Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 08:56 PM GMT

PDB ID	:	4Y80
Title	:	Yeast 20S proteasome in complex with Ac-LAI-ep
Authors	:	Huber, E.M.; Groll, M.
Deposited on	:	2015-02-16
Resolution	:	2.50 Å(reported)

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

The following versions of software and data (see references (1)) were used in the production of this report:

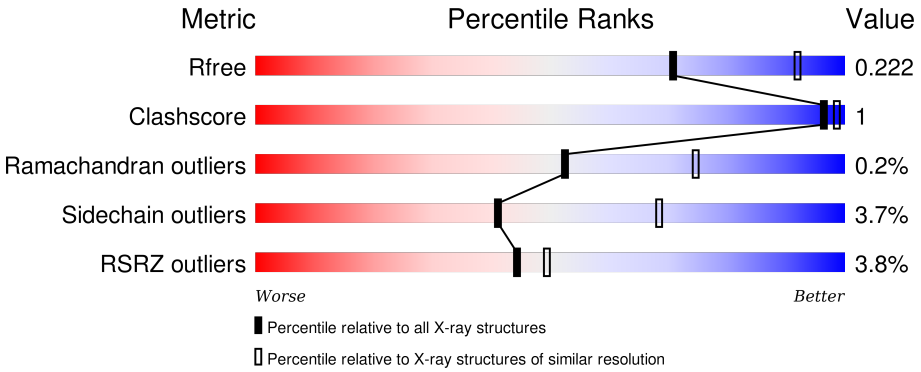
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	4% 96% ·
1	O	250	4% 95% 5%
2	B	258	7% 88% 7% 5%
2	P	258	7% 88% 6% 5%
3	C	254	9% 87% 6% · 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	11% 87% 6% 6%
4	D	260	2% 85% 5% 10%
4	R	260	4% 84% 6% 10%
5	E	234	5% 92% 6%
5	S	234	7% 91% 8%
6	F	288	5% 80% 5% 16%
6	T	288	5% 80% 5% 16%
7	G	252	6% 90% 5%
7	U	252	3% 90% 6%
8	H	232	% 91% 5%
8	V	232	3% 91%
9	I	205	% 93% 6%
9	W	205	2% 92% 7%
10	J	198	% 91% 6%
10	X	198	2% 91% 6%
11	K	212	% 92% 7%
11	Y	212	2% 92% 8%
12	L	222	94% 5%
12	Z	222	94% 5%
13	M	246	3% 91% 6%
13	a	246	% 92% 5%
14	N	196	% 96%
14	b	196	% 98%
15	c	5	100%
15	d	5	100%

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Mol	Chain	Length	Quality of chain
15	e	5	100%
15	f	5	100%
15	g	5	100%
15	h	5	100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	MG	I	301	-	-	-	X
16	MG	Z	301	-	-	-	X
18	MES	H	301	-	-	-	X
18	MES	d	101	-	-	-	X
18	MES	g	101	-	-	-	X

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 50255 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
			1684	1061	293	323	7			
8	V	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			
9	W	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	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	0	0
			1757	1115	303	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	232	Total	C	N	O	S	0	0	0
			1815	1148	311	349	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-LAI-ep.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	c	5	Total	C	N	O	0	0	0
			28	20	3	5			
15	d	5	Total	C	N	O	0	0	0
			28	20	3	5			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
15	e	5	Total C N O 28 20 3 5	0	0	0
15	f	5	Total C N O 28 20 3 5	0	0	0
15	g	5	Total C N O 28 20 3 5	0	0	0
15	h	5	Total C N O 28 20 3 5	0	0	0

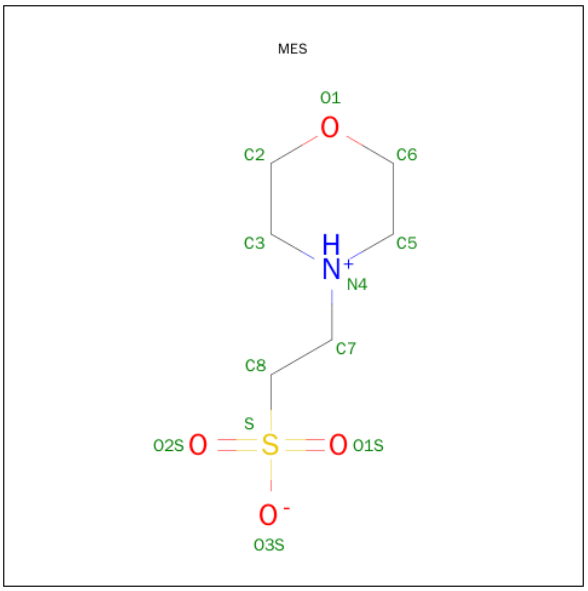
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 17 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 18 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	H	1	Total C N O S 12 6 1 4 1	0	0
18	d	1	Total C N O S 12 6 1 4 1	0	0
18	g	1	Total C N O S 12 6 1 4 1	0	0

- Molecule 19 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	32	Total O 32 32	0	0
19	B	26	Total O 26 26	0	0
19	C	29	Total O 29 29	0	0
19	D	15	Total O 15 15	0	0
19	E	11	Total O 11 11	0	0
19	F	25	Total O 25 25	0	0
19	G	38	Total O 38 38	0	0
19	H	26	Total O 26 26	0	0
19	I	32	Total O 32 32	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	J	37	Total O 37 37	0	0
19	K	33	Total O 33 33	0	0
19	L	28	Total O 28 28	0	0
19	M	39	Total O 39 39	0	0
19	N	23	Total O 23 23	0	0
19	O	23	Total O 23 23	0	0
19	P	21	Total O 21 21	0	0
19	Q	16	Total O 16 16	0	0
19	R	19	Total O 19 19	0	0
19	S	8	Total O 8 8	0	0
19	T	26	Total O 26 26	0	0
19	U	31	Total O 31 31	0	0
19	V	21	Total O 21 21	0	0
19	W	22	Total O 22 22	0	0
19	X	29	Total O 29 29	0	0
19	Y	27	Total O 27 27	0	0
19	Z	36	Total O 36 36	0	0
19	a	38	Total O 38 38	0	0
19	b	26	Total O 26 26	0	0
19	d	1	Total O 1 1	0	0
19	e	2	Total O 2 2	0	0

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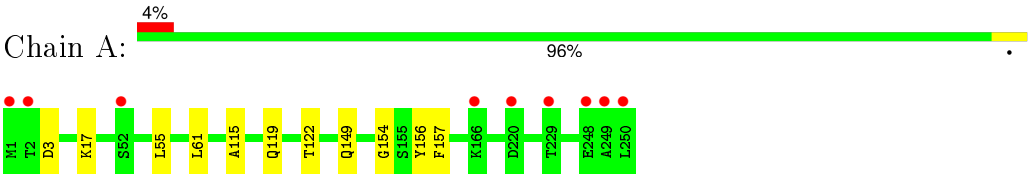
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	f	1	Total O 1 1	0	0
19	g	3	Total O 3 3	0	0
19	h	2	Total O 2 2	0	0

3 Residue-property plots (i)

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

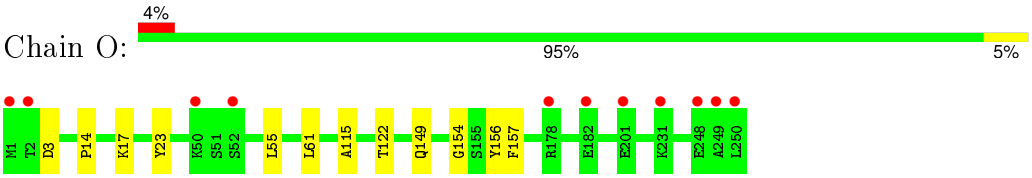
- Molecule 1: Proteasome subunit alpha type-2

Chain A:



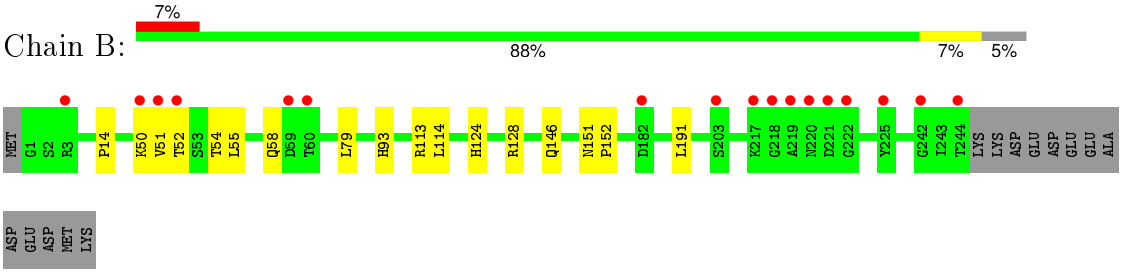
- Molecule 1: Proteasome subunit alpha type-2

Chain O:



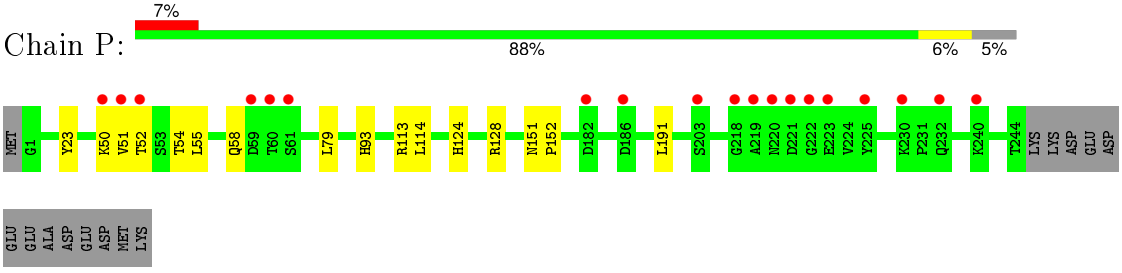
- Molecule 2: Proteasome subunit alpha type-3

Chain B:



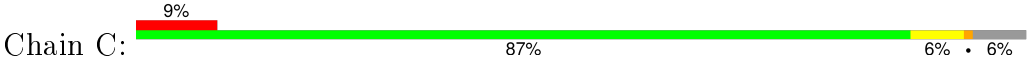
- Molecule 2: Proteasome subunit alpha type-3

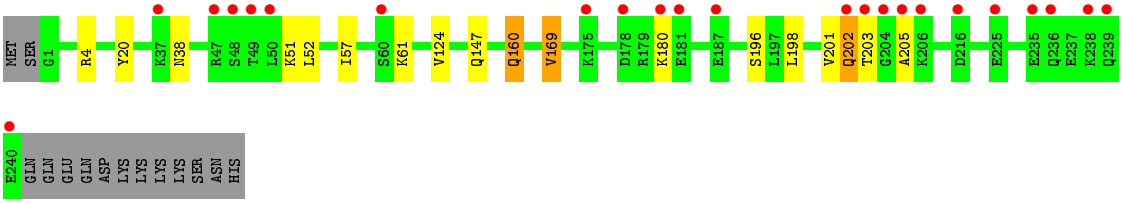
Chain P:



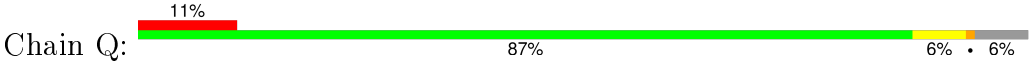
- Molecule 3: Proteasome subunit alpha type-4

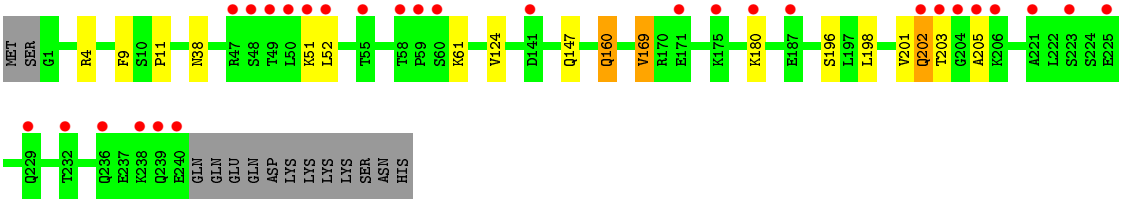
Chain C:



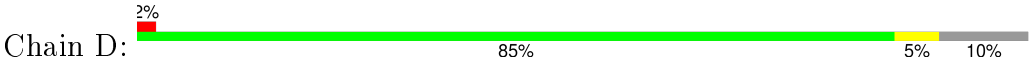


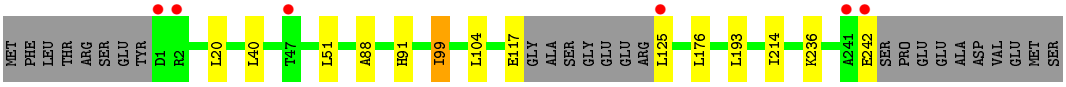
• Molecule 3: Proteasome subunit alpha type-4



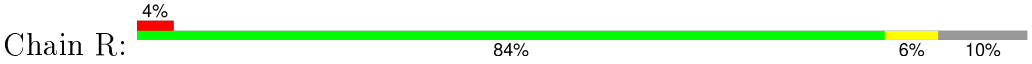


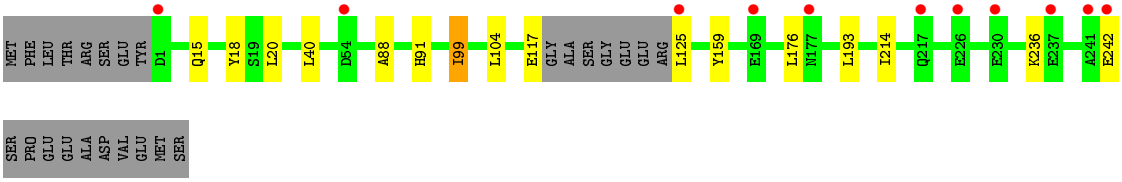
• Molecule 4: Proteasome subunit alpha type-5



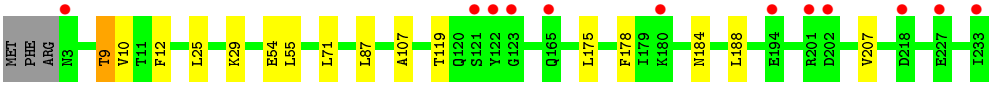


• Molecule 4: Proteasome subunit alpha type-5

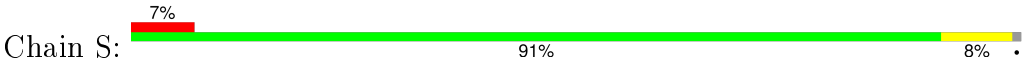


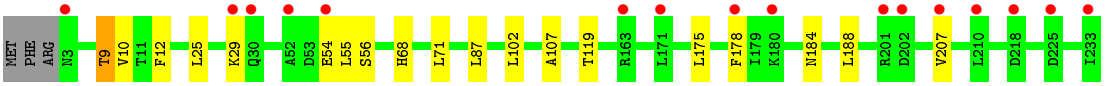


• Molecule 5: Proteasome subunit alpha type-6



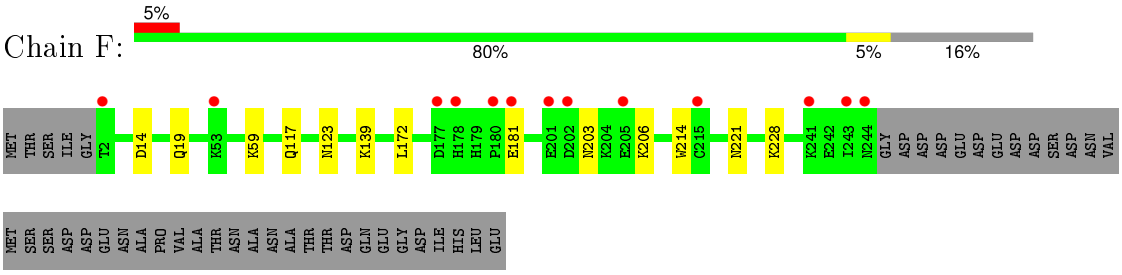
• Molecule 5: Proteasome subunit alpha type-6





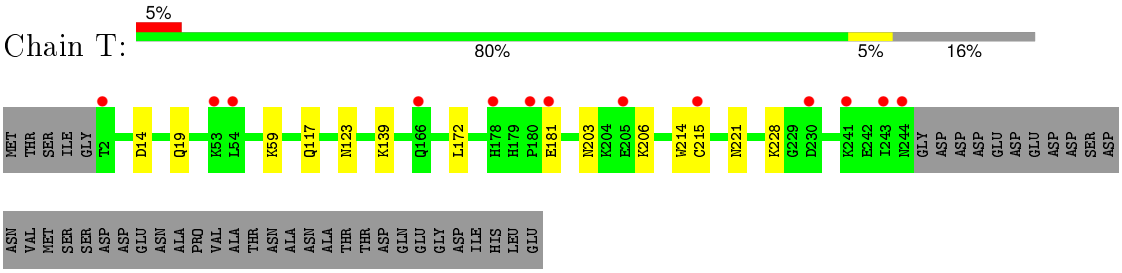
• Molecule 6: Probable proteasome subunit alpha type-7

Chain F:



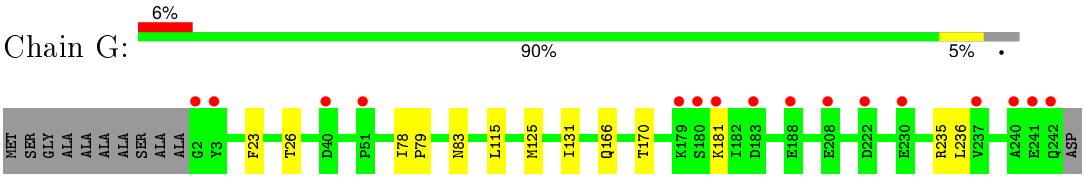
• Molecule 6: Probable proteasome subunit alpha type-7

Chain T:



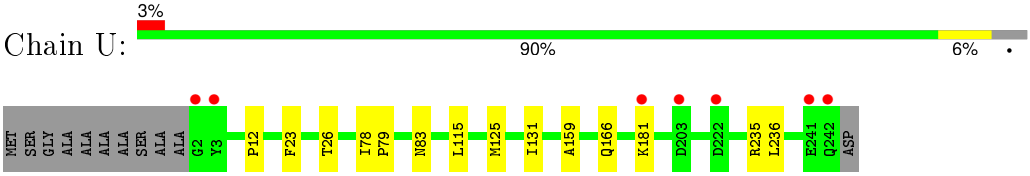
• Molecule 7: Proteasome subunit alpha type-1

Chain G:



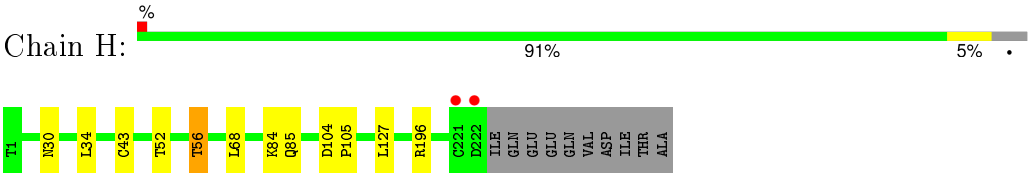
• Molecule 7: Proteasome subunit alpha type-1

Chain U:



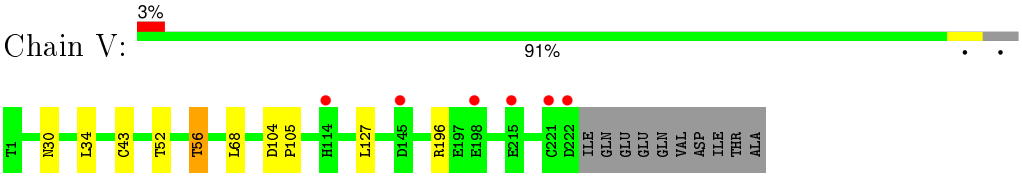
• Molecule 8: Proteasome subunit beta type-2

Chain H:



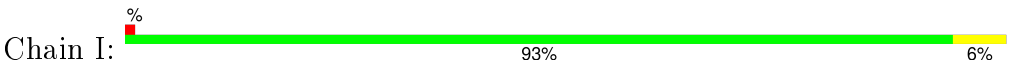
• Molecule 8: Proteasome subunit beta type-2

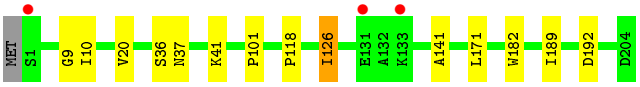
Chain V:



• Molecule 9: Proteasome subunit beta type-3

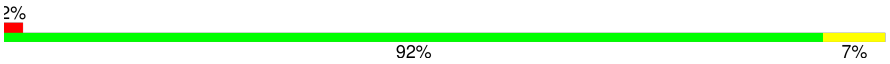
Chain I:

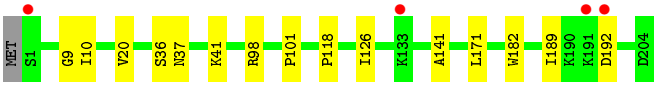




• Molecule 9: Proteasome subunit beta type-3

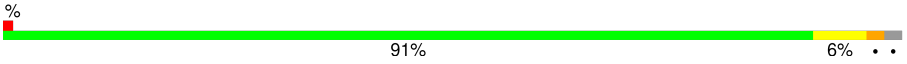
Chain W:

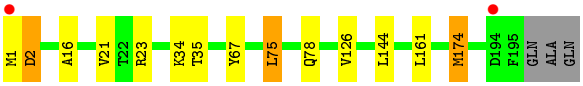




• Molecule 10: Proteasome subunit beta type-4

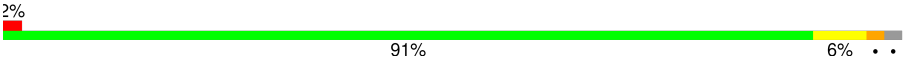
Chain J:

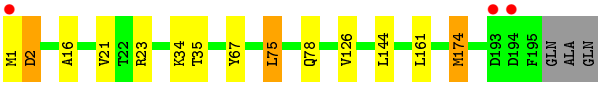




• Molecule 10: Proteasome subunit beta type-4

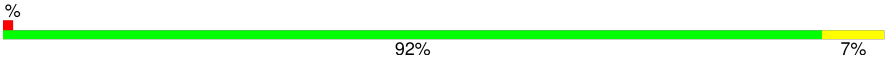
Chain X:

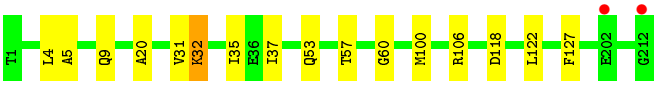




• Molecule 11: Proteasome subunit beta type-5

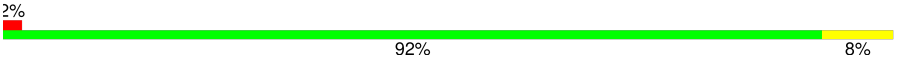
Chain K:





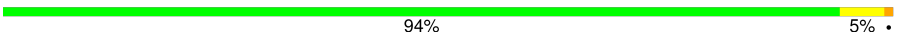
• Molecule 11: Proteasome subunit beta type-5

Chain Y:



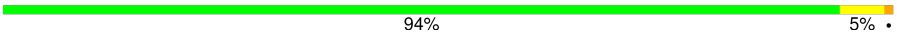
• Molecule 12: Proteasome subunit beta type-6

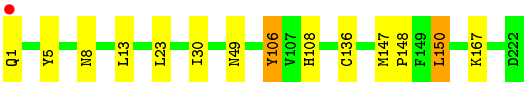
Chain L:



• Molecule 12: Proteasome subunit beta type-6

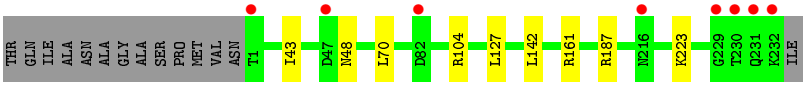
Chain Z:





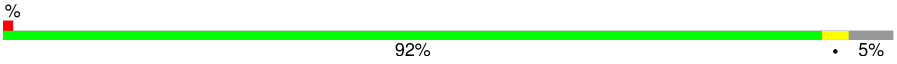
• Molecule 13: Proteasome subunit beta type-7

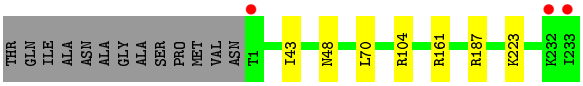
Chain M:



• Molecule 13: Proteasome subunit beta type-7

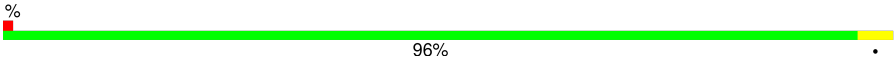
Chain a:

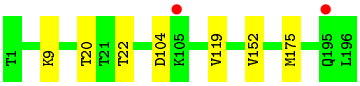




• Molecule 14: Proteasome subunit beta type-1

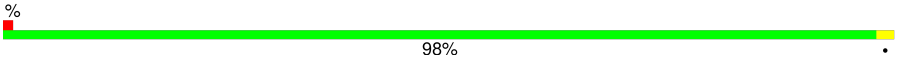
Chain N:

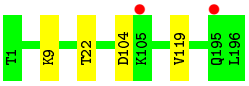




• Molecule 14: Proteasome subunit beta type-1

Chain b:





• Molecule 15: Ac-LAI-ep

Chain c:

There are no outlier residues recorded for this chain.

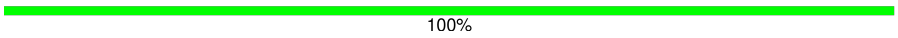
• Molecule 15: Ac-LAI-ep

Chain d:

There are no outlier residues recorded for this chain.

• Molecule 15: Ac-LAI-ep

Chain e:



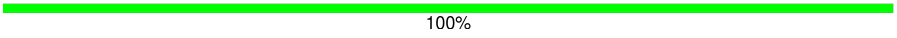
There are no outlier residues recorded for this chain.

• Molecule 15: Ac-LAI-ep

Chain f: 

There are no outlier residues recorded for this chain.

- Molecule 15: Ac-LAI-ep

Chain g: 

There are no outlier residues recorded for this chain.

- Molecule 15: Ac-LAI-ep

Chain h: 

There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	136.63Å 300.15Å 145.43Å 90.00° 113.22° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 14.99 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.4 (15.00-2.50) 97.4 (14.99-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.79 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.202 , 0.219 0.205 , 0.222	Depositor DCC
R_{free} test set	17918 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	50.2	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 28.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 358359 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	50255	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MES, ACE, CL, POL, IL0

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	0.27	0/1952	0.48	0/2642
1	O	0.27	0/1952	0.48	0/2642
2	B	0.28	0/1934	0.50	0/2618
2	P	0.27	0/1934	0.50	0/2618
3	C	0.28	0/1910	0.51	0/2586
3	Q	0.28	0/1910	0.51	0/2586
4	D	0.27	0/1837	0.48	0/2475
4	R	0.27	0/1837	0.48	0/2475
5	E	0.27	0/1800	0.48	0/2433
5	S	0.27	0/1800	0.48	0/2433
6	F	0.27	0/1932	0.46	0/2609
6	T	0.27	0/1932	0.46	0/2609
7	G	0.27	0/1945	0.48	0/2634
7	U	0.28	0/1945	0.48	0/2634
8	H	0.27	0/1715	0.49	0/2326
8	V	0.26	0/1715	0.49	0/2326
9	I	0.28	0/1611	0.49	0/2174
9	W	0.28	0/1611	0.48	0/2174
10	J	0.26	0/1589	0.49	0/2142
10	X	0.26	0/1589	0.49	0/2142
11	K	0.29	0/1681	0.54	1/2274 (0.0%)
11	Y	0.27	0/1681	0.55	1/2274 (0.0%)
12	L	0.28	0/1795	0.48	0/2420
12	Z	0.35	2/1806 (0.1%)	0.56	4/2435 (0.2%)
13	M	0.28	0/1846	0.52	0/2503
13	a	0.27	0/1855	0.52	0/2514
14	N	0.32	0/1541	0.50	0/2087
14	b	0.29	0/1541	0.49	0/2087
15	c	1.03	0/13	1.43	0/17
15	d	1.27	0/13	1.31	0/17
15	e	0.70	0/13	1.36	0/17
15	f	0.50	0/13	1.14	0/17

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
15	g	0.36	0/13	1.23	0/17
15	h	0.46	0/13	1.17	0/17
All	All	0.28	2/50274 (0.0%)	0.50	6/67974 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	Z	108[A]	HIS	CA-C	5.85	1.68	1.52
12	Z	108[B]	HIS	CA-C	5.85	1.68	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	Y	32	LYS	CB-CG-CD	8.75	134.35	111.60
11	K	32	LYS	CB-CG-CD	8.27	133.09	111.60
12	Z	108[A]	HIS	CA-C-O	6.64	134.04	120.10
12	Z	108[B]	HIS	CA-C-O	6.64	134.04	120.10
12	Z	108[A]	HIS	CA-C-N	-5.01	106.18	117.20
12	Z	108[B]	HIS	CA-C-N	-5.01	106.18	117.20

There are no chirality outliers.

There are no planarity outliers.

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	5	0
1	O	1915	0	1929	6	0
2	B	1904	0	1904	7	0
2	P	1904	0	1904	6	0
3	C	1881	0	1895	10	0
3	Q	1881	0	1895	10	0
4	D	1813	0	1797	3	0
4	R	1813	0	1797	6	0
5	E	1773	0	1775	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	S	1773	0	1775	6	0
6	F	1892	0	1883	2	0
6	T	1892	0	1883	3	0
7	G	1907	0	1901	4	0
7	U	1907	0	1901	5	0
8	H	1684	0	1685	3	0
8	V	1684	0	1685	2	0
9	I	1581	0	1574	7	0
9	W	1581	0	1574	7	0
10	J	1561	0	1569	9	0
10	X	1561	0	1569	8	0
11	K	1644	0	1592	8	0
11	Y	1644	0	1592	8	0
12	L	1757	0	1711	4	0
12	Z	1764	0	1718	4	0
13	M	1815	0	1821	1	0
13	a	1824	0	1832	0	0
14	N	1512	0	1478	1	0
14	b	1512	0	1478	0	0
15	c	28	0	36	0	0
15	d	28	0	36	0	0
15	e	28	0	36	0	0
15	f	28	0	36	0	0
15	g	28	0	36	0	0
15	h	28	0	36	0	0
16	G	1	0	0	0	0
16	I	2	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	Z	1	0	0	0	0
17	G	1	0	0	0	0
17	N	1	0	0	0	0
17	U	1	0	0	0	0
17	b	1	0	0	0	0
18	H	12	0	13	0	0
18	d	12	0	13	0	0
18	g	12	0	13	0	0
19	A	32	0	0	0	0
19	B	26	0	0	0	0
19	C	29	0	0	0	0
19	D	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	E	11	0	0	0	0
19	F	25	0	0	0	0
19	G	38	0	0	0	0
19	H	26	0	0	0	0
19	I	32	0	0	0	0
19	J	37	0	0	0	0
19	K	33	0	0	0	0
19	L	28	0	0	0	0
19	M	39	0	0	0	0
19	N	23	0	0	0	0
19	O	23	0	0	0	0
19	P	21	0	0	0	0
19	Q	16	0	0	0	0
19	R	19	0	0	0	0
19	S	8	0	0	0	0
19	T	26	0	0	1	0
19	U	31	0	0	0	0
19	V	21	0	0	0	0
19	W	22	0	0	0	0
19	X	29	0	0	0	0
19	Y	27	0	0	0	0
19	Z	36	0	0	0	0
19	a	38	0	0	0	0
19	b	26	0	0	0	0
19	d	1	0	0	0	0
19	e	2	0	0	0	0
19	f	1	0	0	0	0
19	g	3	0	0	0	0
19	h	2	0	0	0	0
All	All	50255	0	49301	119	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 1.

All (119) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:1:MET:O	10:J:2:ASP:HB2	1.84	0.76
10:X:1:MET:O	10:X:2:ASP:HB2	1.84	0.75
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.75	0.68
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:99:ILE:HD11	4:D:104:LEU:HB2	1.78	0.66
4:R:99:ILE:HD11	4:R:104:LEU:HB2	1.77	0.65
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.78	0.64
11:Y:5:ALA:HB3	11:Y:100:MET:HE2	1.82	0.61
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.85	0.59
3:C:51:LYS:O	3:C:52:LEU:HB2	2.05	0.56
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.06	0.56
11:K:5:ALA:HB3	11:K:100:MET:HE2	1.88	0.55
10:J:174:MET:HA	10:X:174:MET:HA	1.88	0.55
7:G:23:PHE:O	7:G:26:THR:HB	2.07	0.55
7:U:23:PHE:O	7:U:26:THR:HB	2.07	0.55
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.73	0.54
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.73	0.54
11:K:100:MET:CE	11:K:127:PHE:HB2	2.39	0.52
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	1.92	0.52
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.75	0.52
11:Y:100:MET:CE	11:Y:127:PHE:HB2	2.39	0.51
9:I:101:PRO:HB3	9:I:126:ILE:HD12	1.91	0.51
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.93	0.51
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.93	0.51
5:E:12:PHE:H	6:F:19:GLN:HE22	1.57	0.50
12:Z:5:TYR:CE1	12:Z:106:TYR:CD1	3.00	0.50
12:L:5:TYR:CE1	12:L:106:TYR:CD1	3.00	0.49
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.94	0.49
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.94	0.49
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.95	0.49
3:C:201:VAL:HG13	3:C:202:GLN:N	2.27	0.49
2:B:146:GLN:HG2	3:C:57:ILE:HG21	1.93	0.49
2:B:124:HIS:HB3	3:C:124:VAL:HG12	1.93	0.49
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.95	0.49
3:C:201:VAL:O	3:C:202:GLN:CB	2.61	0.49
5:S:12:PHE:H	6:T:19:GLN:HE22	1.59	0.49
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.61	0.48
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.28	0.48
9:W:98:ARG:O	9:W:126:ILE:HD11	2.13	0.48
14:N:152:VAL:HA	14:N:175:MET:HE1	1.95	0.48
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.95	0.48
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.96	0.48
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.77	0.48
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.94	0.48
10:X:1:MET:O	10:X:2:ASP:CB	2.59	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:215:CYS:HB3	19:T:305:HOH:O	2.13	0.47
1:O:55:LEU:HB3	7:U:159:ALA:O	2.15	0.47
8:H:52:THR:O	8:H:56:THR:HB	2.15	0.47
3:Q:201:VAL:O	3:Q:202:GLN:HB2	2.14	0.47
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.97	0.47
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.96	0.47
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.97	0.47
3:C:201:VAL:O	3:C:202:GLN:HB2	2.14	0.46
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.96	0.46
9:W:36:SER:HB2	10:X:126:VAL:HG11	1.98	0.46
6:F:228:LYS:HB2	6:F:228:LYS:HE3	1.81	0.46
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.98	0.46
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	1.98	0.45
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.52	0.45
2:P:151:ASN:HB2	2:P:152:PRO:HD2	1.99	0.45
5:E:9:THR:HG21	5:E:119:THR:HA	1.99	0.45
8:V:52:THR:O	8:V:56:THR:HB	2.16	0.44
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.17	0.44
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.52	0.44
10:J:1:MET:O	10:J:2:ASP:CB	2.59	0.44
2:B:151:ASN:HB2	2:B:152:PRO:HD2	1.99	0.44
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.51	0.44
5:S:9:THR:HG21	5:S:119:THR:HA	1.99	0.44
9:W:101:PRO:HB3	9:W:126:ILE:HD12	2.00	0.44
12:L:8:ASN:HA	12:L:30:ILE:O	2.17	0.44
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.66	0.44
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.33	0.44
3:Q:11:PRO:HA	4:R:18:TYR:CD1	2.53	0.43
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.53	0.43
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.53	0.43
9:W:20:VAL:HG23	9:W:189:ILE:HB	2.00	0.43
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.53	0.43
3:C:169:VAL:HG23	3:C:196:SER:HB2	2.00	0.43
9:I:20:VAL:HG23	9:I:189:ILE:HB	2.00	0.43
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.00	0.43
2:B:93:HIS:HB3	2:B:113:ARG:HH21	1.83	0.43
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	2.00	0.43
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.00	0.43
12:L:147:MET:N	12:L:148:PRO:HD2	2.33	0.43
2:P:93:HIS:HB3	2:P:113:ARG:HH21	1.83	0.43
7:U:26:THR:HG21	7:U:131:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.49	0.42
1:A:149:GLN:O	1:A:156:TYR:HA	2.20	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.42
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.02	0.42
1:O:14:PRO:HA	2:P:23:TYR:CD1	2.55	0.42
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.49	0.42
3:C:198:LEU:HA	3:C:201:VAL:HG12	2.02	0.42
3:Q:198:LEU:HA	3:Q:201:VAL:HG12	2.02	0.42
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.49	0.42
11:K:53:GLN:O	11:K:57:THR:HG23	2.20	0.42
1:O:149:GLN:O	1:O:156:TYR:HA	2.19	0.42
11:Y:53:GLN:O	11:Y:57:THR:HG23	2.20	0.42
7:G:26:THR:HG21	7:G:131:ILE:HD12	2.01	0.42
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.49	0.42
1:A:115:ALA:HB1	1:A:154:GLY:O	2.21	0.41
1:A:55:LEU:HD12	7:G:170:THR:HG23	2.01	0.41
10:J:1:MET:HA	10:J:34:LYS:CE	2.50	0.41
11:K:5:ALA:HB3	11:K:100:MET:CE	2.49	0.41
8:H:84:LYS:HG3	8:H:85:GLN:N	2.36	0.41
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.56	0.41
10:X:1:MET:HA	10:X:34:LYS:CE	2.50	0.41
11:K:20:ALA:HB2	11:K:31:VAL:HG21	2.02	0.41
6:T:228:LYS:HB2	6:T:228:LYS:HE3	1.81	0.41
1:O:115:ALA:HB1	1:O:154:GLY:O	2.21	0.41
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	2.02	0.41
10:J:1:MET:HA	10:J:34:LYS:HE3	2.03	0.41
1:A:119:GLN:O	1:A:122:THR:HB	2.21	0.40
11:K:37:ILE:HG23	11:K:60:GLY:HA2	2.02	0.40
5:S:68:HIS:HE1	5:S:102:LEU:O	2.04	0.40
11:Y:37:ILE:HG23	11:Y:60:GLY:HA2	2.02	0.40
9:I:101:PRO:HB3	9:I:126:ILE:CD1	2.51	0.40
11:Y:5:ALA:HB3	11:Y:100:MET:CE	2.50	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%)	241 (97%)	6 (2%)	1 (0%)	39	61
1	O	248/250 (99%)	241 (97%)	6 (2%)	1 (0%)	39	61
2	B	242/258 (94%)	234 (97%)	7 (3%)	1 (0%)	39	61
2	P	242/258 (94%)	234 (97%)	7 (3%)	1 (0%)	39	61
3	C	238/254 (94%)	230 (97%)	6 (2%)	2 (1%)	24	41
3	Q	238/254 (94%)	230 (97%)	6 (2%)	2 (1%)	24	41
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%)	223 (97%)	6 (3%)	0	100	100
5	S	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
6	F	241/288 (84%)	234 (97%)	7 (3%)	0	100	100
6	T	241/288 (84%)	234 (97%)	7 (3%)	0	100	100
7	G	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
7	U	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
8	H	220/232 (95%)	215 (98%)	5 (2%)	0	100	100
8	V	220/232 (95%)	215 (98%)	5 (2%)	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%)	189 (98%)	3 (2%)	1 (0%)	34	55
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	34	55
11	K	210/212 (99%)	207 (99%)	3 (1%)	0	100	100
11	Y	210/212 (99%)	207 (99%)	3 (1%)	0	100	100
12	L	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
12	Z	221/222 (100%)	217 (98%)	4 (2%)	0	100	100
13	M	230/246 (94%)	223 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	231/246 (94%)	224 (97%)	7 (3%)	0	100	100
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
14	b	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
15	c	2/5 (40%)	2 (100%)	0	0	100	100
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	6288/6644 (95%)	6132 (98%)	146 (2%)	10 (0%)	52	75

All (10) 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
1	A	3	ASP
1	O	3	ASP

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%)	74	91
1	O	209/209 (100%)	206 (99%)	3 (1%)	74	91
2	B	203/216 (94%)	195 (96%)	8 (4%)	39	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	203/216 (94%)	195 (96%)	8 (4%)	39	66
3	C	212/226 (94%)	204 (96%)	8 (4%)	40	67
3	Q	212/226 (94%)	204 (96%)	8 (4%)	40	67
4	D	194/215 (90%)	183 (94%)	11 (6%)	25	46
4	R	194/215 (90%)	184 (95%)	10 (5%)	29	51
5	E	190/193 (98%)	180 (95%)	10 (5%)	28	50
5	S	190/193 (98%)	180 (95%)	10 (5%)	28	50
6	F	201/239 (84%)	190 (94%)	11 (6%)	27	48
6	T	201/239 (84%)	190 (94%)	11 (6%)	27	48
7	G	206/210 (98%)	199 (97%)	7 (3%)	44	72
7	U	206/210 (98%)	199 (97%)	7 (3%)	44	72
8	H	181/190 (95%)	174 (96%)	7 (4%)	39	66
8	V	181/190 (95%)	174 (96%)	7 (4%)	39	66
9	I	172/173 (99%)	167 (97%)	5 (3%)	50	77
9	W	172/173 (99%)	168 (98%)	4 (2%)	58	83
10	J	173/175 (99%)	167 (96%)	6 (4%)	43	70
10	X	173/175 (99%)	167 (96%)	6 (4%)	43	70
11	K	169/169 (100%)	163 (96%)	6 (4%)	42	69
11	Y	169/169 (100%)	163 (96%)	6 (4%)	42	69
12	L	185/185 (100%)	178 (96%)	7 (4%)	40	67
12	Z	186/185 (100%)	179 (96%)	7 (4%)	40	67
13	M	198/208 (95%)	191 (96%)	7 (4%)	43	70
13	a	199/208 (96%)	192 (96%)	7 (4%)	43	70
14	N	162/162 (100%)	157 (97%)	5 (3%)	47	75
14	b	162/162 (100%)	158 (98%)	4 (2%)	55	82
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5318/5546 (96%)	5119 (96%)	199 (4%)	41 68

All (199) 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	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	51	LEU
4	D	99	ILE
4	D	117	GLU
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	55	LEU
5	E	71	LEU

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Mol	Chain	Res	Type
5	E	184	ASN
5	E	188	LEU
5	E	207	VAL
6	F	14	ASP
6	F	59	LYS
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
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	34	LEU
8	H	43	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	32	LYS

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Mol	Chain	Res	Type
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	106	TYR
12	L	136	CYS
12	L	150	LEU
12	L	167	LYS
13	M	43	ILE
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	20	THR
14	N	22	THR
14	N	104	ASP
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	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	203	THR
4	R	20	LEU

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Mol	Chain	Res	Type
4	R	40	LEU
4	R	99	ILE
4	R	117	GLU
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
5	S	29	LYS
5	S	54	GLU
5	S	55	LEU
5	S	71	LEU
5	S	184	ASN
5	S	188	LEU
5	S	207	VAL
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	34	LEU
8	V	43	CYS
8	V	56	THR
8	V	68	LEU

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Mol	Chain	Res	Type
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	7	ARG
11	Y	9	GLN
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	106	TYR
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	104	ASP
14	b	119	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN

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Mol	Chain	Res	Type
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
3	C	38	ASN
3	C	77	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	146	GLN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
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	191	GLN
6	F	240	GLN
7	G	6	HIS
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	167	GLN
8	H	57	GLN
8	H	66	HIS
10	J	55	GLN
11	K	85	ASN
11	K	176	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	158	ASN
13	M	18	ASN
13	M	48	ASN

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Mol	Chain	Res	Type
13	M	102	GLN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	161	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	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	146	GLN
4	R	225	ASN
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	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
10	X	55	GLN
10	X	86	GLN
11	Y	85	ASN
11	Y	176	ASN
12	Z	3	ASN
12	Z	49	ASN

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Mol	Chain	Res	Type
12	Z	70	ASN
12	Z	158	ASN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN
14	b	161	GLN

5.3.3 RNA (i)

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	IL0	c	4	8,15	7,7,8	0.68	0	6,8,10	1.62	2 (33%)
15	IL0	d	4	11,15	7,7,8	1.06	1 (14%)	6,8,10	1.40	2 (33%)
15	IL0	e	4	15,14	7,7,8	1.29	1 (14%)	6,8,10	1.69	2 (33%)
15	IL0	f	4	8,15	7,7,8	0.79	0	6,8,10	1.11	0
15	IL0	g	4	11,15	7,7,8	0.98	1 (14%)	6,8,10	1.08	0
15	IL0	h	4	15,14	7,7,8	1.37	1 (14%)	6,8,10	1.40	1 (16%)

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	IL0	c	4	8,15	-	0/8/8/10	0/0/0/0
15	IL0	d	4	11,15	-	0/8/8/10	0/0/0/0
15	IL0	e	4	15,14	-	0/8/8/10	0/0/0/0
15	IL0	f	4	8,15	-	0/8/8/10	0/0/0/0
15	IL0	g	4	11,15	-	0/8/8/10	0/0/0/0
15	IL0	h	4	15,14	-	0/8/8/10	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	g	4	IL0	C-CA	2.28	1.55	1.52
15	d	4	IL0	C-CA	2.33	1.55	1.52
15	e	4	IL0	C-CA	3.16	1.56	1.52
15	h	4	IL0	C-CA	3.32	1.57	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	h	4	IL0	CG2-CB-CA	-3.04	107.30	111.44
15	e	4	IL0	O-C-CA	-2.95	105.25	111.44
15	c	4	IL0	O-C-CA	-2.94	105.27	111.44
15	d	4	IL0	O-C-CA	-2.50	106.18	111.44
15	e	4	IL0	CG2-CB-CA	-2.49	108.04	111.44
15	c	4	IL0	CG2-CB-CA	-2.37	108.21	111.44
15	d	4	IL0	CG2-CB-CG1	-2.22	106.17	111.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 11 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
18	MES	H	301	-	12,12,12	2.09	1 (8%)	15,16,16	1.87	3 (20%)
18	MES	d	101	-	12,12,12	2.11	1 (8%)	15,16,16	1.54	3 (20%)
18	MES	g	101	-	12,12,12	2.10	1 (8%)	15,16,16	1.59	2 (13%)

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
18	MES	H	301	-	-	0/6/14/14	0/1/1/1
18	MES	d	101	-	-	0/6/14/14	0/1/1/1
18	MES	g	101	-	-	0/6/14/14	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	d	101	MES	C8-S	-6.97	1.67	1.77
18	g	101	MES	C8-S	-6.95	1.67	1.77
18	H	301	MES	C8-S	-6.94	1.67	1.77

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	H	301	MES	O3S-S-C8	2.23	109.63	104.99
18	d	101	MES	O1S-S-C8	2.44	108.59	106.87
18	g	101	MES	O3S-S-C8	2.67	110.53	104.99
18	d	101	MES	O3S-S-C8	2.68	110.56	104.99
18	d	101	MES	O2S-S-C8	3.59	109.41	106.87
18	H	301	MES	O1S-S-C8	4.08	109.75	106.87
18	g	101	MES	O2S-S-C8	4.42	109.99	106.87
18	H	301	MES	O2S-S-C8	4.70	110.19	106.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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%)	-0.12	9 (3%) 46 51	35, 49, 84, 127	0
1	O	250/250 (100%)	0.01	11 (4%) 38 43	38, 55, 99, 130	0
2	B	244/258 (94%)	0.09	17 (6%) 19 22	34, 53, 104, 159	0
2	P	244/258 (94%)	0.20	19 (7%) 16 17	38, 57, 109, 163	0
3	C	240/254 (94%)	0.22	23 (9%) 10 11	35, 56, 122, 164	0
3	Q	240/254 (94%)	0.51	29 (12%) 6 5	43, 73, 157, 202	0
4	D	235/260 (90%)	0.03	6 (2%) 59 63	42, 61, 97, 144	0
4	R	235/260 (90%)	0.15	11 (4%) 35 40	46, 65, 103, 156	0
5	E	231/234 (98%)	0.13	12 (5%) 31 35	42, 62, 97, 142	0
5	S	231/234 (98%)	0.24	16 (6%) 20 22	44, 68, 110, 145	0
6	F	243/288 (84%)	-0.04	13 (5%) 30 34	37, 57, 106, 134	0
6	T	243/288 (84%)	0.19	13 (5%) 30 34	41, 66, 119, 158	0
7	G	241/252 (95%)	-0.06	16 (6%) 22 24	34, 51, 94, 146	0
7	U	241/252 (95%)	-0.10	7 (2%) 55 60	36, 52, 85, 129	0
8	H	222/232 (95%)	-0.10	2 (0%) 85 88	36, 48, 75, 116	0
8	V	222/232 (95%)	-0.02	6 (2%) 58 62	37, 52, 80, 125	1 (0%)
9	I	204/205 (99%)	-0.34	3 (1%) 76 79	31, 44, 77, 95	0
9	W	204/205 (99%)	-0.30	4 (1%) 68 72	33, 48, 78, 102	0
10	J	195/198 (98%)	-0.31	2 (1%) 84 86	32, 46, 72, 117	0
10	X	195/198 (98%)	-0.27	3 (1%) 76 79	34, 49, 74, 126	0
11	K	212/212 (100%)	-0.30	2 (0%) 85 88	34, 46, 75, 91	0
11	Y	212/212 (100%)	-0.26	4 (1%) 70 73	36, 48, 77, 103	0
12	L	222/222 (100%)	-0.29	0 100 100	33, 49, 75, 103	0
12	Z	222/222 (100%)	-0.25	1 (0%) 91 92	33, 49, 78, 104	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	232/246 (94%)	-0.23	8 (3%) 49 54	29, 48, 77, 98	0
13	a	233/246 (94%)	-0.25	3 (1%) 79 82	31, 46, 72, 94	0
14	N	196/196 (100%)	-0.32	2 (1%) 84 86	33, 44, 72, 98	0
14	b	196/196 (100%)	-0.28	2 (1%) 84 86	34, 45, 74, 95	0
15	c	2/5 (40%)	-0.62	0 100 100	55, 55, 55, 57	0
15	d	2/5 (40%)	-0.72	0 100 100	55, 55, 55, 61	0
15	e	2/5 (40%)	0.99	0 100 100	55, 55, 55, 62	0
15	f	2/5 (40%)	0.03	0 100 100	56, 56, 56, 62	0
15	g	2/5 (40%)	-0.47	0 100 100	55, 55, 55, 64	0
15	h	2/5 (40%)	1.27	0 100 100	61, 61, 61, 69	0
All	All	6347/6644 (95%)	-0.06	244 (3%) 44 49	29, 53, 99, 202	1 (0%)

All (244) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	219	ALA	12.5
1	O	1	MET	10.4
2	B	220	ASN	9.1
3	Q	49	THR	8.4
3	C	206	LYS	8.3
1	A	1	MET	8.0
8	H	221	CYS	7.9
8	V	222	ASP	7.8
3	Q	50	LEU	7.4
3	Q	206	LYS	7.1
2	P	51	VAL	6.9
8	V	221	CYS	6.9
8	H	222	ASP	6.6
10	X	1	MET	6.4
2	P	222	GLY	6.2
2	P	218	GLY	6.1
3	Q	48	SER	6.0
9	W	1	SER	5.9
3	C	49	THR	5.9
10	J	1	MET	5.7
2	B	219	ALA	5.2
5	E	233	ILE	5.2
5	E	202	ASP	5.1

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Mol	Chain	Res	Type	RSRZ
2	B	51	VAL	5.1
7	U	222	ASP	5.1
3	Q	236	GLN	5.1
5	S	202	ASP	5.0
2	P	221	ASP	4.9
2	B	221	ASP	4.8
2	P	220	ASN	4.8
3	C	236	GLN	4.7
1	A	250	LEU	4.7
13	M	232	LYS	4.7
2	B	222	GLY	4.7
3	C	202	GLN	4.7
10	X	194	ASP	4.6
3	Q	225	GLU	4.6
10	J	194	ASP	4.5
9	I	1	SER	4.4
3	Q	239	GLN	4.4
4	D	241	ALA	4.4
3	Q	240	GLU	4.4
2	P	52	THR	4.4
2	B	218	GLY	4.3
3	Q	51	LYS	4.3
13	M	230	THR	4.3
13	M	1	THR	4.3
5	S	233	ILE	4.3
4	D	242	GLU	4.2
13	M	231	GLN	4.2
3	Q	238	LYS	4.1
3	C	238	LYS	4.1
3	C	225	GLU	4.0
2	P	59	ASP	4.0
1	O	249	ALA	4.0
3	C	205	ALA	4.0
3	Q	202	GLN	3.9
13	M	229	GLY	3.9
13	a	1	THR	3.8
3	Q	205	ALA	3.8
11	Y	106	ARG	3.7
3	C	50	LEU	3.7
6	F	243	ILE	3.7
13	a	233	ILE	3.7
10	X	193	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	242	GLY	3.6
7	U	2	GLY	3.6
7	G	179	LYS	3.6
6	T	215	CYS	3.6
1	O	201	GLU	3.5
7	U	181	LYS	3.5
3	C	239	GLN	3.5
1	O	231	LYS	3.5
11	Y	212	GLY	3.5
1	O	250	LEU	3.4
3	C	240	GLU	3.4
7	G	3	TYR	3.4
11	K	212	GLY	3.4
6	F	53	LYS	3.4
6	T	181	GLU	3.3
6	F	180	PRO	3.3
1	O	52	SER	3.3
4	R	241	ALA	3.3
5	S	54	GLU	3.3
4	R	242	GLU	3.3
6	T	241	LYS	3.3
4	R	125	LEU	3.2
3	Q	223	SER	3.2
3	Q	141	ASP	3.2
14	N	105	LYS	3.2
6	T	244	ASN	3.2
6	T	243	ILE	3.2
2	P	225	TYR	3.2
7	U	241	GLU	3.1
4	R	217	GLN	3.1
1	A	248	GLU	3.1
3	Q	55	THR	3.1
9	W	133	LYS	3.1
2	B	225	TYR	3.1
3	C	180	LYS	3.1
7	G	242	GLN	3.0
13	a	232	LYS	3.0
13	M	216	ASN	3.0
3	Q	203	THR	3.0
6	F	241	LYS	3.0
4	D	125	LEU	3.0
8	V	114	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
8	V	145	ASP	2.9
6	F	244	ASN	2.9
3	Q	232	THR	2.9
6	F	205	GLU	2.9
6	F	202	ASP	2.9
9	W	192	ASP	2.9
1	O	248	GLU	2.9
2	B	59	ASP	2.8
6	T	2	THR	2.8
2	B	182	ASP	2.8
5	E	180	LYS	2.8
3	C	235	GLU	2.8
7	G	188	GLU	2.8
5	S	218	ASP	2.8
1	A	249	ALA	2.8
2	P	182	ASP	2.8
6	F	215	CYS	2.8
7	U	242	GLN	2.8
14	N	195	GLN	2.8
14	b	105	LYS	2.8
3	C	204	GLY	2.8
2	P	223	GLU	2.8
3	C	216	ASP	2.8
5	E	3	ASN	2.8
7	U	203	ASP	2.8
1	A	2	THR	2.7
3	Q	52	LEU	2.7
6	T	205	GLU	2.7
6	T	178	HIS	2.7
3	C	175	LYS	2.7
2	P	203	SER	2.7
3	Q	60	SER	2.7
6	F	2	THR	2.7
5	E	201	ARG	2.7
3	Q	229	GLN	2.7
13	M	47	ASP	2.7
5	S	201	ARG	2.7
5	E	218	ASP	2.7
3	Q	187	GLU	2.6
2	B	52	THR	2.6
1	O	2	THR	2.6
6	F	201	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
3	C	60	SER	2.6
7	G	2	GLY	2.6
7	G	240	ALA	2.6
2	B	3	ARG	2.6
14	b	195	GLN	2.6
3	C	37	LYS	2.6
5	S	225	ASP	2.6
12	Z	1	GLN	2.6
2	P	60	THR	2.6
3	C	47	ARG	2.6
3	Q	175	LYS	2.5
7	U	3	TYR	2.5
2	B	244	THR	2.5
2	B	60	THR	2.5
5	E	227	GLU	2.5
6	F	177	ASP	2.5
5	S	163	ARG	2.5
2	P	240	LYS	2.5
9	I	133	LYS	2.5
9	I	131	GLU	2.5
5	E	123	GLY	2.5
5	S	29	LYS	2.4
5	S	207	VAL	2.4
4	D	2	ARG	2.4
4	R	1	ASP	2.4
6	F	181	GLU	2.4
3	Q	59	PRO	2.4
5	S	52	ALA	2.4
3	Q	180	LYS	2.4
3	C	181	GLU	2.4
6	T	180	PRO	2.4
7	G	181	LYS	2.4
3	C	48	SER	2.4
4	R	237	GLU	2.4
7	G	208	GLU	2.3
2	B	217	LYS	2.3
5	E	194	GLU	2.3
7	G	241	GLU	2.3
3	Q	58	THR	2.3
3	C	187	GLU	2.3
4	D	1	ASP	2.3
6	T	230	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
11	Y	147	ASP	2.3
7	G	51	PRO	2.3
7	G	222	ASP	2.3
1	O	182	GLU	2.3
5	S	180	LYS	2.2
7	G	237	VAL	2.2
2	B	203	SER	2.2
1	O	178	ARG	2.2
3	C	203	THR	2.2
2	P	232	GLN	2.2
3	Q	47	ARG	2.2
11	Y	202	GLU	2.2
7	G	180	SER	2.2
5	E	122	TYR	2.2
2	P	50	LYS	2.2
5	S	3	ASN	2.2
6	T	54	LEU	2.2
5	S	30	GLN	2.1
13	M	82	ASP	2.1
2	P	186	ASP	2.1
4	R	169	GLU	2.1
1	A	229	THR	2.1
4	D	47	THR	2.1
1	O	50	LYS	2.1
5	S	171	LEU	2.1
1	A	220	ASP	2.1
2	B	50	LYS	2.1
3	Q	221	ALA	2.1
2	P	61	SER	2.1
4	R	226	GLU	2.1
6	F	178	HIS	2.1
5	S	178	PHE	2.1
3	C	178	ASP	2.1
5	S	210	LEU	2.1
5	E	121	SER	2.1
7	G	40	ASP	2.1
9	W	191	LYS	2.1
6	T	166	GLN	2.1
8	V	215	GLU	2.1
2	P	230	LYS	2.1
4	R	54	ASP	2.1
11	K	202	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
6	T	53	LYS	2.1
4	R	230	GLU	2.0
8	V	198	GLU	2.0
3	Q	204	GLY	2.0
3	Q	171	GLU	2.0
4	R	177	ASN	2.0
7	G	183	ASP	2.0
1	A	52	SER	2.0
7	G	230	GLU	2.0
1	A	166	LYS	2.0
5	E	165	GLN	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å^2)	Q<0.9
15	IL0	h	4	8/9	0.76	0.34	-	61,63,67,68	0
15	IL0	e	4	8/9	0.75	0.32	-	56,58,58,58	0
15	IL0	f	4	8/9	0.93	0.18	-	62,65,73,75	0
15	IL0	c	4	8/9	0.93	0.16	-	60,63,67,67	0
15	IL0	d	4	8/9	0.95	0.17	-	52,62,66,67	0
15	IL0	g	4	8/9	0.94	0.17	-	56,64,71,74	0

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å^2)	Q<0.9
18	MES	g	101	12/12	0.84	0.37	10.09	79,82,85,91	0
18	MES	d	101	12/12	0.85	0.39	9.94	79,85,87,90	0
18	MES	H	301	12/12	0.71	0.36	8.54	89,111,129,131	0
16	MG	Z	301	1/1	0.89	0.22	4.32	66,66,66,66	0
16	MG	I	301	1/1	0.95	0.21	3.61	56,56,56,56	0
17	CL	b	201	1/1	0.93	0.15	1.98	83,83,83,83	0
16	MG	N	201	1/1	0.95	0.10	-0.72	42,42,42,42	0
16	MG	K	301	1/1	0.95	0.08	-0.81	46,46,46,46	0
16	MG	G	301	1/1	0.83	0.09	-0.85	48,48,48,48	0
16	MG	I	302	1/1	0.99	0.04	-2.73	39,39,39,39	0
17	CL	N	202	1/1	0.99	0.06	-2.76	58,58,58,58	0
16	MG	L	301	1/1	0.99	0.06	-2.93	46,46,46,46	0
17	CL	G	302	1/1	0.99	0.14	-	30,30,30,30	0
17	CL	U	301	1/1	0.97	0.16	-	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.