	5:E:188:LEU:HD13	2.00	0.42
10:X:36:ARG:NH1	10:X:58:GLU:OE2	2.52	0.42
9:I:62:LEU:CD1	9:I:104:VAL:HG21	2.49	0.42
2:B:180:LYS:O	2:B:183:MET:HB2	2.19	0.42
2:B:204:ALA:O	2:B:209:ARG:NH2	2.52	0.42
3:C:71:LEU:C	3:C:71:LEU:HD23	2.39	0.42
4:D:149:HIS:O	4:D:156:PHE:HA	2.19	0.42
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.55	0.42
12:L:196:ILE:HG12	8:V:24:PRO:O	2.18	0.42
13:M:26:ASN:HA	13:M:39:VAL:O	2.19	0.42
7:U:34:LEU:HD23	7:U:35:ALA:N	2.35	0.42
2:B:213:ALA:HA	2:B:227:LYS:O	2.19	0.42
1:O:83:ARG:HE	7:U:114:ASN:HD21	1.67	0.42
2:P:95:GLN:HE21	9:W:68:TYR:HA	1.84	0.42
14:N:14:LEU:HD11	14:N:100:ALA:HB3	2.01	0.42
5:S:197:SER:HA	5:S:200:LEU:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:111:ILE:HD12	9:W:189:ILE:HG22	2.01	0.42
3:C:46:ARG:NH1	3:C:206:LYS:HG2	2.35	0.42
12:L:195:HIS:HD2	12:L:197:GLN:H	1.66	0.42
9:W:62:LEU:CD1	9:W:104:VAL:HG21	2.49	0.42
5:S:200:LEU:HD13	5:S:204:SER:HA	2.01	0.42
7:U:227:LEU:HB3	7:U:231:ASN:HB2	2.01	0.42
11:Y:73:ARG:HH21	11:Y:73:ARG:HG2	1.84	0.42
7:G:147:LYS:O	7:G:154:TYR:HA	2.20	0.42
2:P:134:PHE:O	2:P:149:THR:HA	2.20	0.42
2:P:139:TYR:CD1	2:P:224:VAL:HG21	2.55	0.42
9:W:20:VAL:HG23	9:W:189:ILE:HB	2.02	0.42
11:Y:37:ILE:HG23	11:Y:60:GLY:HA2	2.01	0.42
10:J:60:ILE:O	10:J:64:ILE:HG12	2.19	0.42
4:D:37:GLY:HA2	4:D:145:TYR:CE1	2.55	0.41
5:E:197:SER:HA	5:E:200:LEU:CD1	2.49	0.41
8:H:112:SER:OG	8:H:120:ASP:HB2	2.20	0.41
13:M:159:VAL:HG23	13:M:159:VAL:O	2.20	0.41
5:E:200:LEU:HD13	5:E:204:SER:HA	2.01	0.41
7:G:52:ASP:HB3	7:G:55:LEU:HG	2.02	0.41
7:G:73:VAL:CG1	7:G:133:THR:HB	2.50	0.41
3:Q:46:ARG:NH1	3:Q:206:LYS:HG2	2.35	0.41
5:S:9:THR:CG2	5:S:119:THR:HA	2.50	0.41
5:S:71:LEU:HA	5:S:132:LEU:O	2.19	0.41
11:Y:41:LEU:HD23	11:Y:41:LEU:HA	1.87	0.41
7:U:147:LYS:O	7:U:154:TYR:HA	2.20	0.41
3:Q:51:LYS:HB3	18:Q:305:HOH:O	2.20	0.41
7:G:239:ILE:O	7:G:242:GLN:HB3	2.21	0.41
5:S:77:ALA:N	5:S:78:PRO:CD	2.83	0.41
9:I:111:ILE:HD12	9:I:189:ILE:HG22	2.02	0.41
11:K:25:TRP:CH2	12:L:144:SER:HA	2.55	0.41
11:K:41:LEU:HD23	11:K:41:LEU:HA	1.87	0.41
3:Q:71:LEU:C	3:Q:71:LEU:HD23	2.41	0.41
12:Z:152:ASN:O	12:Z:156:PHE:HA	2.20	0.41
5:E:71:LEU:HA	5:E:132:LEU:O	2.21	0.41
7:U:73:VAL:CG1	7:U:133:THR:HB	2.51	0.41
2:B:134:PHE:O	2:B:149:THR:HA	2.20	0.41
5:E:80:ALA:HB2	5:E:129:VAL:HG21	2.03	0.41
6:F:116:VAL:HG21	6:F:147:LEU:HD21	2.02	0.41
7:G:115:LEU:HD12	7:G:115:LEU:HA	1.93	0.41
10:J:91:SER:HA	10:J:94:SER:OG	2.20	0.41
4:R:97:GLU:OE1	12:Z:75:TYR:OH	2.26	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:52:ASP:HB3	7:U:55:LEU:HG	2.02	0.41
7:G:106:ASP:HB3	7:G:146:TYR:CZ	2.56	0.41
8:H:102:GLY:HA2	8:H:178:MET:SD	2.61	0.41
3:Q:160:GLN:HA	3:Q:160:GLN:NE2	2.22	0.41
5:S:80:ALA:HB2	5:S:129:VAL:HG21	2.03	0.41
6:F:87:ARG:HG2	6:F:115:TYR:CD2	2.56	0.41
12:L:152:ASN:O	12:L:156:PHE:HA	2.21	0.41
9:W:167:SER:O	9:W:171:LEU:HB2	2.21	0.41
5:E:77:ALA:N	5:E:78:PRO:CD	2.84	0.40
9:I:20:VAL:HG23	9:I:189:ILE:HB	2.02	0.40
7:U:78:ILE:HG22	7:U:79:PRO:HD3	2.03	0.40
7:G:227:LEU:HB3	7:G:231:ASN:HB2	2.03	0.40
12:L:100:LYS:HD3	12:L:105:TYR:CZ	2.56	0.40
4:R:58:LYS:HE2	4:R:74:THR:HG21	2.03	0.40
6:T:87:ARG:HG2	6:T:115:TYR:CD2	2.56	0.40
12:Z:13:LEU:HD12	12:Z:13:LEU:C	2.42	0.40
6:F:78:ILE:N	6:F:79:PRO:CD	2.85	0.40
1:O:37:ILE:HD12	1:O:192:ALA:HB2	2.03	0.40
1:O:122:THR:CG2	2:P:128:ARG:HH21	2.34	0.40
2:P:8:ARG:HD2	3:Q:4:ARG:NH2	2.36	0.40
2:P:55:LEU:HD12	2:P:55:LEU:HA	1.98	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%)	240 (97%)	5 (2%)	3 (1%)	13	27
1	O	248/250 (99%)	240 (97%)	5 (2%)	3 (1%)	13	27
2	B	242/258 (94%)	234 (97%)	6 (2%)	2 (1%)	19	39
2	P	242/258 (94%)	234 (97%)	6 (2%)	2 (1%)	19	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	238/254 (94%)	225 (94%)	10 (4%)	3 (1%)	12	24
3	Q	238/254 (94%)	225 (94%)	10 (4%)	3 (1%)	12	24
4	D	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
4	R	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
5	E	229/234 (98%)	217 (95%)	12 (5%)	0	100	100
5	S	229/234 (98%)	216 (94%)	13 (6%)	0	100	100
6	F	241/288 (84%)	232 (96%)	8 (3%)	1 (0%)	34	57
6	T	241/288 (84%)	232 (96%)	8 (3%)	1 (0%)	34	57
7	G	239/252 (95%)	231 (97%)	7 (3%)	1 (0%)	34	57
7	U	239/252 (95%)	229 (96%)	9 (4%)	1 (0%)	34	57
8	H	219/231 (95%)	215 (98%)	4 (2%)	0	100	100
8	V	219/231 (95%)	215 (98%)	4 (2%)	0	100	100
9	I	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
9	W	202/205 (98%)	193 (96%)	9 (4%)	0	100	100
10	J	193/198 (98%)	190 (98%)	1 (0%)	2 (1%)	15	32
10	X	193/198 (98%)	190 (98%)	1 (0%)	2 (1%)	15	32
11	K	209/211 (99%)	202 (97%)	7 (3%)	0	100	100
11	Y	209/211 (99%)	202 (97%)	7 (3%)	0	100	100
12	L	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
12	Z	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
13	M	231/246 (94%)	223 (96%)	8 (4%)	0	100	100
13	a	231/246 (94%)	223 (96%)	8 (4%)	0	100	100
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	b	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
All	All	6272/6610 (95%)	6061 (97%)	187 (3%)	24 (0%)	34	57

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	202	GLN
6	F	203	ASN
3	Q	202	GLN
6	T	203	ASN
3	C	239	GLN

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Mol	Chain	Res	Type
1	O	2	THR
3	Q	239	GLN
1	A	2	THR
1	A	50	LYS
1	A	166	LYS
3	C	205	ALA
1	O	166	LYS
3	Q	205	ALA
2	B	221	ASP
1	O	50	LYS
2	B	51	VAL
10	J	2	ASP
2	P	51	VAL
2	P	221	ASP
10	X	2	ASP
7	G	51	PRO
10	J	9	VAL
7	U	51	PRO
10	X	9	VAL

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	209/209 (100%)	201 (96%)	8 (4%)	33	59
1	O	209/209 (100%)	201 (96%)	8 (4%)	33	59
2	B	203/216 (94%)	188 (93%)	15 (7%)	13	28
2	P	203/216 (94%)	188 (93%)	15 (7%)	13	28
3	C	212/226 (94%)	196 (92%)	16 (8%)	13	27
3	Q	212/226 (94%)	196 (92%)	16 (8%)	13	27
4	D	194/215 (90%)	180 (93%)	14 (7%)	14	29
4	R	194/215 (90%)	180 (93%)	14 (7%)	14	29
5	E	190/193 (98%)	172 (90%)	18 (10%)	8	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	S	190/193 (98%)	172 (90%)	18 (10%)	8	16
6	F	201/239 (84%)	184 (92%)	17 (8%)	10	21
6	T	201/239 (84%)	185 (92%)	16 (8%)	12	24
7	G	206/210 (98%)	192 (93%)	14 (7%)	16	32
7	U	206/210 (98%)	192 (93%)	14 (7%)	16	32
8	H	180/189 (95%)	172 (96%)	8 (4%)	28	53
8	V	180/189 (95%)	171 (95%)	9 (5%)	24	47
9	I	172/173 (99%)	165 (96%)	7 (4%)	30	56
9	W	172/173 (99%)	165 (96%)	7 (4%)	30	56
10	J	173/175 (99%)	164 (95%)	9 (5%)	23	46
10	X	173/175 (99%)	166 (96%)	7 (4%)	31	57
11	K	168/168 (100%)	161 (96%)	7 (4%)	30	55
11	Y	168/168 (100%)	161 (96%)	7 (4%)	30	55
12	L	185/185 (100%)	176 (95%)	9 (5%)	25	48
12	Z	185/185 (100%)	177 (96%)	8 (4%)	29	54
13	M	199/208 (96%)	186 (94%)	13 (6%)	17	34
13	a	199/208 (96%)	186 (94%)	13 (6%)	17	34
14	N	162/162 (100%)	158 (98%)	4 (2%)	47	73
14	b	162/162 (100%)	158 (98%)	4 (2%)	47	73
All	All	5308/5536 (96%)	4993 (94%)	315 (6%)	19	39

All (315) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	29	LYS
1	A	59	GLU
1	A	61	LEU
1	A	122	THR
1	A	157	PHE
1	A	228	PRO
1	A	231	LYS
2	B	3	ARG
2	B	8	ARG
2	B	17	ARG

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Mol	Chain	Res	Type
2	B	50	LYS
2	B	56	LEU
2	B	58	GLN
2	B	62	THR
2	B	79	LEU
2	B	119	GLN
2	B	180	LYS
2	B	184	LYS
2	B	185	VAL
2	B	191	LEU
2	B	194	LYS
2	B	197	SER
3	C	4	ARG
3	C	26	LYS
3	C	38	ASN
3	C	49	THR
3	C	51	LYS
3	C	61	LYS
3	C	138	PRO
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	175	LYS
3	C	180	LYS
3	C	228	ASN
3	C	232	THR
3	C	235	GLU
3	C	240	GLU
4	D	40	LEU
4	D	51	LEU
4	D	54	ASP
4	D	60	VAL
4	D	117	GLU
4	D	125	LEU
4	D	176	LEU
4	D	190	LEU
4	D	193	LEU
4	D	202	GLU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU

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Mol	Chain	Res	Type
5	E	3	ASN
5	E	4	ASN
5	E	9	THR
5	E	25	LEU
5	E	29	LYS
5	E	55	LEU
5	E	71	LEU
5	E	87	LEU
5	E	92	ASN
5	E	116	GLN
5	E	118	ASN
5	E	147	GLN
5	E	184	ASN
5	E	186	ASP
5	E	188	LEU
5	E	202	ASP
5	E	207	VAL
5	E	219	THR
6	F	14	ASP
6	F	47	GLU
6	F	58	GLN
6	F	94	SER
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	172	LEU
6	F	181	GLU
6	F	198	LEU
6	F	203	ASN
6	F	206	LYS
6	F	214	TRP
6	F	221	ASN
6	F	231	LEU
6	F	240	GLN
6	F	244	ASN
7	G	26	THR
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	122	ARG
7	G	125	MET
7	G	166	GLN

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Mol	Chain	Res	Type
7	G	171	THR
7	G	178	LYS
7	G	181	LYS
7	G	215	GLU
7	G	230	GLU
7	G	235	ARG
7	G	236	LEU
8	H	3	ILE
8	H	30	ASN
8	H	34	LEU
8	H	68	LEU
8	H	113	ILE
8	H	127	LEU
8	H	153	LYS
8	H	191	LEU
9	I	31	GLN
9	I	114	LYS
9	I	117	LYS
9	I	123	PHE
9	I	151	SER
9	I	171	LEU
9	I	182	TRP
10	J	22	THR
10	J	23	ARG
10	J	35	THR
10	J	75	LEU
10	J	78	GLN
10	J	91	SER
10	J	144	LEU
10	J	163	LEU
10	J	174	MET
11	K	4	LEU
11	K	9	GLN
11	K	31	VAL
11	K	35	ILE
11	K	41	LEU
11	K	73	ARG
11	K	148	LEU
12	L	1	GLN
12	L	11	THR
12	L	13	LEU
12	L	23	LEU

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Mol	Chain	Res	Type
12	L	49	ASN
12	L	137	ARG
12	L	150	LEU
12	L	157	LYS
12	L	167	LYS
13	M	2	GLN
13	M	10	SER
13	M	43	ILE
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	106	LYS
13	M	161	ARG
13	M	187	ARG
13	M	192	SER
13	M	212	LEU
13	M	213	GLN
13	M	215	GLU
14	N	9	LYS
14	N	36	ARG
14	N	119	VAL
14	N	144	GLU
1	O	2	THR
1	O	29	LYS
1	O	59	GLU
1	O	61	LEU
1	O	122	THR
1	O	157	PHE
1	O	228	PRO
1	O	231	LYS
2	P	3	ARG
2	P	8	ARG
2	P	17	ARG
2	P	50	LYS
2	P	56	LEU
2	P	58	GLN
2	P	62	THR
2	P	79	LEU
2	P	119	GLN
2	P	180	LYS
2	P	184	LYS
2	P	185	VAL

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Mol	Chain	Res	Type
2	P	191	LEU
2	P	194	LYS
2	P	197	SER
3	Q	4	ARG
3	Q	26	LYS
3	Q	38	ASN
3	Q	49	THR
3	Q	51	LYS
3	Q	61	LYS
3	Q	138	PRO
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	175	LYS
3	Q	180	LYS
3	Q	228	ASN
3	Q	232	THR
3	Q	235	GLU
3	Q	240	GLU
4	R	40	LEU
4	R	51	LEU
4	R	60	VAL
4	R	117	GLU
4	R	125	LEU
4	R	176	LEU
4	R	182	SER
4	R	190	LEU
4	R	193	LEU
4	R	202	GLU
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	3	ASN
5	S	4	ASN
5	S	9	THR
5	S	25	LEU
5	S	29	LYS
5	S	55	LEU
5	S	71	LEU
5	S	87	LEU
5	S	92	ASN

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Mol	Chain	Res	Type
5	S	116	GLN
5	S	118	ASN
5	S	147	GLN
5	S	184	ASN
5	S	186	ASP
5	S	188	LEU
5	S	202	ASP
5	S	207	VAL
5	S	219	THR
6	T	14	ASP
6	T	47	GLU
6	T	58	GLN
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	172	LEU
6	T	181	GLU
6	T	198	LEU
6	T	203	ASN
6	T	206	LYS
6	T	214	TRP
6	T	221	ASN
6	T	231	LEU
6	T	240	GLN
6	T	244	ASN
7	U	26	THR
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	122	ARG
7	U	125	MET
7	U	166	GLN
7	U	171	THR
7	U	178	LYS
7	U	181	LYS
7	U	215	GLU
7	U	230	GLU
7	U	235	ARG
7	U	236	LEU
8	V	3	ILE
8	V	30	ASN
8	V	34	LEU

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Mol	Chain	Res	Type
8	V	43	CYS
8	V	68	LEU
8	V	113	ILE
8	V	127	LEU
8	V	153	LYS
8	V	191	LEU
9	W	31	GLN
9	W	114	LYS
9	W	117	LYS
9	W	123	PHE
9	W	151	SER
9	W	171	LEU
9	W	182	TRP
10	X	35	THR
10	X	75	LEU
10	X	78	GLN
10	X	91	SER
10	X	144	LEU
10	X	163	LEU
10	X	174	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	31	VAL
11	Y	35	ILE
11	Y	41	LEU
11	Y	73	ARG
11	Y	148	LEU
12	Z	1	GLN
12	Z	11	THR
12	Z	13	LEU
12	Z	23	LEU
12	Z	49	ASN
12	Z	150	LEU
12	Z	157	LYS
12	Z	167	LYS
13	a	2	GLN
13	a	10	SER
13	a	43	ILE
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	106	LYS

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Mol	Chain	Res	Type
13	a	161	ARG
13	a	187	ARG
13	a	192	SER
13	a	212	LEU
13	a	213	GLN
13	a	215	GLU
14	b	9	LYS
14	b	36	ARG
14	b	119	VAL
14	b	144	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (135) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
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	100	ASN
4	D	198	GLN
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	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

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Mol	Chain	Res	Type
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	175	ASN
7	G	186	ASN
8	H	22	GLN
8	H	30	ASN
8	H	57	GLN
8	H	66	HIS
8	H	165	ASN
8	H	172	ASN
8	H	189	ASN
9	I	88	GLN
10	J	55	GLN
10	J	118	GLN
10	J	146	HIS
10	J	147	HIS
10	J	191	GLN
11	K	9	GLN
11	K	85	ASN
11	K	176	ASN
12	L	3	ASN
12	L	49	ASN
12	L	80	ASN
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	69	GLN
14	N	161	GLN
1	O	94	HIS
2	P	20	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN

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Mol	Chain	Res	Type
2	P	155	ASN
2	P	176	GLN
3	Q	17	GLN
3	Q	38	ASN
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	160	ASN
4	R	198	GLN
4	R	225	ASN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
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	175	ASN
7	U	186	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	88	GLN
10	X	55	GLN

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Mol	Chain	Res	Type
10	X	118	GLN
10	X	147	HIS
10	X	191	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	143	ASN
11	Y	176	ASN
12	Z	1	GLN
12	Z	3	ASN
12	Z	36	ASN
12	Z	49	ASN
12	Z	80	ASN
12	Z	158	ASN
13	a	18	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	38	HIS
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 ⓘ

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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
15	SEM	g	2	15	12,13,14	1.80	1 (8%)	11,15,17	1.21	1 (9%)
15	0A1	g	3	15	12,13,14	1.92	1 (8%)	13,16,18	0.82	0
15	0A1	h	3	15	12,13,14	2.42	2 (16%)	13,16,18	1.08	2 (15%)
15	SEM	e	2	15	12,13,14	1.67	1 (8%)	11,15,17	0.71	0
15	0A1	f	3	15	12,13,14	2.42	3 (25%)	13,16,18	1.15	2 (15%)
15	0A1	e	3	15	12,13,14	2.26	1 (8%)	13,16,18	1.17	1 (7%)
15	SEM	h	2	15	12,13,14	1.84	1 (8%)	11,15,17	0.64	0
15	SEM	f	2	15	12,13,14	1.57	1 (8%)	11,15,17	0.49	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
15	SEM	g	2	15	-	1/6/8/10	0/1/1/1
15	0A1	g	3	15	-	2/7/8/10	0/1/1/1
15	0A1	h	3	15	-	2/7/8/10	0/1/1/1
15	SEM	e	2	15	-	0/6/8/10	0/1/1/1
15	0A1	f	3	15	-	2/7/8/10	0/1/1/1
15	0A1	e	3	15	-	2/7/8/10	0/1/1/1
15	SEM	h	2	15	-	1/6/8/10	0/1/1/1
15	SEM	f	2	15	-	1/6/8/10	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	e	3	0A1	CB-CG	-6.79	1.35	1.51
15	f	3	0A1	CB-CG	-6.76	1.35	1.51
15	h	3	0A1	CB-CG	-6.66	1.35	1.51
15	h	2	SEM	C'-C1'	-5.83	1.36	1.50
15	g	3	0A1	CB-CG	-5.73	1.37	1.51
15	g	2	SEM	C'-C1'	-5.68	1.37	1.50
15	e	2	SEM	C'-C1'	-5.27	1.38	1.50
15	f	2	SEM	C'-C1'	-4.89	1.39	1.50
15	h	3	0A1	OH-CZ	-2.38	1.32	1.37
15	f	3	0A1	CD1-CG	-2.13	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	f	3	0A1	OH-CZ	-2.11	1.33	1.37

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	g	2	SEM	C'-OG-CB	-2.61	106.73	112.67
15	h	3	0A1	CM-OH-CZ	-2.47	112.16	117.51
15	h	3	0A1	CB-CA-C	-2.29	107.17	111.47
15	f	3	0A1	CB-CA-C	-2.26	107.23	111.47
15	f	3	0A1	CM-OH-CZ	-2.14	112.87	117.51
15	e	3	0A1	CB-CA-C	-2.11	107.52	111.47

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	h	2	SEM	CA-CB-OG-C'
15	f	3	0A1	C-CA-CB-CG
15	e	3	0A1	N-CA-CB-CG
15	g	3	0A1	N-CA-CB-CG
15	h	3	0A1	N-CA-CB-CG
15	f	2	SEM	N-CA-CB-OG
15	g	2	SEM	CA-CB-OG-C'
15	f	3	0A1	N-CA-CB-CG
15	e	3	0A1	C-CA-CB-CG
15	g	3	0A1	C-CA-CB-CG
15	h	3	0A1	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 7 are monoatomic - leaving 5 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	f	101	-	12,12,12	0.79	0	14,16,16	0.54	0
17	MES	X	201	-	12,12,12	0.74	0	14,16,16	0.36	0
17	MES	b	201	-	12,12,12	0.82	0	14,16,16	0.93	1 (7%)
17	MES	H	301	-	12,12,12	0.73	0	14,16,16	0.39	0
17	MES	V	301	-	12,12,12	0.73	0	14,16,16	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	MES	f	101	-	-	5/6/14/14	0/1/1/1
17	MES	X	201	-	-	2/6/14/14	0/1/1/1
17	MES	b	201	-	-	0/6/14/14	0/1/1/1
17	MES	H	301	-	-	2/6/14/14	0/1/1/1
17	MES	V	301	-	-	1/6/14/14	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	201	MES	O1S-S-C8	-3.00	103.31	106.92

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	f	101	MES	C8-C7-N4-C3
17	f	101	MES	C7-C8-S-O2S
17	f	101	MES	C7-C8-S-O3S
17	V	301	MES	N4-C7-C8-S

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Mol	Chain	Res	Type	Atoms
17	H	301	MES	C8-C7-N4-C3
17	H	301	MES	C8-C7-N4-C5
17	f	101	MES	C7-C8-S-O1S
17	f	101	MES	C8-C7-N4-C5
17	X	201	MES	C7-C8-S-O2S
17	X	201	MES	C8-C7-N4-C5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	X	201	MES	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%)	-0.44	4 (1%) 72 68	45, 60, 95, 136	0
1	O	250/250 (100%)	-0.32	6 (2%) 59 53	49, 67, 104, 131	0
2	B	244/258 (94%)	-0.25	8 (3%) 46 39	43, 64, 121, 166	0
2	P	244/258 (94%)	-0.20	13 (5%) 26 20	48, 67, 122, 153	0
3	C	240/254 (94%)	-0.25	11 (4%) 32 26	44, 66, 126, 155	0
3	Q	240/254 (94%)	-0.02	18 (7%) 14 10	53, 80, 142, 171	0
4	D	235/260 (90%)	-0.45	1 (0%) 92 91	47, 69, 101, 134	0
4	R	235/260 (90%)	-0.30	2 (0%) 84 82	51, 72, 109, 134	0
5	E	231/234 (98%)	-0.31	5 (2%) 62 56	50, 71, 103, 129	0
5	S	231/234 (98%)	-0.20	9 (3%) 39 32	49, 77, 113, 132	0
6	F	243/288 (84%)	-0.39	6 (2%) 57 51	42, 65, 106, 135	0
6	T	243/288 (84%)	-0.26	7 (2%) 51 45	47, 71, 113, 136	0
7	G	241/252 (95%)	-0.45	6 (2%) 57 51	43, 62, 98, 133	0
7	U	241/252 (95%)	-0.46	3 (1%) 79 76	46, 63, 97, 118	0
8	H	221/231 (95%)	-0.49	2 (0%) 84 82	44, 58, 84, 135	0
8	V	221/231 (95%)	-0.48	2 (0%) 84 82	44, 63, 84, 130	0
9	I	204/205 (99%)	-0.67	2 (0%) 82 80	41, 55, 82, 111	0
9	W	204/205 (99%)	-0.56	2 (0%) 82 80	40, 57, 82, 112	0
10	J	195/198 (98%)	-0.54	0 100 100	38, 55, 82, 118	0
10	X	195/198 (98%)	-0.62	3 (1%) 73 70	43, 58, 80, 130	0
11	K	211/211 (100%)	-0.50	1 (0%) 91 89	42, 55, 76, 101	0
11	Y	211/211 (100%)	-0.54	2 (0%) 84 82	45, 57, 81, 102	0
12	L	222/222 (100%)	-0.66	0 100 100	39, 58, 81, 91	0
12	Z	222/222 (100%)	-0.59	1 (0%) 91 89	41, 59, 87, 105	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.59	4 (1%) 70 66	41, 58, 84, 121	0
13	a	233/246 (94%)	-0.59	3 (1%) 77 73	43, 58, 80, 127	0
14	N	196/196 (100%)	-0.62	1 (0%) 91 89	40, 54, 80, 111	0
14	b	196/196 (100%)	-0.62	1 (0%) 91 89	41, 54, 84, 104	0
15	e	0/4	-	-	-	-
15	f	0/4	-	-	-	-
15	g	0/4	-	-	-	-
15	h	0/4	-	-	-	-
All	All	6332/6626 (95%)	-0.43	123 (1%) 66 62	38, 62, 104, 171	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	V	222	ASP	7.0
8	H	222	ASP	6.9
2	B	219	ALA	6.7
2	P	219	ALA	6.2
3	Q	49	THR	6.1
13	a	233	ILE	6.0
3	C	49	THR	6.0
5	S	202	ASP	5.2
2	B	220	ASN	5.2
3	Q	203	THR	5.0
3	Q	48	SER	4.9
3	C	206	LYS	4.7
3	Q	50	LEU	4.7
3	Q	204	GLY	4.7
2	P	51	VAL	4.5
2	P	241	THR	4.5
3	C	48	SER	4.4
8	V	221	CYS	4.4
2	P	220	ASN	4.3
6	T	180	PRO	4.2
6	F	243	ILE	4.1
3	C	203	THR	4.1
5	S	204	SER	4.0
5	E	202	ASP	4.0
3	Q	235	GLU	3.9
2	P	52	THR	3.9
1	A	1	MET	3.8
1	A	2	THR	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	240	LYS	3.8
2	B	222	GLY	3.8
13	M	1	THR	3.8
1	O	250	LEU	3.6
1	A	250	LEU	3.5
2	B	221	ASP	3.5
13	M	232	LYS	3.4
9	I	1	SER	3.4
3	Q	206	LYS	3.4
2	P	240	LYS	3.4
8	H	221	CYS	3.4
3	C	50	LEU	3.3
6	T	177	ASP	3.3
11	Y	212	GLY	3.3
13	a	232	LYS	3.3
11	K	212	GLY	3.2
5	S	233	ILE	3.2
3	Q	202	GLN	3.2
3	Q	240	GLU	3.2
7	U	2	GLY	3.2
2	P	243	ILE	3.1
6	T	2	THR	3.1
5	E	233	ILE	3.1
5	S	54	GLU	3.1
6	F	205	GLU	3.1
3	Q	236	GLN	3.1
13	M	233	ILE	3.0
2	P	244	THR	3.0
1	O	249	ALA	3.0
2	P	218	GLY	3.0
13	a	1	THR	2.9
3	C	202	GLN	2.9
5	E	201	ARG	2.9
10	X	194	ASP	2.9
11	Y	106	ARG	2.8
10	X	193	ASP	2.7
5	S	225	ASP	2.7
2	P	203	SER	2.7
6	T	244	ASN	2.7
3	C	238	LYS	2.7
7	G	188	GLU	2.7
9	W	1	SER	2.7

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Mol	Chain	Res	Type	RSRZ
13	M	81	ALA	2.6
14	b	195	GLN	2.6
1	O	201	GLU	2.6
6	F	177	ASP	2.6
6	T	181	GLU	2.6
3	Q	47	ARG	2.6
5	E	54	GLU	2.6
3	C	47	ARG	2.6
7	G	241	GLU	2.5
3	Q	238	LYS	2.5
2	B	244	THR	2.4
2	B	203	SER	2.4
1	O	52	SER	2.4
3	Q	201	VAL	2.4
14	N	195	GLN	2.4
2	P	223	GLU	2.4
5	S	55	LEU	2.4
2	P	221	ASP	2.4
4	R	1	ASP	2.4
2	B	204	ALA	2.4
6	F	202	ASP	2.4
10	X	1	MET	2.4
5	S	201	ARG	2.3
7	U	241	GLU	2.3
5	S	207	VAL	2.3
7	G	179	LYS	2.3
3	Q	205	ALA	2.3
1	O	2	THR	2.3
12	Z	1	GLN	2.3
4	R	242	GLU	2.3
5	S	228	ALA	2.3
3	Q	180	LYS	2.2
7	U	222	ASP	2.2
6	T	241	LYS	2.2
7	G	178	LYS	2.2
4	D	142	ASP	2.2
6	F	203	ASN	2.2
9	W	191	LYS	2.1
3	C	240	GLU	2.1
3	Q	234	ILE	2.1
3	Q	239	GLN	2.1
3	Q	141	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	235	GLU	2.1
2	P	222	GLY	2.1
5	E	163	ARG	2.1
3	C	204	GLY	2.1
9	I	192	ASP	2.1
6	F	230	ASP	2.1
1	A	228	PRO	2.0
7	G	240	ALA	2.0
1	O	50	LYS	2.0
6	T	53	LYS	2.0
7	G	237	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
15	SEM	h	2	13/14	0.95	0.13	38,44,47,48	0
15	SEM	g	2	13/14	0.96	0.15	45,50,53,58	0
15	SEM	f	2	13/14	0.96	0.13	36,43,44,46	0
15	0A1	e	3	13/14	0.96	0.14	34,37,50,53	0
15	0A1	g	3	13/14	0.96	0.19	36,41,53,58	0
15	0A1	h	3	13/14	0.96	0.14	29,31,40,45	0
15	SEM	e	2	13/14	0.97	0.14	41,47,52,54	0
15	0A1	f	3	13/14	0.97	0.13	30,33,41,44	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(\AA^2)	Q<0.9
16	MG	H	302	1/1	0.80	0.21	101,101,101,101	0
17	MES	b	201	12/12	0.85	0.56	20,20,20,20	0
16	MG	G	301	1/1	0.94	0.18	81,81,81,81	0
16	MG	Z	301	1/1	0.96	0.15	127,127,127,127	0
17	MES	V	301	12/12	0.96	0.19	94,101,107,108	0
17	MES	X	201	12/12	0.96	0.14	79,81,88,88	0
16	MG	I	301	1/1	0.96	0.29	149,149,149,149	0
17	MES	H	301	12/12	0.97	0.17	79,95,98,99	0
16	MG	N	201	1/1	0.97	0.18	74,74,74,74	0
17	MES	f	101	12/12	0.97	0.12	66,82,89,89	0
16	MG	K	301	1/1	0.99	0.15	85,85,85,85	0
16	MG	Y	301	1/1	0.99	0.18	93,93,93,93	0

6.5 Other polymers [i](#)

There are no such residues in this entry.