Full wwPDB X-ray Structure Validation Report (i)

Jan 2, 2024 – 03:26 pm GMT

PDB ID	:	4YA9
Title	:	Yeast 20S proteasome beta2-H114D mutant in complex with Ac-LAD-ep
Authors	:	Huber, E.M.; Groll, M.
Deposited on	:	2015-02-17
Resolution	:	2.70 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 (i) 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 (1)) were used in the production of this report:

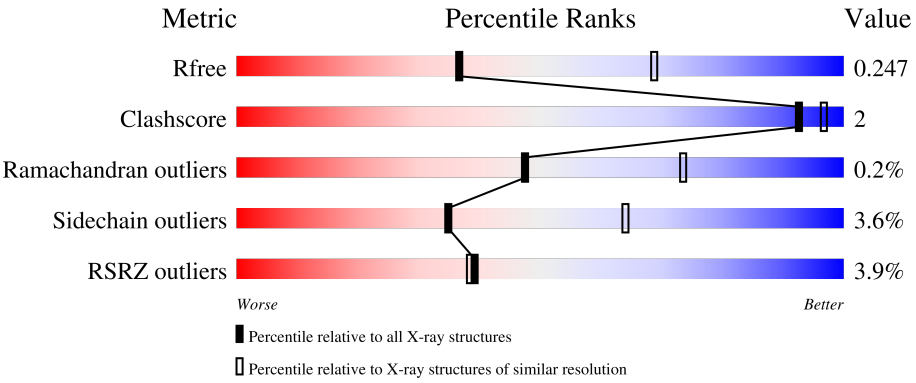
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	6% 97% ·
1	O	250	5% 97% ·
2	B	258	6% 88% 5% · 5%
2	P	258	5% 88% 5% · 5%
3	C	254	8% 87% 6% · 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	12% 87% 6% 6%
4	D	260	3% 85% 5% 10%
4	R	260	3% 84% 6% 10%
5	E	234	4% 92% 6%
5	S	234	6% 90% 8%
6	F	288	6% 80% 16%
6	T	288	6% 80% 16%
7	G	252	5% 90% 6%
7	U	252	3% 90% 6%
8	H	232	89% 6%
8	V	232	89% 6%
9	I	205	93% 6%
9	W	205	94% 5%
10	J	198	91% 6%
10	X	198	3% 91% 6%
11	K	212	92% 8%
11	Y	212	94% 6%
12	L	222	95% 5%
12	Z	222	95% 5%
13	M	246	89% 5% 5%
13	a	246	92% 5%
14	N	196	95% 5%
14	b	196	97%
15	c	5	80% 20%
15	d	5	80% 20%

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Mol	Chain	Length	Quality of chain
15	e	5	80% 20%
15	f	5	80% 20%
15	g	5	80% 20%
15	h	5	80% 20%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	ASJ	c	4	-	X	-	-

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 50343 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 subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	222	Total	C	N	O	S	0	0	0
			1682	1059	291	325	7			
8	V	222	Total	C	N	O	S	0	0	0
			1682	1059	291	325	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	114	ASP	HIS	engineered mutation	UNP P25043
V	114	ASP	HIS	engineered mutation	UNP P25043

- 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			
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	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	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	1	0
			1764	1120	305	335	4			
12	Z	222	Total	C	N	O	S	0	1	0
			1764	1120	305	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			

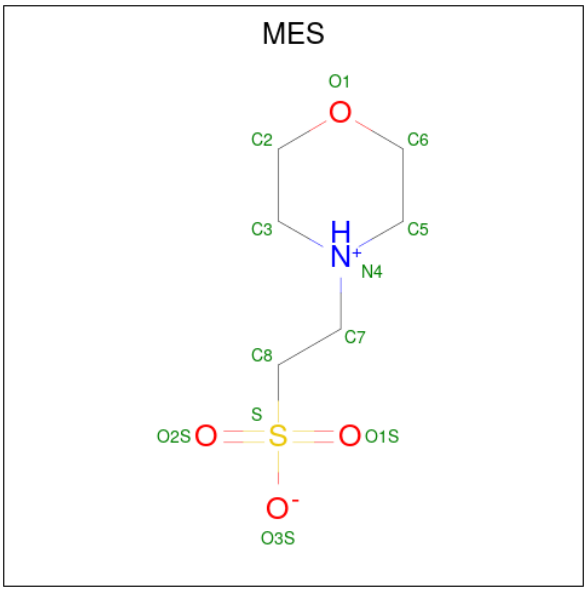
- Molecule 15 is a protein called Ac-LAD-ep.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
15	c	5	Total C N O 28 18 3 7	0	0	0
15	d	5	Total C N O 28 18 3 7	0	0	0
15	e	5	Total C N O 28 18 3 7	0	0	0
15	f	5	Total C N O 28 18 3 7	0	0	0
15	g	5	Total C N O 28 18 3 7	0	0	0
15	h	5	Total C N O 28 18 3 7	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Mg 1 1	0	0
16	I	2	Total Mg 2 2	0	0
16	J	1	Total Mg 1 1	0	0
16	K	1	Total Mg 1 1	0	0
16	L	1	Total Mg 1 1	0	0
16	N	1	Total Mg 1 1	0	0
16	W	1	Total Mg 1 1	0	0

- Molecule 17 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	K	1	Total C N O S 12 6 1 4 1	0	0
17	Y	1	Total C N O S 12 6 1 4 1	0	0
17	c	1	Total C N O S 12 6 1 4 1	0	0
17	f	1	Total C N O S 12 6 1 4 1	0	0

- Molecule 18 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	U	1	Total Cl 1 1	0	0

- Molecule 19 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	c	1	Total K 1 1	0	0
19	f	1	Total K 1 1	0	0

- Molecule 20 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	40	Total O 40 40	0	0
20	B	31	Total O 31 31	0	0
20	C	23	Total O 23 23	0	0
20	D	15	Total O 15 15	0	0
20	E	14	Total O 14 14	0	0
20	F	26	Total O 26 26	0	0
20	G	33	Total O 33 33	0	0
20	H	33	Total O 33 33	0	0
20	I	33	Total O 33 33	0	0
20	J	31	Total O 31 31	0	0
20	K	35	Total O 35 35	0	0
20	L	35	Total O 35 35	0	0
20	M	34	Total O 34 34	0	0
20	N	27	Total O 27 27	0	0
20	O	21	Total O 21 21	0	0
20	P	21	Total O 21 21	0	0
20	Q	16	Total O 16 16	0	0
20	R	18	Total O 18 18	0	0
20	S	15	Total O 15 15	0	0
20	T	24	Total O 24 24	0	0
20	U	35	Total O 35 35	0	0
20	V	38	Total O 38 38	0	0

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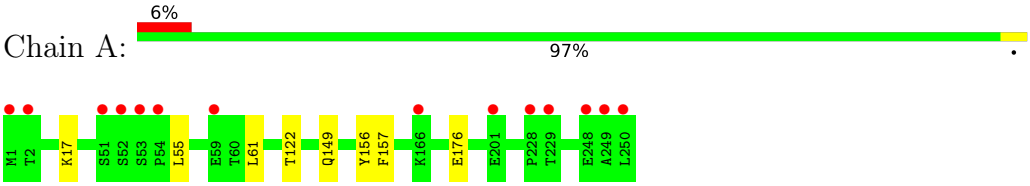
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	W	32	Total O 32 32	0	0
20	X	38	Total O 38 38	0	0
20	Y	32	Total O 32 32	0	0
20	Z	30	Total O 30 30	0	0
20	a	45	Total O 45 45	0	0
20	b	28	Total O 28 28	0	0
20	c	3	Total O 3 3	0	0
20	d	1	Total O 1 1	0	0
20	e	1	Total O 1 1	0	0
20	g	1	Total O 1 1	0	0
20	h	1	Total O 1 1	0	0

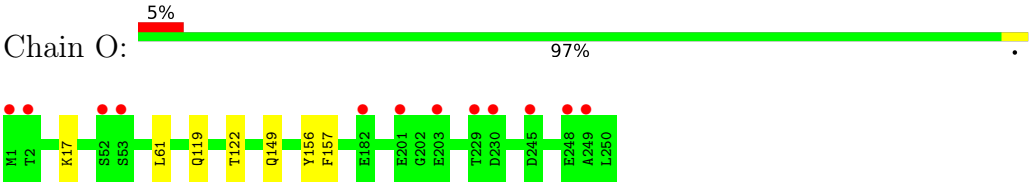
3 Residue-property plots (i)

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.

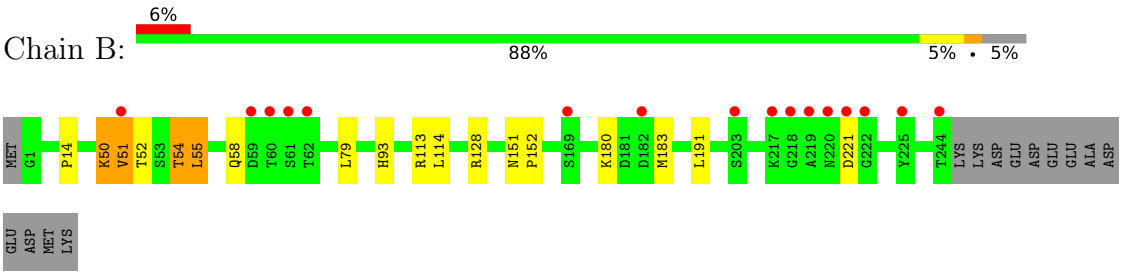
• Molecule 1: Proteasome subunit alpha type-2



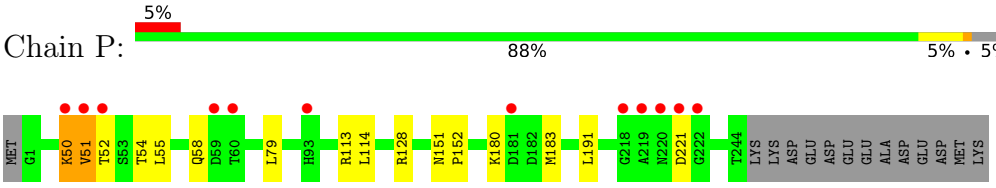
• Molecule 1: Proteasome subunit alpha type-2



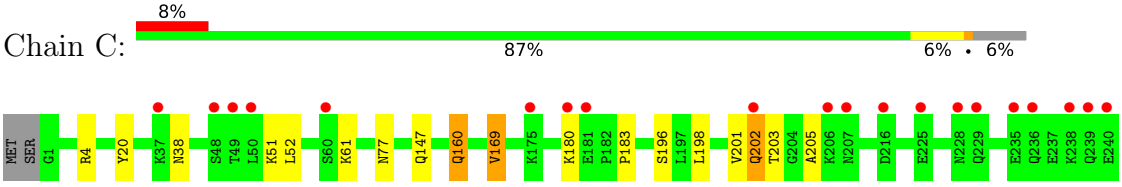
• Molecule 2: Proteasome subunit alpha type-3



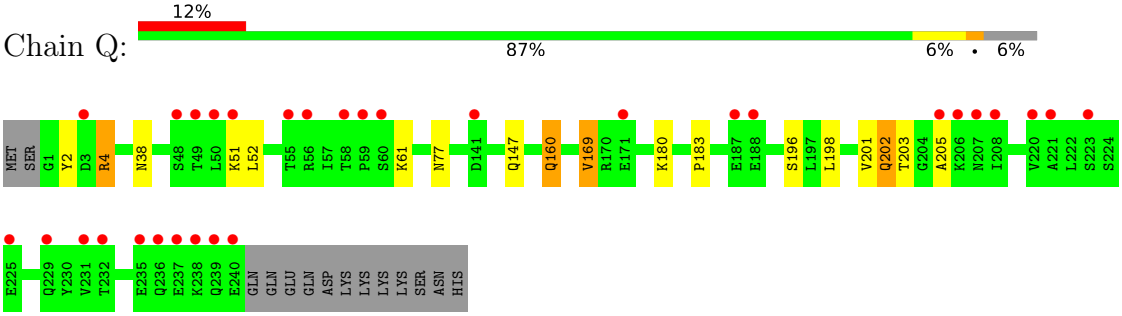
• Molecule 2: Proteasome subunit alpha type-3



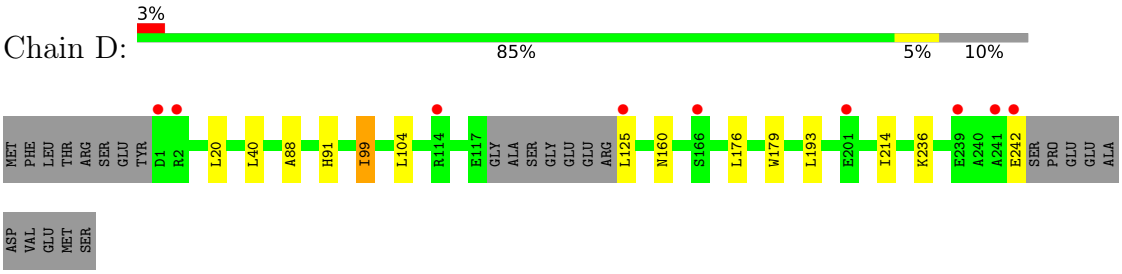
• Molecule 3: Proteasome subunit alpha type-4



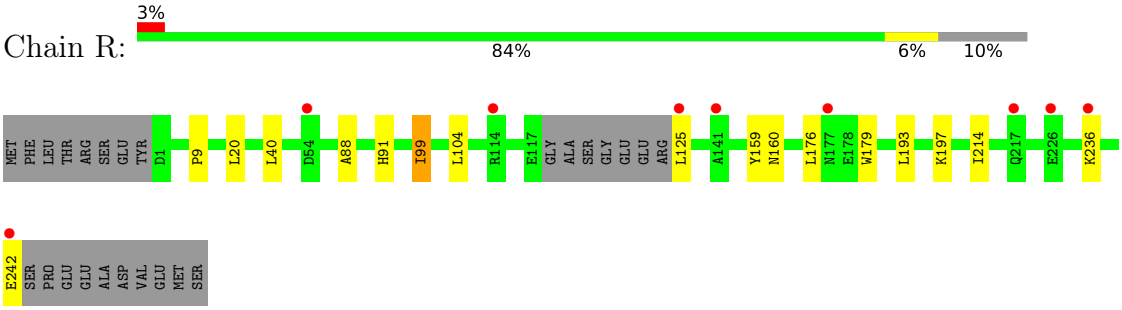
• Molecule 3: Proteasome subunit alpha type-4



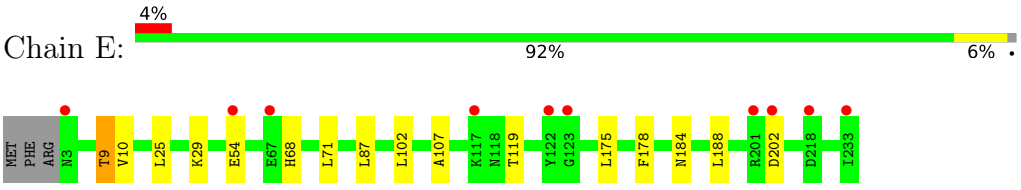
• Molecule 4: Proteasome subunit alpha type-5



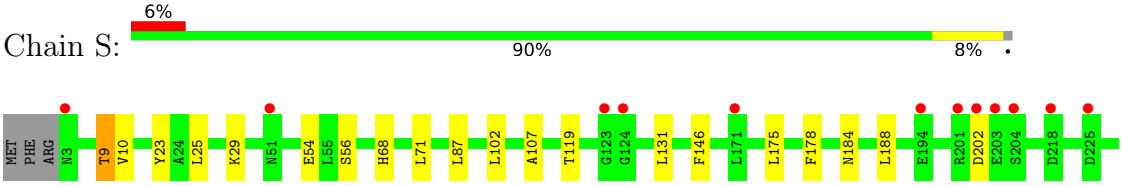
• Molecule 4: Proteasome subunit alpha type-5



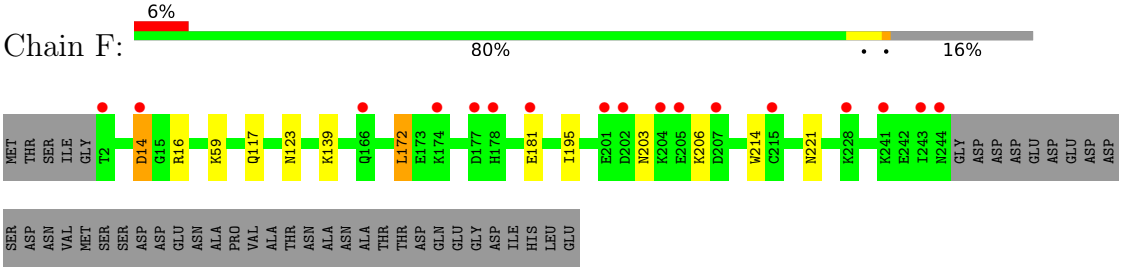
• Molecule 5: Proteasome subunit alpha type-6



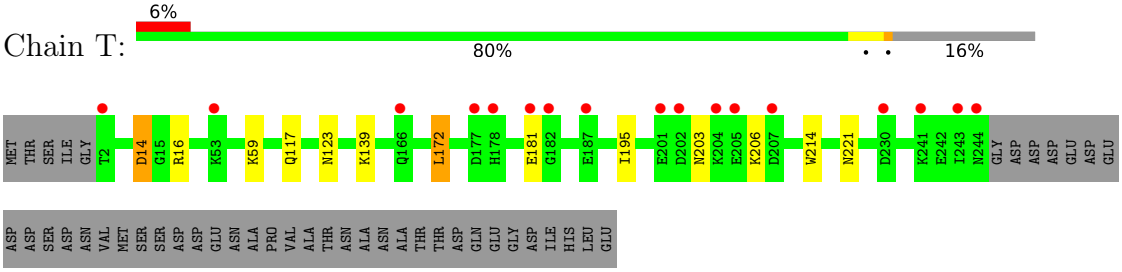
• Molecule 5: Proteasome subunit alpha type-6



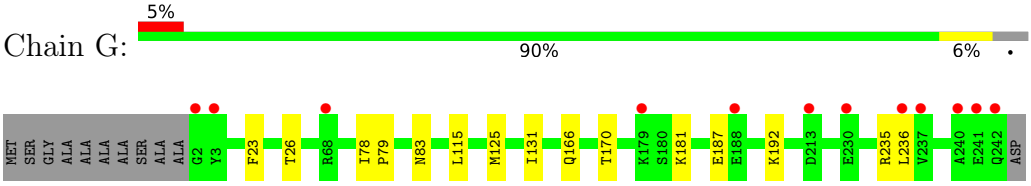
• Molecule 6: Probable proteasome subunit alpha type-7



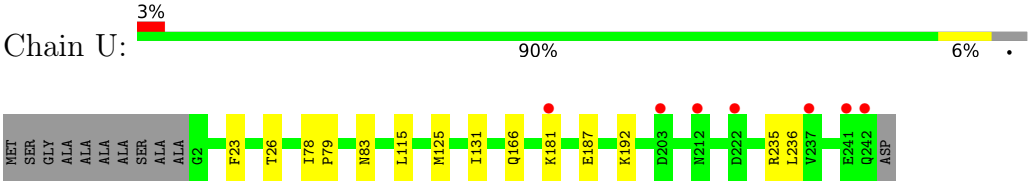
• Molecule 6: Probable proteasome subunit alpha type-7



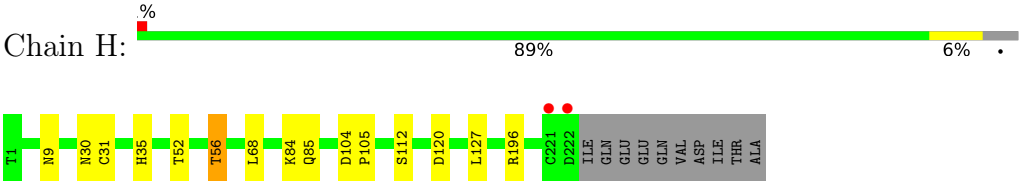
• Molecule 7: Proteasome subunit alpha type-1



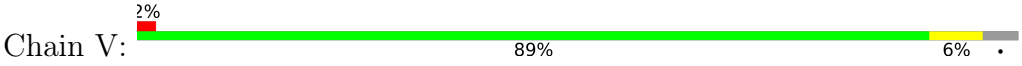
• Molecule 7: Proteasome subunit alpha type-1

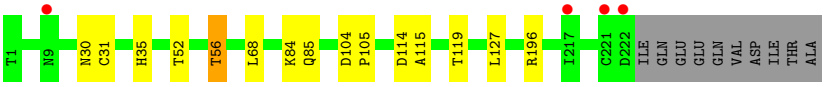


• Molecule 8: Proteasome subunit beta type-2

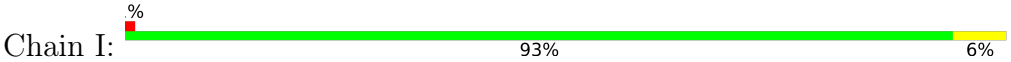


• Molecule 8: Proteasome subunit beta type-2

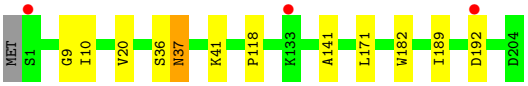




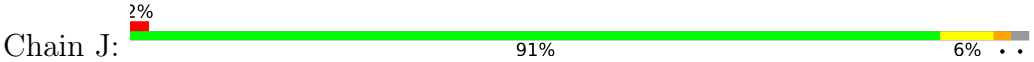
• Molecule 9: Proteasome subunit beta type-3

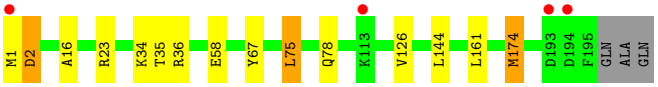


• Molecule 9: Proteasome subunit beta type-3

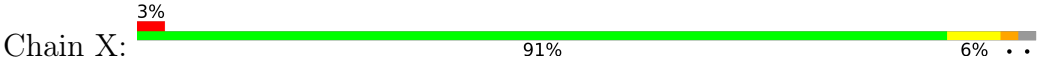


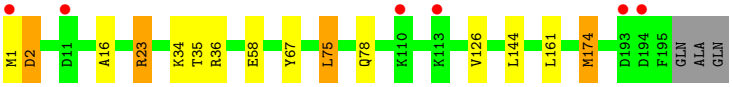
• Molecule 10: Proteasome subunit beta type-4



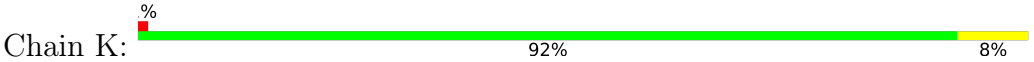


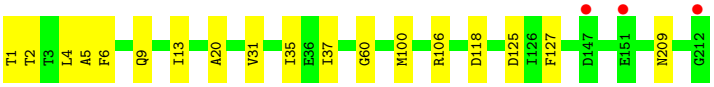
• Molecule 10: Proteasome subunit beta type-4



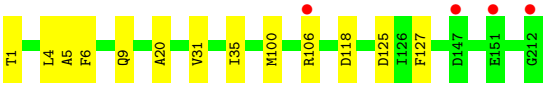


• Molecule 11: Proteasome subunit beta type-5



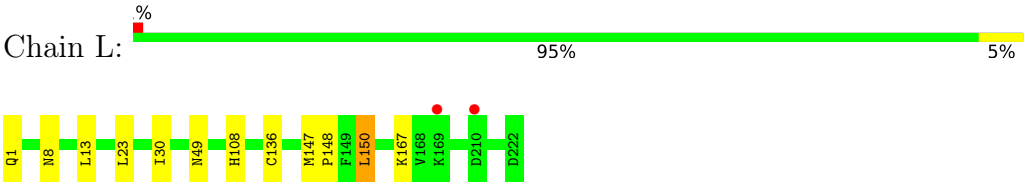


• Molecule 11: Proteasome subunit beta type-5



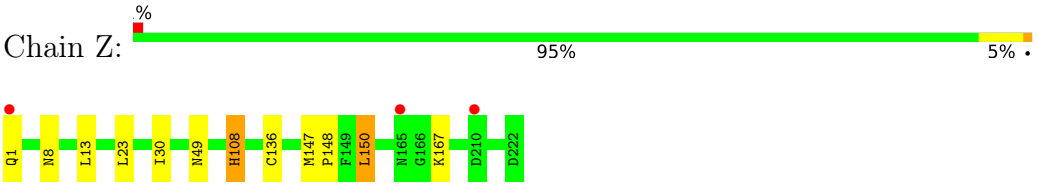
• Molecule 12: Proteasome subunit beta type-6

Chain L:



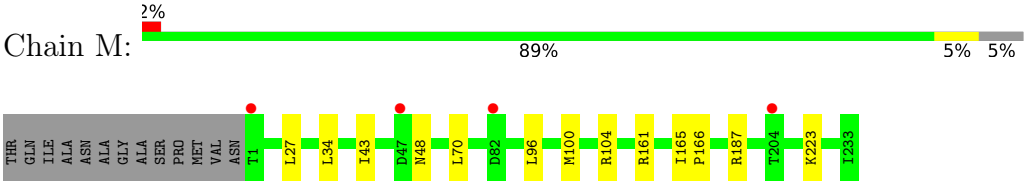
• Molecule 12: Proteasome subunit beta type-6

Chain Z:



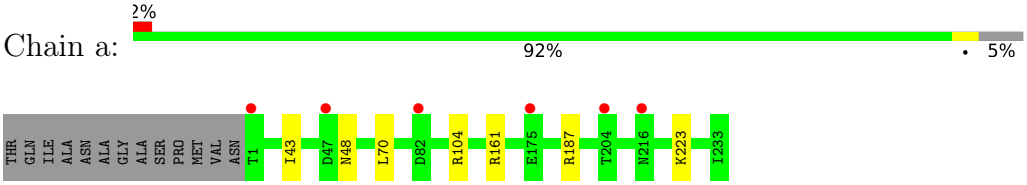
• Molecule 13: Proteasome subunit beta type-7

Chain M:



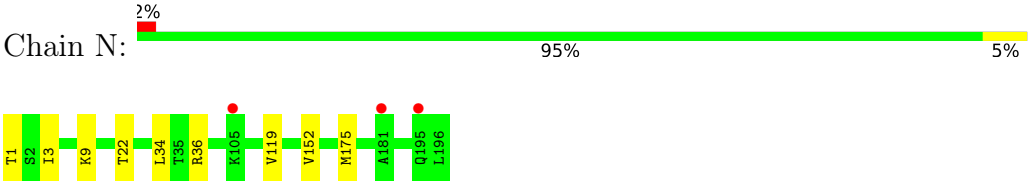
• Molecule 13: Proteasome subunit beta type-7

Chain a:



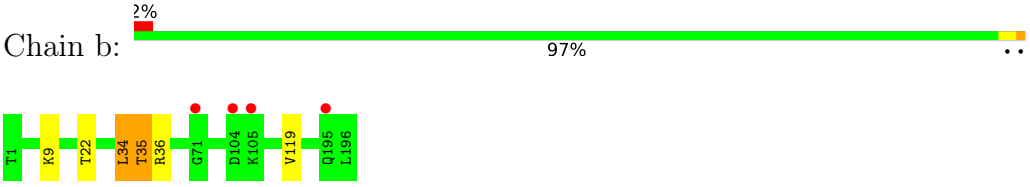
• Molecule 14: Proteasome subunit beta type-1

Chain N:



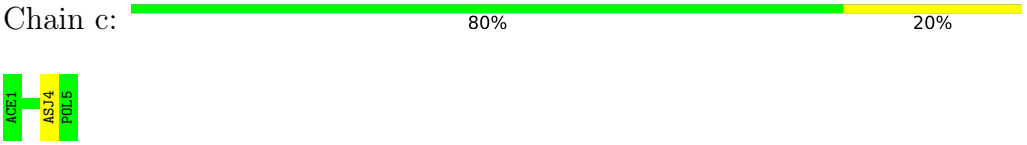
• Molecule 14: Proteasome subunit beta type-1

Chain b:



• Molecule 15: Ac-LAD-ep

Chain c:



• Molecule 15: Ac-LAD-ep

Chain d:

• Molecule 15: Ac-LAD-ep

Chain e:

• Molecule 15: Ac-LAD-ep

Chain f:

• Molecule 15: Ac-LAD-ep

Chain g:

• Molecule 15: Ac-LAD-ep

Chain h:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	135.38Å 299.69Å 145.31Å 90.00° 112.83° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.5 (15.00-2.70) 95.6 (15.00-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.85 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.220 , 0.241 0.227 , 0.247	Depositor DCC
R_{free} test set	13823 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	48.5	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 41.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	50343	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: K, MG, ASJ, ACE, MES, POL, CL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.26	0/1952	0.48	0/2642
1	O	0.26	0/1952	0.48	0/2642
2	B	0.26	0/1934	0.50	0/2618
2	P	0.26	0/1934	0.49	0/2618
3	C	0.26	0/1910	0.51	0/2586
3	Q	0.26	0/1910	0.51	0/2586
4	D	0.26	0/1837	0.48	0/2475
4	R	0.26	0/1837	0.48	0/2475
5	E	0.26	0/1800	0.48	0/2433
5	S	0.26	0/1800	0.48	0/2433
6	F	0.27	0/1932	0.46	0/2609
6	T	0.26	0/1932	0.47	0/2609
7	G	0.27	0/1945	0.48	0/2634
7	U	0.27	0/1945	0.48	0/2634
8	H	0.27	0/1712	0.50	0/2322
8	V	0.25	0/1712	0.49	0/2322
9	I	0.27	0/1611	0.56	1/2174 (0.0%)
9	W	0.31	0/1611	0.51	0/2174
10	J	0.25	0/1589	0.49	0/2142
10	X	0.26	0/1589	0.49	0/2142
11	K	0.27	0/1681	0.51	0/2274
11	Y	0.27	0/1681	0.52	1/2274 (0.0%)
12	L	0.35	2/1806 (0.1%)	0.57	4/2435 (0.2%)
12	Z	0.36	2/1806 (0.1%)	0.59	4/2435 (0.2%)
13	M	0.26	0/1855	0.51	0/2514
13	a	0.27	0/1855	0.52	0/2514
14	N	0.35	1/1541 (0.1%)	0.55	2/2087 (0.1%)
14	b	0.43	2/1541 (0.1%)	0.68	3/2087 (0.1%)
15	c	1.19	0/13	1.70	0/17
15	d	0.99	0/13	1.04	0/17
15	e	0.34	0/13	1.30	0/17
15	f	0.41	0/13	1.19	0/17

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
15	g	1.18	0/13	1.40	0/17
15	h	0.37	0/13	1.27	0/17
All	All	0.28	7/50288 (0.0%)	0.51	15/67992 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
14	b	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	34	LEU	C-N	-12.49	1.05	1.34
14	N	34	LEU	C-N	-8.89	1.13	1.34
12	Z	108[A]	HIS	CA-C	6.62	1.70	1.52
12	Z	108[B]	HIS	CA-C	6.62	1.70	1.52
12	L	108[A]	HIS	CA-C	6.22	1.69	1.52
12	L	108[B]	HIS	CA-C	6.22	1.69	1.52
14	b	35	THR	C-N	5.58	1.46	1.34

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	34	LEU	C-N-CA	13.43	155.28	121.70
14	b	34	LEU	O-C-N	-13.33	101.37	122.70
9	I	126	ILE	CG1-CB-CG2	-10.59	88.10	111.40
14	b	34	LEU	CA-C-N	9.67	138.47	117.20
12	Z	108[A]	HIS	CA-C-O	7.94	136.77	120.10
12	Z	108[B]	HIS	CA-C-O	7.94	136.77	120.10
14	N	34	LEU	C-N-CA	7.73	141.02	121.70
14	N	34	LEU	O-C-N	-6.81	111.81	122.70
12	L	108[A]	HIS	CA-C-O	6.54	133.83	120.10
12	L	108[B]	HIS	CA-C-O	6.54	133.83	120.10
12	Z	108[A]	HIS	CA-C-N	-5.66	104.75	117.20
12	Z	108[B]	HIS	CA-C-N	-5.66	104.75	117.20
11	Y	1	THR	N-CA-C	5.36	125.48	111.00
12	L	108[A]	HIS	CA-C-N	-5.09	106.01	117.20
12	L	108[B]	HIS	CA-C-N	-5.09	106.01	117.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	b	34	LEU	Peptide
14	b	35	THR	Mainchain

5.2 Too-close contacts (i)

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	3	0
2	B	1904	0	1904	9	0
2	P	1904	0	1904	6	0
3	C	1881	0	1895	8	0
3	Q	1881	0	1895	8	0
4	D	1813	0	1797	4	0
4	R	1813	0	1797	7	0
5	E	1773	0	1775	4	0
5	S	1773	0	1775	7	0
6	F	1892	0	1883	2	0
6	T	1892	0	1883	2	0
7	G	1907	0	1901	5	0
7	U	1907	0	1901	4	0
8	H	1682	0	1682	6	0
8	V	1682	0	1682	6	0
9	I	1581	0	1574	14	0
9	W	1581	0	1574	6	0
10	J	1561	0	1569	7	0
10	X	1561	0	1569	8	0
11	K	1644	0	1592	10	0
11	Y	1644	0	1592	6	0
12	L	1764	0	1718	3	0
12	Z	1764	0	1718	3	0
13	M	1824	0	1832	3	0
13	a	1824	0	1832	0	0
14	N	1512	0	1477	2	0
14	b	1512	0	1477	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	c	28	0	29	0	0
15	d	28	0	29	0	0
15	e	28	0	29	0	0
15	f	28	0	29	0	0
15	g	28	0	29	0	0
15	h	28	0	29	0	0
16	G	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	K	1	0	0	0	0
16	L	1	0	0	0	0
16	N	1	0	0	0	0
16	W	1	0	0	0	0
17	K	12	0	13	0	0
17	Y	12	0	13	0	0
17	c	12	0	13	0	0
17	f	12	0	13	0	0
18	U	1	0	0	0	0
19	c	1	0	0	0	0
19	f	1	0	0	0	0
20	A	40	0	0	0	0
20	B	31	0	0	1	0
20	C	23	0	0	0	0
20	D	15	0	0	0	0
20	E	14	0	0	0	0
20	F	26	0	0	0	0
20	G	33	0	0	0	0
20	H	33	0	0	1	0
20	I	33	0	0	0	0
20	J	31	0	0	0	0
20	K	35	0	0	0	0
20	L	35	0	0	0	0
20	M	34	0	0	0	0
20	N	27	0	0	0	0
20	O	21	0	0	0	0
20	P	21	0	0	1	0
20	Q	16	0	0	0	0
20	R	18	0	0	1	0
20	S	15	0	0	0	0
20	T	24	0	0	0	0
20	U	35	0	0	0	0
20	V	38	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	W	32	0	0	0	0
20	X	38	0	0	0	0
20	Y	32	0	0	1	0
20	Z	30	0	0	0	0
20	a	45	0	0	0	0
20	b	28	0	0	0	0
20	c	3	0	0	0	0
20	d	1	0	0	0	0
20	e	1	0	0	0	0
20	g	1	0	0	0	0
20	h	1	0	0	0	0
All	All	50343	0	49282	136	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 2.

All (136) 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)
9:I:98:ARG:HD2	9:I:126:ILE:HD12	1.58	0.83
10:X:1:MET:O	10:X:2:ASP:HB2	1.85	0.75
10:J:1:MET:O	10:J:2:ASP:HB2	1.85	0.74
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.76	0.67
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.76	0.67
9:I:98:ARG:HD2	9:I:126:ILE:CD1	2.27	0.65
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.83	0.59
11:Y:5:ALA:HB3	11:Y:100:MET:HE2	1.84	0.59
4:R:99:ILE:HD11	4:R:104:LEU:HB2	1.86	0.58
4:D:99:ILE:HD11	4:D:104:LEU:HB2	1.86	0.57
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.88	0.56
9:I:125:LEU:HD23	9:I:126:ILE:HG22	1.89	0.55
11:K:5:ALA:HB3	11:K:100:MET:HE2	1.89	0.54
9:I:125:LEU:CD2	9:I:126:ILE:HG22	2.37	0.53
9:I:98:ARG:CD	9:I:126:ILE:CD1	2.87	0.52
14:N:152:VAL:HA	14:N:175:MET:HE1	1.90	0.52
7:U:23:PHE:O	7:U:26:THR:HB	2.10	0.52
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.92	0.52
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.93	0.51
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.75	0.51
7:G:23:PHE:O	7:G:26:THR:HB	2.11	0.51
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:201:VAL:O	3:C:202:GLN:CB	2.59	0.51
9:W:36:SER:HB2	10:X:126:VAL:HG11	1.91	0.51
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.93	0.51
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.92	0.50
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.59	0.50
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.93	0.50
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.11	0.50
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.76	0.50
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.94	0.49
3:C:51:LYS:O	3:C:52:LEU:HB2	2.11	0.49
11:K:100:MET:CE	11:K:127:PHE:HB2	2.42	0.49
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.94	0.49
11:Y:100:MET:CE	11:Y:127:PHE:HB2	2.43	0.48
3:Q:201:VAL:O	3:Q:202:GLN:HB2	2.13	0.48
3:C:201:VAL:HG13	3:C:202:GLN:N	2.28	0.48
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.49	0.48
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.48	0.48
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.28	0.48
8:H:52:THR:O	8:H:56:THR:HB	2.13	0.48
1:A:176:GLU:HG2	2:B:55:LEU:HD13	1.95	0.47
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.96	0.47
8:V:52:THR:O	8:V:56:THR:HB	2.14	0.47
11:K:209:ASN:O	9:W:37:ASN:ND2	2.47	0.47
8:V:114:ASP:OD2	8:V:115:ALA:N	2.47	0.47
4:R:197:LYS:HD2	20:R:312:HOH:O	2.14	0.47
3:C:201:VAL:O	3:C:202:GLN:HB2	2.13	0.47
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.80	0.47
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.96	0.47
13:M:27:LEU:HD21	13:M:34:LEU:HD22	1.97	0.47
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.96	0.46
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.80	0.46
12:L:8:ASN:HA	12:L:30:ILE:O	2.16	0.46
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.96	0.46
9:I:126:ILE:HD13	9:I:126:ILE:HG21	1.63	0.45
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.52	0.45
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.99	0.44
10:X:23:ARG:HG2	20:Y:421:HOH:O	2.17	0.44
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.52	0.44
10:J:36:ARG:NH1	10:J:58:GLU:OE2	2.50	0.44
7:G:78:ILE:N	7:G:79:PRO:CD	2.80	0.44
9:I:98:ARG:CD	9:I:126:ILE:HD12	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:98:ARG:NE	9:I:126:ILE:HD11	2.32	0.44
5:S:9:THR:HG21	5:S:119:THR:HA	2.00	0.44
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.99	0.44
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.99	0.44
9:I:9:GLY:HA3	9:I:41:LYS:HE2	2.00	0.44
11:K:20:ALA:HB2	11:K:31:VAL:HG21	2.00	0.44
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.99	0.44
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.53	0.44
7:U:78:ILE:N	7:U:79:PRO:CD	2.81	0.44
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.52	0.44
10:X:36:ARG:NH1	10:X:58:GLU:OE2	2.51	0.43
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.48	0.43
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.53	0.43
7:U:26:THR:HG21	7:U:131:ILE:HD12	2.01	0.43
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.18	0.43
3:C:198:LEU:HA	3:C:201:VAL:HG12	2.00	0.43
5:E:9:THR:HG21	5:E:119:THR:HA	2.00	0.43
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.99	0.43
3:Q:198:LEU:HA	3:Q:201:VAL:HG12	2.00	0.43
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.01	0.43
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.33	0.43
2:P:113:ARG:NH1	20:P:301:HOH:O	2.40	0.43
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.01	0.43
2:B:180:LYS:O	2:B:183:MET:HB2	2.19	0.43
1:A:149:GLN:O	1:A:156:TYR:HA	2.19	0.43
6:T:172:LEU:CD1	6:T:195:ILE:HD13	2.49	0.43
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.49	0.42
8:H:84:LYS:HG3	8:H:85:GLN:N	2.34	0.42
11:K:1:THR:HG22	11:K:2:THR:N	2.33	0.42
2:P:180:LYS:O	2:P:183:MET:HB2	2.19	0.42
1:O:149:GLN:O	1:O:156:TYR:HA	2.19	0.42
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	2.00	0.42
9:I:36:SER:HB2	10:J:126:VAL:HG11	2.00	0.42
11:K:6:PHE:HA	11:K:125:ASP:O	2.19	0.42
4:R:9:PRO:HA	5:S:23:TYR:CD1	2.53	0.42
2:B:151:ASN:HB2	2:B:152:PRO:HD2	2.01	0.42
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.49	0.42
8:V:84:LYS:HG3	8:V:85:GLN:N	2.34	0.42
14:N:1:THR:CG2	14:N:3:ILE:HG23	2.50	0.42
6:T:14:ASP:HB2	6:T:16:ARG:HD3	2.02	0.42
6:F:14:ASP:HB2	6:F:16:ARG:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:187:GLU:HG2	7:G:192:LYS:HB2	2.01	0.42
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.49	0.42
9:I:98:ARG:CD	9:I:126:ILE:HD11	2.50	0.42
1:O:119:GLN:O	1:O:122:THR:HB	2.19	0.42
7:G:26:THR:HG21	7:G:131:ILE:HD12	2.01	0.42
5:E:68:HIS:HE1	5:E:102:LEU:O	2.03	0.41
11:Y:6:PHE:HA	11:Y:125:ASP:O	2.20	0.41
1:A:55:LEU:HD12	7:G:170:THR:HG23	2.02	0.41
2:B:54:THR:HG22	20:B:308:HOH:O	2.19	0.41
8:H:9:ASN:HB2	20:H:307:HOH:O	2.20	0.41
6:F:172:LEU:CD1	6:F:195:ILE:HD13	2.50	0.41
12:L:147:MET:N	12:L:148:PRO:HD2	2.34	0.41
2:P:50:LYS:O	2:P:51:VAL:C	2.58	0.41
7:U:187:GLU:HG2	7:U:192:LYS:HB2	2.01	0.41
5:S:68:HIS:HE1	5:S:102:LEU:O	2.04	0.41
10:X:1:MET:HA	10:X:34:LYS:CE	2.50	0.41
2:B:50:LYS:O	2:B:51:VAL:C	2.59	0.41
2:B:93:HIS:HB3	2:B:113:ARG:HH21	1.85	0.41
10:J:1:MET:HA	10:J:34:LYS:CE	2.51	0.41
8:H:112:SER:OG	8:H:120:ASP:HB2	2.21	0.41
11:K:37:ILE:HG23	11:K:60:GLY:HA2	2.03	0.41
13:M:96:LEU:O	13:M:100:MET:HG2	2.21	0.41
9:W:20:VAL:HG23	9:W:189:ILE:HB	2.03	0.41
11:K:5:ALA:HB3	11:K:100:MET:CE	2.50	0.40
3:Q:2:TYR:CZ	3:Q:4:ARG:HB2	2.56	0.40
9:I:126:ILE:O	9:I:126:ILE:HG13	2.21	0.40
10:J:174:MET:HA	10:X:174:MET:HA	2.03	0.40
11:K:5:ALA:HA	11:K:13:ILE:O	2.22	0.40
5:S:131:LEU:HB2	5:S:146:PHE:HB3	2.03	0.40
8:V:84:LYS:HE2	8:V:119:THR:HG23	2.04	0.40
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.57	0.40
11:Y:5:ALA:HB3	11:Y:100:MET:CE	2.49	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%)	242 (98%)	6 (2%)	0	100	100
1	O	248/250 (99%)	242 (98%)	6 (2%)	0	100	100
2	B	242/258 (94%)	233 (96%)	7 (3%)	2 (1%)	19	43
2	P	242/258 (94%)	233 (96%)	7 (3%)	2 (1%)	19	43
3	C	238/254 (94%)	230 (97%)	5 (2%)	3 (1%)	12	30
3	Q	238/254 (94%)	230 (97%)	5 (2%)	3 (1%)	12	30
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%)	224 (98%)	5 (2%)	0	100	100
5	S	229/234 (98%)	224 (98%)	5 (2%)	0	100	100
6	F	241/288 (84%)	233 (97%)	8 (3%)	0	100	100
6	T	241/288 (84%)	233 (97%)	8 (3%)	0	100	100
7	G	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
7	U	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
8	H	220/232 (95%)	213 (97%)	7 (3%)	0	100	100
8	V	220/232 (95%)	213 (97%)	7 (3%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	188 (97%)	4 (2%)	1 (0%)	29	54
10	X	193/198 (98%)	188 (97%)	4 (2%)	1 (0%)	29	54
11	K	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
11	Y	210/212 (99%)	207 (99%)	3 (1%)	0	100	100
12	L	221/222 (100%)	217 (98%)	4 (2%)	0	100	100
12	Z	221/222 (100%)	217 (98%)	4 (2%)	0	100	100
13	M	231/246 (94%)	224 (97%)	7 (3%)	0	100	100
13	a	231/246 (94%)	225 (97%)	6 (3%)	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
15	c	2/5 (40%)	2 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	d	2/5 (40%)	2 (100%)	0	0	100	100
15	e	2/5 (40%)	2 (100%)	0	0	100	100
15	f	2/5 (40%)	2 (100%)	0	0	100	100
15	g	2/5 (40%)	2 (100%)	0	0	100	100
15	h	2/5 (40%)	2 (100%)	0	0	100	100
All	All	6290/6644 (95%)	6124 (97%)	154 (2%)	12 (0%)	47	73

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
10	J	2	ASP
2	P	51	VAL
3	Q	202	GLN
10	X	2	ASP
3	C	205	ALA
3	Q	205	ALA
2	B	221	ASP
2	P	221	ASP
3	C	183	PRO
3	Q	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%)	206 (99%)	3 (1%)	67	86
1	O	209/209 (100%)	206 (99%)	3 (1%)	67	86
2	B	203/216 (94%)	195 (96%)	8 (4%)	32	61
2	P	203/216 (94%)	195 (96%)	8 (4%)	32	61
3	C	212/226 (94%)	203 (96%)	9 (4%)	30	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Q	212/226 (94%)	203 (96%)	9 (4%)	30	58
4	D	194/215 (90%)	185 (95%)	9 (5%)	27	54
4	R	194/215 (90%)	185 (95%)	9 (5%)	27	54
5	E	190/193 (98%)	181 (95%)	9 (5%)	26	54
5	S	190/193 (98%)	181 (95%)	9 (5%)	26	54
6	F	201/239 (84%)	190 (94%)	11 (6%)	21	46
6	T	201/239 (84%)	190 (94%)	11 (6%)	21	46
7	G	206/210 (98%)	199 (97%)	7 (3%)	37	66
7	U	206/210 (98%)	199 (97%)	7 (3%)	37	66
8	H	181/190 (95%)	175 (97%)	6 (3%)	38	67
8	V	181/190 (95%)	175 (97%)	6 (3%)	38	67
9	I	172/173 (99%)	167 (97%)	5 (3%)	42	71
9	W	172/173 (99%)	168 (98%)	4 (2%)	50	78
10	J	173/175 (99%)	167 (96%)	6 (4%)	36	65
10	X	173/175 (99%)	167 (96%)	6 (4%)	36	65
11	K	169/169 (100%)	164 (97%)	5 (3%)	41	70
11	Y	169/169 (100%)	164 (97%)	5 (3%)	41	70
12	L	186/185 (100%)	180 (97%)	6 (3%)	39	68
12	Z	186/185 (100%)	178 (96%)	8 (4%)	29	57
13	M	199/208 (96%)	192 (96%)	7 (4%)	36	65
13	a	199/208 (96%)	192 (96%)	7 (4%)	36	65
14	N	162/162 (100%)	158 (98%)	4 (2%)	47	76
14	b	162/162 (100%)	158 (98%)	4 (2%)	47	76
15	c	1/1 (100%)	1 (100%)	0	100	100
15	d	1/1 (100%)	1 (100%)	0	100	100
15	e	1/1 (100%)	1 (100%)	0	100	100
15	f	1/1 (100%)	1 (100%)	0	100	100
15	g	1/1 (100%)	1 (100%)	0	100	100
15	h	1/1 (100%)	1 (100%)	0	100	100
All	All	5320/5546 (96%)	5129 (96%)	191 (4%)	35	64

All (191) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	61	LEU
1	A	157	PHE
2	B	50	LYS
2	B	52	THR
2	B	54	THR
2	B	55	LEU
2	B	58	GLN
2	B	79	LEU
2	B	114	LEU
2	B	191	LEU
3	C	4	ARG
3	C	38	ASN
3	C	61	LYS
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	203	THR
4	D	20	LEU
4	D	40	LEU
4	D	99	ILE
4	D	125	LEU
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	10	VAL
5	E	25	LEU
5	E	29	LYS
5	E	54	GLU
5	E	71	LEU
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
6	F	14	ASP
6	F	59	LYS
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS

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Mol	Chain	Res	Type
6	F	172	LEU
6	F	181	GLU
6	F	203	ASN
6	F	206	LYS
6	F	214	TRP
6	F	221	ASN
7	G	83	ASN
7	G	115	LEU
7	G	125	MET
7	G	166	GLN
7	G	181	LYS
7	G	235	ARG
7	G	236	LEU
8	H	30	ASN
8	H	31	CYS
8	H	56	THR
8	H	68	LEU
8	H	127	LEU
8	H	196	ARG
9	I	37	ASN
9	I	126	ILE
9	I	171	LEU
9	I	182	TRP
9	I	192	ASP
10	J	23	ARG
10	J	35	THR
10	J	75	LEU
10	J	78	GLN
10	J	144	LEU
10	J	174	MET
11	K	4	LEU
11	K	9	GLN
11	K	35	ILE
11	K	106	ARG
11	K	118	ASP
12	L	1	GLN
12	L	23	LEU
12	L	49	ASN
12	L	136	CYS
12	L	150	LEU
12	L	167	LYS
13	M	43	ILE

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Mol	Chain	Res	Type
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
13	M	223	LYS
14	N	9	LYS
14	N	22	THR
14	N	36	ARG
14	N	119	VAL
1	O	17	LYS
1	O	61	LEU
1	O	157	PHE
2	P	50	LYS
2	P	52	THR
2	P	54	THR
2	P	55	LEU
2	P	58	GLN
2	P	79	LEU
2	P	114	LEU
2	P	191	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	61	LYS
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	203	THR
4	R	20	LEU
4	R	40	LEU
4	R	99	ILE
4	R	125	LEU
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	10	VAL
5	S	25	LEU

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Mol	Chain	Res	Type
5	S	29	LYS
5	S	54	GLU
5	S	71	LEU
5	S	184	ASN
5	S	188	LEU
5	S	202	ASP
6	T	14	ASP
6	T	59	LYS
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	172	LEU
6	T	181	GLU
6	T	203	ASN
6	T	206	LYS
6	T	214	TRP
6	T	221	ASN
7	U	83	ASN
7	U	115	LEU
7	U	125	MET
7	U	166	GLN
7	U	181	LYS
7	U	235	ARG
7	U	236	LEU
8	V	30	ASN
8	V	31	CYS
8	V	56	THR
8	V	68	LEU
8	V	127	LEU
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
9	W	182	TRP
9	W	192	ASP
10	X	23	ARG
10	X	35	THR
10	X	75	LEU
10	X	78	GLN
10	X	144	LEU
10	X	174	MET
11	Y	4	LEU
11	Y	9	GLN

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Mol	Chain	Res	Type
11	Y	35	ILE
11	Y	106	ARG
11	Y	118	ASP
12	Z	1	GLN
12	Z	23	LEU
12	Z	49	ASN
12	Z	108[A]	HIS
12	Z	108[B]	HIS
12	Z	136	CYS
12	Z	150	LEU
12	Z	167	LYS
13	a	43	ILE
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
13	a	223	LYS
14	b	9	LYS
14	b	22	THR
14	b	36	ARG
14	b	119	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN
2	B	102	ASN
2	B	119	GLN
2	B	123	GLN
2	B	176	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	146	GLN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN

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Mol	Chain	Res	Type
5	E	99	ASN
5	E	116	GLN
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	240	GLN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	167	GLN
8	H	57	GLN
9	I	203	GLN
10	J	55	GLN
11	K	9	GLN
11	K	85	ASN
11	K	176	ASN
12	L	3	ASN
12	L	70	ASN
12	L	158	ASN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
1	O	94	HIS
2	P	20	GLN
2	P	119	GLN
2	P	123	GLN
2	P	176	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	146	GLN
4	R	225	ASN

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Mol	Chain	Res	Type
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
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	240	GLN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	167	GLN
8	V	57	GLN
8	V	66	HIS
8	V	200	GLN
10	X	55	GLN
10	X	86	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	176	ASN
12	Z	3	ASN
12	Z	70	ASN
12	Z	158	ASN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	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 (i)

6 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	ASJ	g	4	11,15	7,7,7	1.16	1 (14%)	5,8,8	1.31	1 (20%)
15	ASJ	e	4	14,15	7,7,7	1.00	0	5,8,8	1.88	1 (20%)
15	ASJ	c	4	8,19,15	7,7,7	2.57	4 (57%)	5,8,8	1.01	0
15	ASJ	f	4	8,19,15	7,7,7	1.13	1 (14%)	5,8,8	1.76	1 (20%)
15	ASJ	d	4	11,15	7,7,7	1.17	1 (14%)	5,8,8	1.32	0
15	ASJ	h	4	14,15	7,7,7	0.91	0	5,8,8	1.97	2 (40%)

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	ASJ	g	4	11,15	-	2/6/6/6	-
15	ASJ	e	4	14,15	-	1/6/6/6	-
15	ASJ	c	4	8,19,15	-	5/6/6/6	-
15	ASJ	f	4	8,19,15	-	3/6/6/6	-
15	ASJ	d	4	11,15	-	1/6/6/6	-
15	ASJ	h	4	14,15	-	1/6/6/6	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c	4	ASJ	C-CA	4.80	1.60	1.52
15	c	4	ASJ	CB-CA	3.03	1.58	1.53
15	d	4	ASJ	OD1-CG	-2.93	1.20	1.30
15	c	4	ASJ	OD1-CG	-2.86	1.21	1.30
15	g	4	ASJ	OD1-CG	-2.61	1.22	1.30
15	f	4	ASJ	C-CA	2.02	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c	4	ASJ	OD2-CG	2.02	1.28	1.22

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	h	4	ASJ	CB-CA-C	-3.39	106.09	112.21
15	e	4	ASJ	CB-CA-C	-3.24	106.36	112.21
15	f	4	ASJ	CB-CA-C	-3.07	106.65	112.21
15	g	4	ASJ	O-C-CA	-2.16	102.98	111.52
15	h	4	ASJ	OD2-CG-CB	-2.00	116.38	122.80

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	c	4	ASJ	O-C-CA-N
15	c	4	ASJ	O-C-CA-CB
15	d	4	ASJ	N-CA-CB-CG
15	f	4	ASJ	N-CA-CB-CG
15	g	4	ASJ	N-CA-CB-CG
15	f	4	ASJ	CA-CB-CG-OD2
15	c	4	ASJ	CA-CB-CG-OD1
15	f	4	ASJ	CA-CB-CG-OD1
15	g	4	ASJ	C-CA-CB-CG
15	c	4	ASJ	CA-CB-CG-OD2
15	c	4	ASJ	N-CA-CB-CG
15	e	4	ASJ	N-CA-CB-CG
15	h	4	ASJ	N-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 15 ligands modelled in this entry, 11 are monoatomic - leaving 4 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	c	302	-	12,12,12	2.12	1 (8%)	14,16,16	1.49	3 (21%)
17	MES	K	302	-	12,12,12	2.12	1 (8%)	14,16,16	1.45	3 (21%)
17	MES	Y	301	-	12,12,12	2.08	1 (8%)	14,16,16	1.50	2 (14%)
17	MES	f	101	-	12,12,12	2.19	1 (8%)	14,16,16	1.31	2 (14%)

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	c	302	-	-	3/6/14/14	0/1/1/1
17	MES	K	302	-	-	0/6/14/14	0/1/1/1
17	MES	Y	301	-	-	0/6/14/14	0/1/1/1
17	MES	f	101	-	-	2/6/14/14	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	f	101	MES	C8-S	-7.31	1.67	1.77
17	K	302	MES	C8-S	-7.05	1.67	1.77
17	c	302	MES	C8-S	-7.02	1.67	1.77
17	Y	301	MES	C8-S	-6.89	1.67	1.77

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	c	302	MES	O2S-S-C8	3.41	111.02	106.92
17	Y	301	MES	O2S-S-C8	3.17	110.74	106.92
17	Y	301	MES	O3S-S-C8	3.11	110.80	105.77
17	f	101	MES	O1S-S-C8	3.07	110.62	106.92
17	K	302	MES	O3S-S-C8	2.97	110.58	105.77
17	K	302	MES	O2S-S-C8	2.64	110.09	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	f	101	MES	O3S-S-C8	2.53	109.87	105.77
17	c	302	MES	O3S-S-C8	2.53	109.86	105.77
17	c	302	MES	O1S-S-C8	2.45	109.86	106.92
17	K	302	MES	O1S-S-C8	2.13	109.48	106.92

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	c	302	MES	C7-C8-S-O1S
17	c	302	MES	C7-C8-S-O3S
17	f	101	MES	C8-C7-N4-C5
17	c	302	MES	C7-C8-S-O2S
17	f	101	MES	C8-C7-N4-C3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
14	N	1
14	b	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	34:LEU	C	35:THR	N	1.13
1	b	34:LEU	C	35:THR	N	1.05

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, 95^{th} 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%)	-0.01	14 (5%)	24	23	31, 46, 85, 126	0
1	O	250/250 (100%)	0.09	12 (4%)	30	28	34, 54, 98, 131	0
2	B	244/258 (94%)	0.06	16 (6%)	18	16	30, 50, 99, 151	0
2	P	244/258 (94%)	0.13	12 (4%)	29	28	34, 54, 100, 156	0
3	C	240/254 (94%)	0.21	20 (8%)	11	9	32, 53, 116, 155	0
3	Q	240/254 (94%)	0.55	31 (12%)	3	2	40, 70, 151, 195	0
4	D	235/260 (90%)	-0.02	9 (3%)	40	39	34, 54, 86, 135	0
4	R	235/260 (90%)	0.19	9 (3%)	40	39	42, 61, 98, 151	0
5	E	231/234 (98%)	0.09	10 (4%)	35	33	37, 57, 93, 141	0
5	S	231/234 (98%)	0.17	13 (5%)	24	23	39, 63, 103, 139	0
6	F	243/288 (84%)	-0.04	17 (6%)	16	14	34, 53, 104, 134	0
6	T	243/288 (84%)	0.10	17 (6%)	16	14	34, 56, 107, 140	0
7	G	241/252 (95%)	-0.09	12 (4%)	28	27	29, 47, 88, 138	0
7	U	241/252 (95%)	-0.13	7 (2%)	51	52	33, 47, 79, 117	0
8	H	222/232 (95%)	-0.18	2 (0%)	84	85	30, 42, 73, 106	0
8	V	222/232 (95%)	-0.18	4 (1%)	68	70	28, 44, 75, 114	0
9	I	204/205 (99%)	-0.36	2 (0%)	82	83	27, 41, 70, 100	0
9	W	204/205 (99%)	-0.35	3 (1%)	73	76	26, 43, 70, 101	0
10	J	195/198 (98%)	-0.18	4 (2%)	63	65	28, 43, 70, 116	0
10	X	195/198 (98%)	-0.18	6 (3%)	49	49	31, 46, 74, 123	0
11	K	212/212 (100%)	-0.26	3 (1%)	75	77	28, 43, 73, 91	0
11	Y	212/212 (100%)	-0.24	4 (1%)	66	69	31, 46, 76, 106	0
12	L	222/222 (100%)	-0.22	2 (0%)	84	85	30, 46, 76, 105	0
12	Z	222/222 (100%)	-0.19	3 (1%)	75	77	31, 44, 78, 105	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	233/246 (94%)	-0.27	4 (1%) 70 72	27, 44, 65, 80	0
13	a	233/246 (94%)	-0.18	6 (2%) 56 57	28, 43, 65, 75	0
14	N	196/196 (100%)	-0.25	3 (1%) 73 76	26, 39, 67, 94	0
14	b	196/196 (100%)	-0.20	4 (2%) 65 67	27, 40, 71, 94	0
15	c	2/5 (40%)	-0.66	0 100 100	42, 42, 42, 46	0
15	d	2/5 (40%)	-0.59	0 100 100	53, 53, 53, 60	0
15	e	2/5 (40%)	0.00	0 100 100	41, 41, 41, 49	0
15	f	2/5 (40%)	-0.65	0 100 100	43, 43, 43, 50	0
15	g	2/5 (40%)	-0.18	0 100 100	57, 57, 57, 66	0
15	h	2/5 (40%)	0.30	0 100 100	45, 45, 45, 52	0
All	All	6348/6644 (95%)	-0.06	249 (3%) 39 38	26, 49, 94, 195	0

All (249) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	219	ALA	8.0
1	O	1	MET	7.8
3	Q	206	LYS	7.5
1	O	249	ALA	6.3
3	Q	49	THR	6.1
3	Q	239	GLN	5.9
5	S	202	ASP	5.8
3	Q	238	LYS	5.3
10	X	194	ASP	5.3
3	Q	48	SER	5.2
1	A	1	MET	4.9
14	N	105	LYS	4.9
3	Q	50	LEU	4.8
13	a	204	THR	4.8
2	B	220	ASN	4.8
2	P	51	VAL	4.8
4	D	242	GLU	4.8
8	V	222	ASP	4.7
11	Y	212	GLY	4.7
2	B	218	GLY	4.6
3	C	240	GLU	4.6
10	J	1	MET	4.6
9	W	1	SER	4.4

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Mol	Chain	Res	Type	RSRZ
10	X	1	MET	4.4
3	C	235	GLU	4.3
2	P	218	GLY	4.3
13	M	1	THR	4.3
11	K	212	GLY	4.2
8	H	222	ASP	4.2
5	E	202	ASP	4.1
6	T	230	ASP	4.1
6	F	205	GLU	4.1
6	F	202	ASP	4.1
2	B	221	ASP	4.1
3	C	180	LYS	4.1
6	T	2	THR	4.0
3	Q	240	GLU	4.0
3	C	202	GLN	4.0
1	O	229	THR	4.0
10	J	194	ASP	3.9
2	P	221	ASP	3.9
3	Q	55	THR	3.9
13	a	1	THR	3.8
4	R	242	GLU	3.8
5	S	51	ASN	3.8
6	T	244	ASN	3.8
3	C	225	GLU	3.7
3	Q	60	SER	3.7
2	P	59	ASP	3.7
3	Q	141	ASP	3.7
2	P	220	ASN	3.7
3	C	181	GLU	3.7
3	C	37	LYS	3.7
2	B	244	THR	3.7
2	B	219	ALA	3.7
2	P	222	GLY	3.6
6	T	241	LYS	3.6
3	C	239	GLN	3.6
1	A	248	GLU	3.5
6	T	243	ILE	3.5
7	G	3	TYR	3.5
8	V	221	CYS	3.5
4	R	236	LYS	3.5
13	a	47	ASP	3.5
9	I	1	SER	3.5

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Mol	Chain	Res	Type	RSRZ
3	C	206	LYS	3.4
6	F	201	GLU	3.4
3	Q	223	SER	3.4
6	F	244	ASN	3.4
5	S	233	ILE	3.4
1	O	52	SER	3.4
7	G	179	LYS	3.4
2	B	182	ASP	3.4
4	R	177	ASN	3.4
7	G	242	GLN	3.4
11	Y	106	ARG	3.4
4	R	114	ARG	3.3
14	N	195	GLN	3.3
2	B	222	GLY	3.3
5	E	122	TYR	3.3
3	C	49	THR	3.3
1	A	59	GLU	3.3
2	B	51	VAL	3.3
1	O	248	GLU	3.3
10	X	193	ASP	3.3
1	A	2	THR	3.3
3	Q	59	PRO	3.3
3	Q	229	GLN	3.3
6	T	178	HIS	3.2
3	Q	221	ALA	3.2
7	U	181	LYS	3.2
10	J	193	ASP	3.1
5	E	233	ILE	3.1
11	Y	147	ASP	3.1
5	E	201	ARG	3.1
14	b	195	GLN	3.1
5	S	123	GLY	3.1
1	A	52	SER	3.1
6	F	215	CYS	3.1
7	U	241	GLU	3.1
9	W	133	LYS	3.1
3	Q	207	ASN	3.1
3	Q	236	GLN	3.0
1	A	250	LEU	3.0
13	M	82	ASP	3.0
7	U	242	GLN	3.0
6	T	182	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
3	Q	51	LYS	2.9
3	C	228	ASN	2.9
5	S	204	SER	2.9
2	B	60	THR	2.9
3	C	238	LYS	2.9
6	T	205	GLU	2.9
5	E	3	ASN	2.9
9	I	192	ASP	2.9
12	Z	210	ASP	2.9
3	C	48	SER	2.9
3	C	236	GLN	2.8
6	F	241	LYS	2.8
5	E	218	ASP	2.8
1	O	201	GLU	2.8
3	Q	225	GLU	2.8
6	F	177	ASP	2.8
3	Q	232	THR	2.8
7	G	240	ALA	2.7
2	B	59	ASP	2.7
6	F	181	GLU	2.7
5	S	203	GLU	2.7
1	A	54	PRO	2.7
4	D	166	SER	2.7
12	Z	1	GLN	2.7
6	F	178	HIS	2.7
7	G	188	GLU	2.7
5	S	124	GLY	2.7
1	O	53	SER	2.7
4	D	114	ARG	2.7
6	T	181	GLU	2.7
3	Q	3	ASP	2.6
5	S	3	ASN	2.6
12	L	169	LYS	2.6
5	S	225	ASP	2.6
3	C	229	GLN	2.6
7	G	241	GLU	2.6
6	T	177	ASP	2.6
6	T	53	LYS	2.6
12	Z	165	ASN	2.6
7	G	2	GLY	2.6
2	B	217	LYS	2.5
6	T	166	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
4	R	54	ASP	2.5
9	W	192	ASP	2.5
10	X	11	ASP	2.5
14	b	104	ASP	2.5
6	T	204	LYS	2.5
5	E	54	GLU	2.5
7	G	230	GLU	2.5
7	U	222	ASP	2.5
4	D	125	LEU	2.5
2	B	61	SER	2.5
6	T	202	ASP	2.5
12	L	210	ASP	2.5
4	D	201	GLU	2.5
11	Y	151	GLU	2.5
2	P	60	THR	2.5
14	b	71	GLY	2.5
10	X	110	LYS	2.5
6	F	2	THR	2.4
4	R	125	LEU	2.4
3	C	207	ASN	2.4
13	M	47	ASP	2.4
2	B	62	THR	2.4
2	B	203	SER	2.4
13	M	204	THR	2.4
4	D	2	ARG	2.4
4	D	239	GLU	2.4
1	O	182	GLU	2.4
7	U	203	ASP	2.4
10	J	113	LYS	2.4
14	b	105	LYS	2.4
1	A	201	GLU	2.4
14	N	181	ALA	2.3
2	P	93	HIS	2.3
6	F	207	ASP	2.3
3	C	60	SER	2.3
3	Q	187	GLU	2.3
1	O	203	GLU	2.3
3	Q	188	GLU	2.3
3	Q	205	ALA	2.3
6	F	14	ASP	2.3
1	A	51	SER	2.3
4	D	241	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
6	F	243	ILE	2.3
3	Q	220	VAL	2.3
4	D	1	ASP	2.3
8	V	217	ILE	2.3
2	P	50	LYS	2.2
6	F	228	LYS	2.2
7	G	237	VAL	2.2
3	Q	235	GLU	2.2
11	K	151	GLU	2.2
1	A	249	ALA	2.2
5	S	194	GLU	2.2
6	F	174	LYS	2.2
4	R	141	ALA	2.2
1	O	2	THR	2.2
3	Q	231	VAL	2.2
2	B	169	SER	2.2
8	H	221	CYS	2.2
1	A	229	THR	2.2
6	T	207	ASP	2.2
7	U	212	ASN	2.2
7	G	236	LEU	2.2
6	T	201	GLU	2.2
2	P	52	THR	2.2
7	U	237	VAL	2.2
1	O	245	ASP	2.1
13	a	82	ASP	2.1
3	C	175	LYS	2.1
3	Q	171	GLU	2.1
3	C	216	ASP	2.1
5	S	218	ASP	2.1
4	R	226	GLU	2.1
8	V	9	ASN	2.1
1	O	230	ASP	2.1
3	C	50	LEU	2.1
5	E	117	LYS	2.1
6	F	166	GLN	2.1
13	a	216	ASN	2.1
5	S	171	LEU	2.1
1	A	228	PRO	2.1
3	Q	56	ARG	2.1
11	K	147	ASP	2.1
1	A	166	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	P	181	ASP	2.1
5	E	67	GLU	2.1
6	T	187	GLU	2.1
13	a	175	GLU	2.1
3	Q	208	ILE	2.1
10	X	113	LYS	2.1
5	S	201	ARG	2.0
1	A	53	SER	2.0
7	G	213	ASP	2.0
4	R	217	GLN	2.0
2	B	225	TYR	2.0
6	F	204	LYS	2.0
5	E	123	GLY	2.0
3	Q	58	THR	2.0
3	Q	237	GLU	2.0
7	G	68	ARG	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, 95^{th} 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	ASJ	c	4	8/8	0.84	0.21	45,51,56,57	0
15	ASJ	g	4	8/8	0.92	0.17	58,64,68,70	0
15	ASJ	e	4	8/8	0.93	0.16	43,47,49,50	0
15	ASJ	h	4	8/8	0.93	0.18	47,49,51,51	0
15	ASJ	d	4	8/8	0.95	0.15	46,55,59,59	0
15	ASJ	f	4	8/8	0.95	0.16	46,50,52,56	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, 95^{th} 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
17	MES	f	101	12/12	0.81	0.41	64,111,128,130	0
17	MES	c	302	12/12	0.85	0.30	53,91,109,114	0
16	MG	K	301	1/1	0.86	0.13	55,55,55,55	0
16	MG	G	301	1/1	0.88	0.19	50,50,50,50	0
16	MG	N	201	1/1	0.88	0.17	40,40,40,40	0
17	MES	K	302	12/12	0.89	0.26	51,71,75,76	0
17	MES	Y	301	12/12	0.89	0.28	53,71,75,76	0
19	K	c	301	1/1	0.89	0.35	30,30,30,30	0
16	MG	J	201	1/1	0.94	0.31	30,30,30,30	0
16	MG	I	301	1/1	0.95	0.15	47,47,47,47	0
16	MG	W	301	1/1	0.96	0.13	30,30,30,30	0
16	MG	L	301	1/1	0.97	0.06	46,46,46,46	0
18	CL	U	301	1/1	0.98	0.19	32,32,32,32	0
16	MG	I	302	1/1	0.99	0.09	41,41,41,41	0
19	K	f	102	1/1	0.99	0.07	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.