Full wwPDB X-ray Structure Validation Report (i)

Apr 23, 2024 – 10:23 pm BST

PDB ID	:	8RHK
Title	:	Yeast 20S proteasome in complex with a linear oxindole epoxyketone (compound 6)
Authors	:	Goetz, M.G.; Godwin, K.; Price, R.; Dorn, R.; Merrill-Steskal, G.; Hansen, H.; Klemmer, W.; Produturi, G.; Rocha, M.; Palmer, M.; Molacek, L.; Strater, Z.; Groll, M.
Deposited on	:	2023-12-15
Resolution	:	2.80 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 (i)) were used in the production of this report:

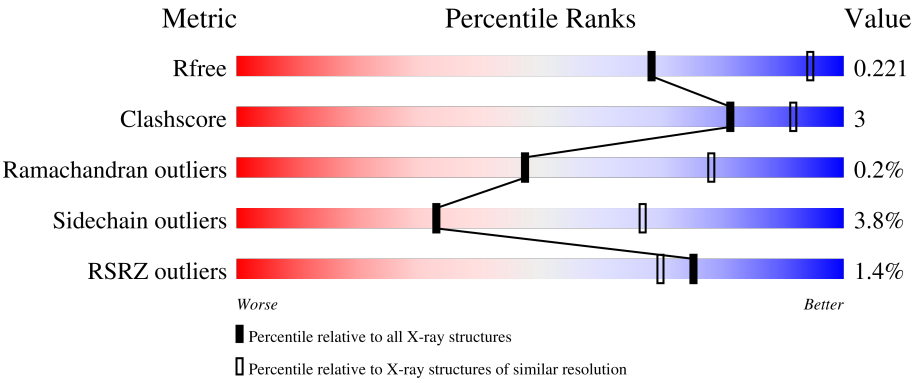
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	4% 96% ·
1	O	250	3% 95% 5%
2	B	258	2% 88% 6% 5%
2	P	258	4% 88% 6% · 5%

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Mol	Chain	Length	Quality of chain
3	C	254	3% 87% 6% 6%
3	Q	254	5% 87% 6% 6%
4	D	260	% 84% 6% 10%
4	R	260	% 85% 5% 10%
5	E	234	% 92% 6%
5	S	234	2% 92% 6%
6	F	288	% 80% 16%
6	T	288	2% 79% 5% 16%
7	G	252	% 88% 7%
7	U	252	% 87% 8%
8	H	232	% 88% 7%
8	V	232	% 88% 8%
9	I	205	91% 8%
9	W	205	91% 8%
10	J	198	% 89% 7%
10	X	198	2% 89% 7%
11	K	212	86% 11%
11	Y	212	87% 11%
12	L	222	91% 9%
12	Z	222	92% 8%
13	M	246	88% 7% 5%
13	a	246	92% 5%
14	N	196	% 95% 5%
14	b	196	% 98%
15	g	5	60% 40%

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Mol	Chain	Length	Quality of chain
15	h	5	60% 40%
16	e	5	60% 40%
16	f	5	40% 60%
16	i	5	60% 40%
16	j	5	60% 40%

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	A1H2H	i	2	-	-	-	X
16	A1H2H	j	2	-	-	-	X

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 49935 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	0	0
			1757	1115	303	335	4			

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

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

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

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

- Molecule 15 is a protein called Linear oxindole epoxyketone.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	g	5	Total	C	F	N	O	0	0	0
			54	37	1	6	10			
15	h	5	Total	C	F	N	O	0	0	0
			54	37	1	6	10			

- Molecule 16 is a protein called Linear oxindole epoxyketone.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	e	5	Total	C	F	N	O	0	0	0
			54	37	1	6	10			
16	i	5	Total	C	F	N	O	0	0	0
			54	37	1	6	10			
16	f	5	Total	C	F	N	O	0	0	0
			54	37	1	6	10			
16	j	5	Total	C	F	N	O	0	0	0
			54	37	1	6	10			

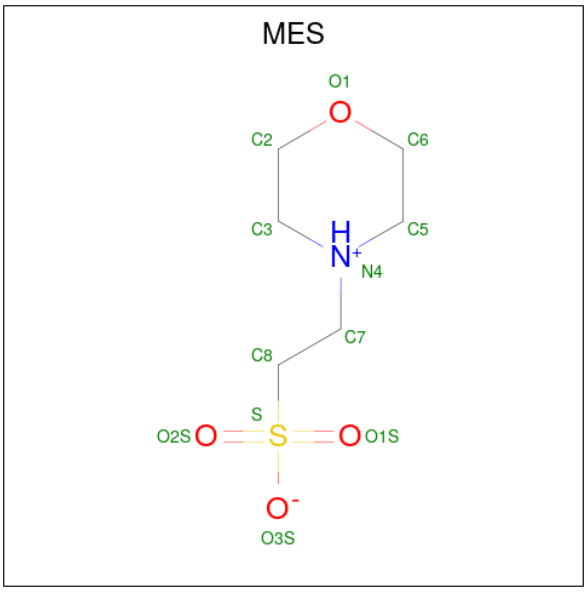
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	G	1	Total	Mg	0	0
			1	1		
17	I	1	Total	Mg	0	0
			1	1		
17	K	1	Total	Mg	0	0
			1	1		
17	N	1	Total	Mg	0	0
			1	1		
17	V	1	Total	Mg	0	0
			1	1		
17	X	1	Total	Mg	0	0
			1	1		
17	Y	1	Total	Mg	0	0
			1	1		
17	Z	1	Total	Mg	0	0
			1	1		

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

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

- Molecule 19 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 20 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	9	Total O 9 9	0	0
20	B	16	Total O 16 16	0	0
20	C	5	Total O 5 5	0	0
20	D	9	Total O 9 9	0	0
20	E	5	Total O 5 5	0	0
20	F	4	Total O 4 4	0	0
20	G	8	Total O 8 8	0	0
20	H	17	Total O 17 17	0	0
20	I	7	Total O 7 7	0	0
20	J	19	Total O 19 19	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	K	12	Total O 12 12	0	0
20	L	21	Total O 21 21	0	0
20	M	14	Total O 14 14	0	0
20	N	13	Total O 13 13	0	0
20	O	2	Total O 2 2	0	0
20	P	10	Total O 10 10	0	0
20	Q	8	Total O 8 8	0	0
20	R	2	Total O 2 2	0	0
20	S	4	Total O 4 4	0	0
20	T	3	Total O 3 3	0	0
20	U	11	Total O 11 11	0	0
20	V	12	Total O 12 12	0	0
20	W	7	Total O 7 7	0	0
20	X	14	Total O 14 14	0	0
20	Y	12	Total O 12 12	0	0
20	Z	11	Total O 11 11	0	0
20	a	12	Total O 12 12	0	0
20	b	7	Total O 7 7	0	0
20	e	2	Total O 2 2	0	0
20	i	2	Total O 2 2	0	0
20	f	1	Total O 1 1	0	0

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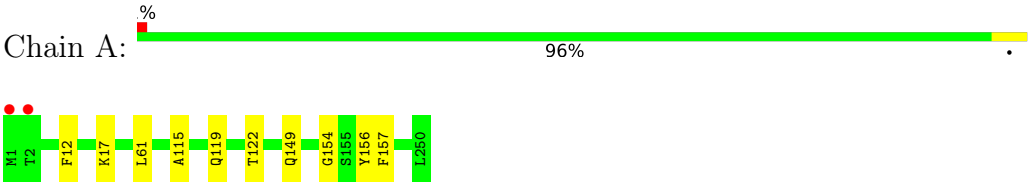
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	h	1	Total O 1 1	0	0
20	j	1	Total O 1 1	0	0

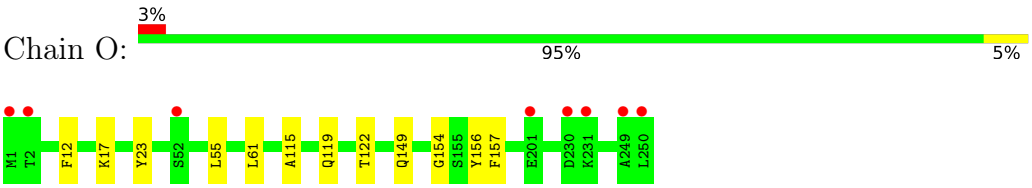
3 Residue-property plots (i)

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.

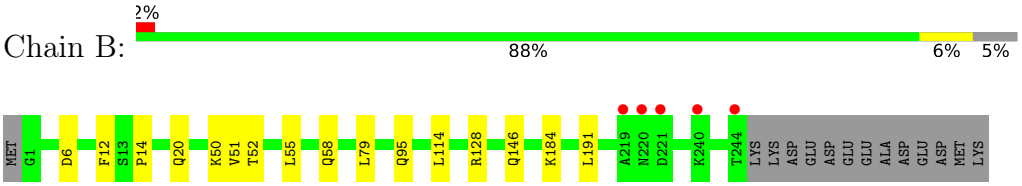
• Molecule 1: Proteasome subunit alpha type-2



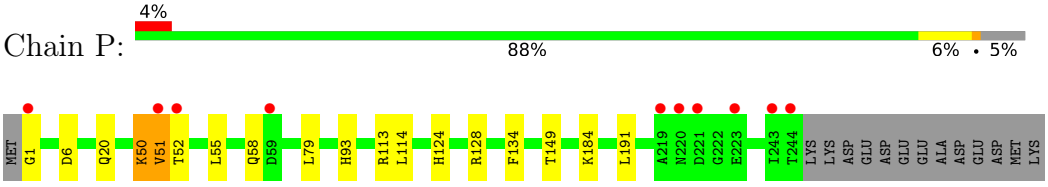
• Molecule 1: Proteasome subunit alpha type-2



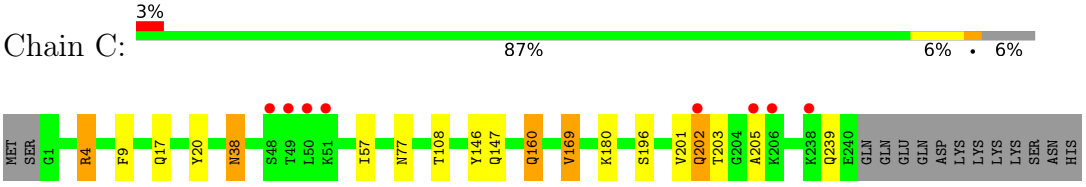
• Molecule 2: Proteasome subunit alpha type-3



• Molecule 2: Proteasome subunit alpha type-3

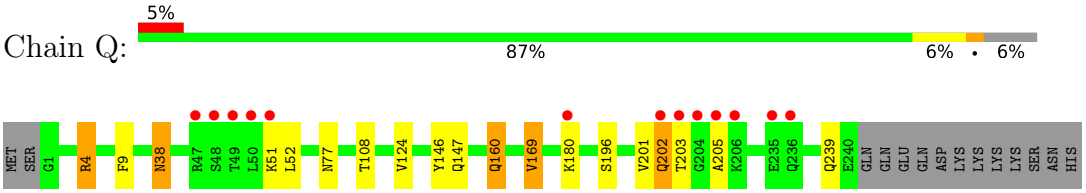


• Molecule 3: Proteasome subunit alpha type-4



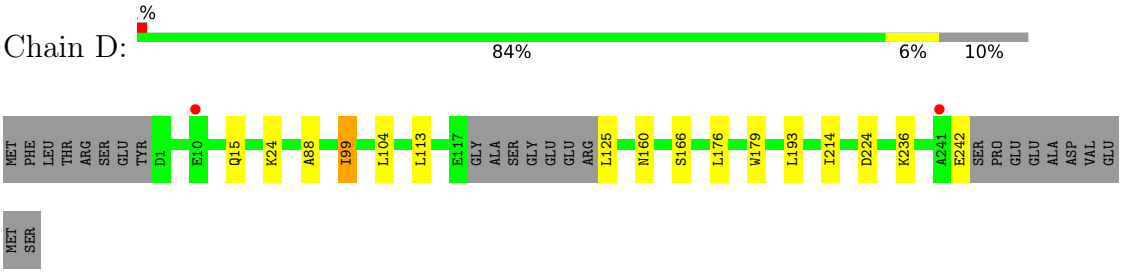
• Molecule 3: Proteasome subunit alpha type-4

Chain Q:



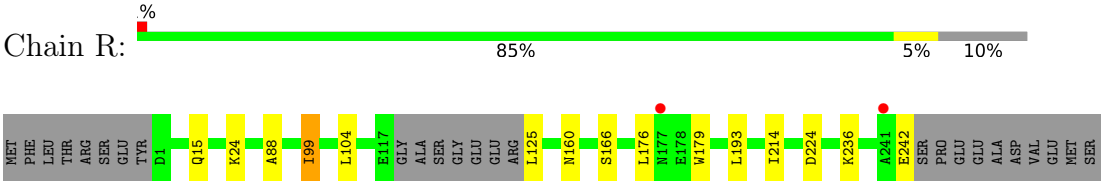
• Molecule 4: Proteasome subunit alpha type-5

Chain D:



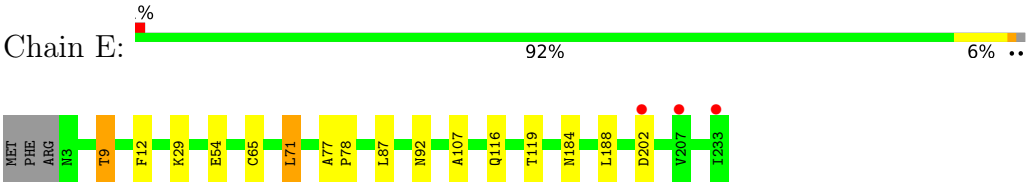
• Molecule 4: Proteasome subunit alpha type-5

Chain R:



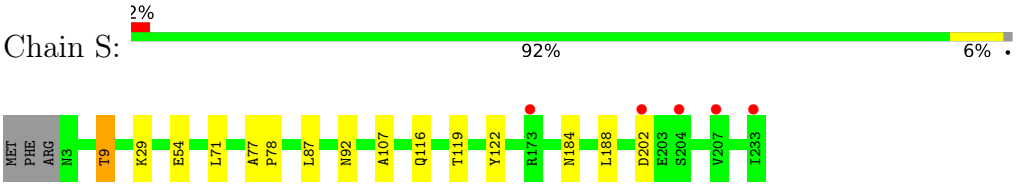
• Molecule 5: Proteasome subunit alpha type-6

Chain E:



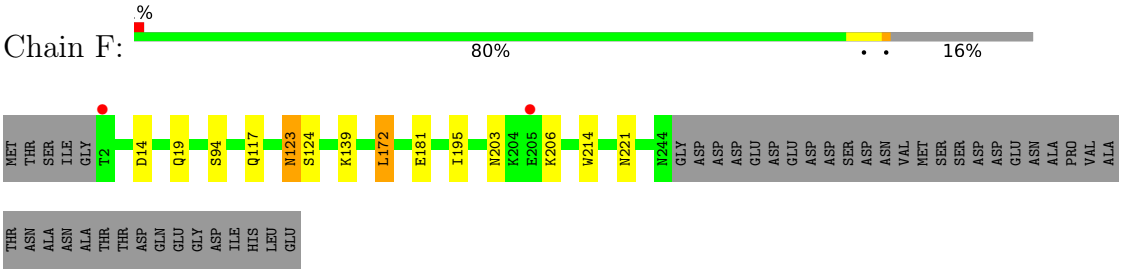
• Molecule 5: Proteasome subunit alpha type-6

Chain S:

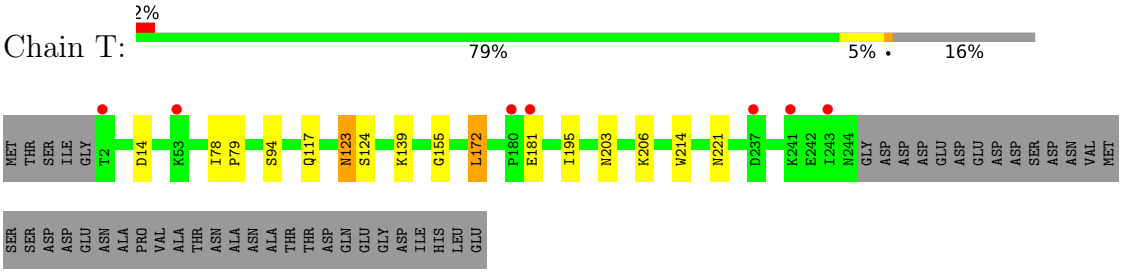


• Molecule 6: Probable proteasome subunit alpha type-7

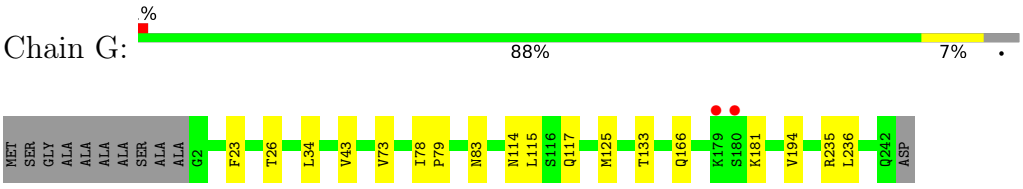
Chain F:



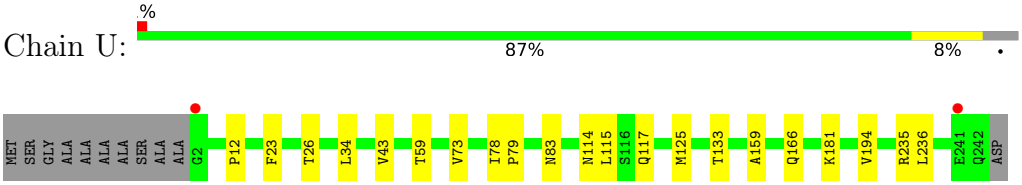
• Molecule 6: Probable proteasome subunit alpha type-7



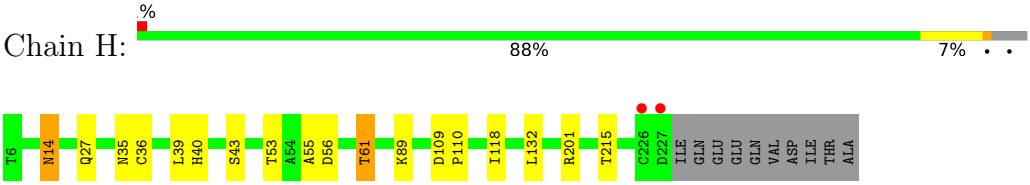
• Molecule 7: Proteasome subunit alpha type-1



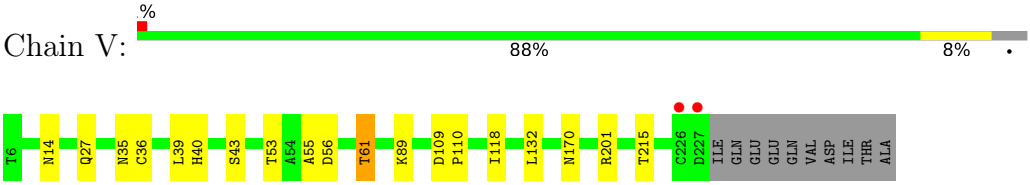
• Molecule 7: Proteasome subunit alpha type-1



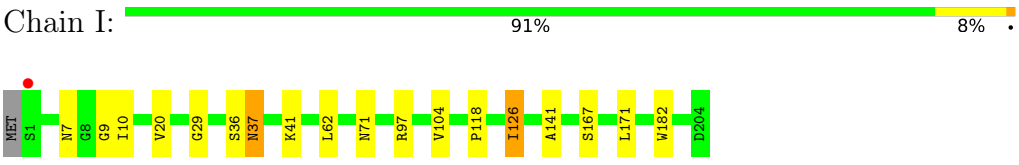
• Molecule 8: Proteasome subunit beta type-2



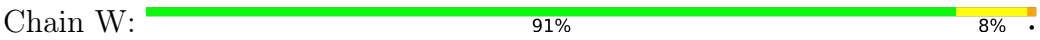
• Molecule 8: Proteasome subunit beta type-2

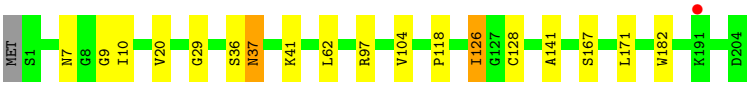


• Molecule 9: Proteasome subunit beta type-3

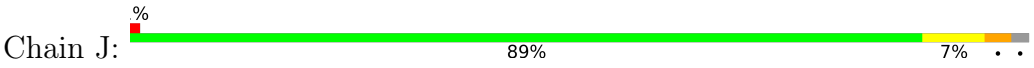


• Molecule 9: Proteasome subunit beta type-3

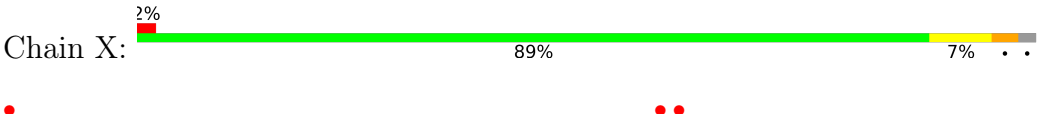




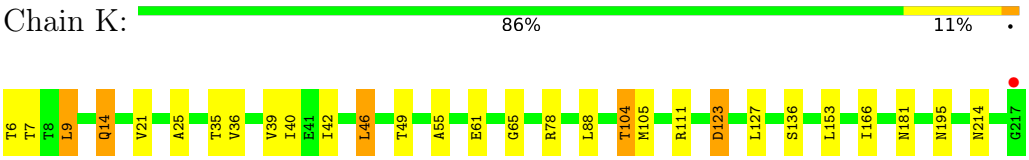
• Molecule 10: Proteasome subunit beta type-4



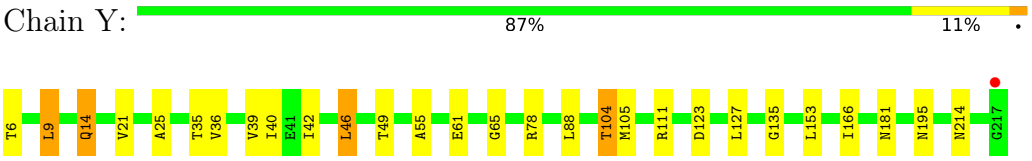
• Molecule 10: Proteasome subunit beta type-4



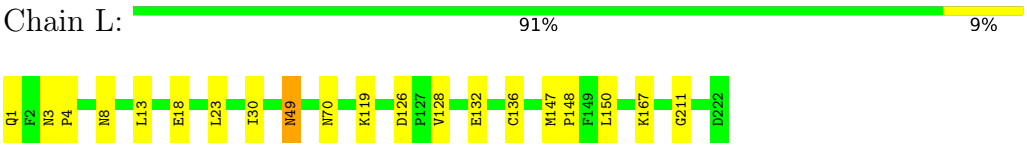
• Molecule 11: Proteasome subunit beta type-5



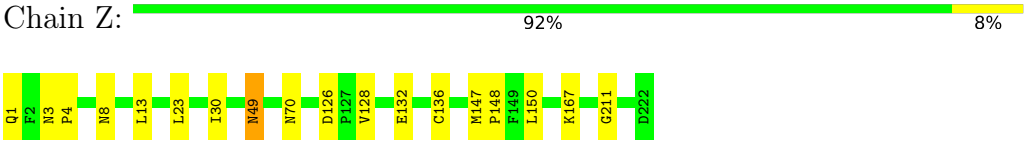
• Molecule 11: Proteasome subunit beta type-5



• Molecule 12: Proteasome subunit beta type-6

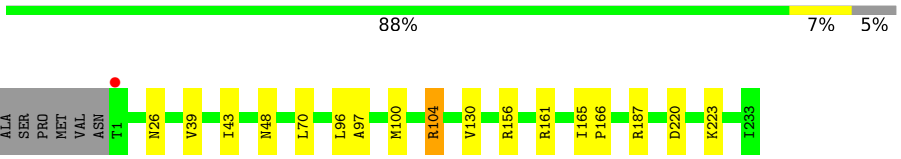


• Molecule 12: Proteasome subunit beta type-6



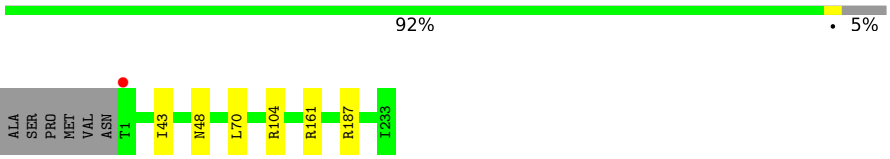
• Molecule 13: Proteasome subunit beta type-7

Chain M:



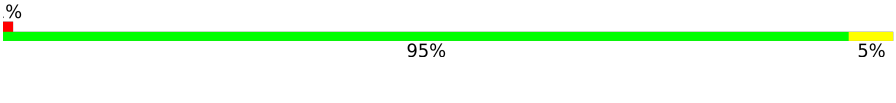
• Molecule 13: Proteasome subunit beta type-7

Chain a:



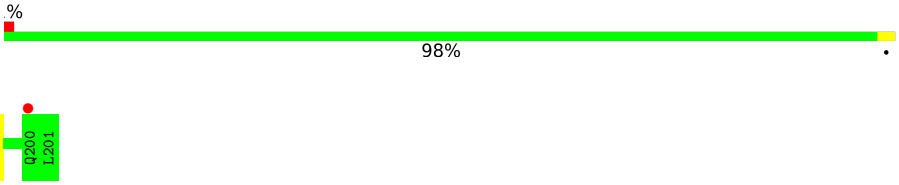
• Molecule 14: Proteasome subunit beta type-1

Chain N:



• Molecule 14: Proteasome subunit beta type-1

Chain b:



• Molecule 15: Linear oxindole epoxyketone

Chain g:

• Molecule 15: Linear oxindole epoxyketone

Chain h:

• Molecule 16: Linear oxindole epoxyketone

Chain e:

• Molecule 16: Linear oxindole epoxyketone

Chain i:

• Molecule 16: Linear oxindole epoxyketone

Chain f:

• Molecule 16: Linear oxindole epoxyketone

Chain j:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	136.10Å 300.68Å 144.70Å 90.00° 113.19° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 29.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.2 (30.00-2.80) 96.3 (29.98-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.50 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.182 , 0.218 0.190 , 0.221	Depositor DCC
R_{free} test set	12577 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	63.1	Xtriage
Anisotropy	0.541	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 41.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	49935	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% 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: 6VO, MES, A1H2H, MG, A1H2I, CL, A1H45, ACE

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	0.65	0/1952	0.70	0/2642
1	O	0.65	0/1952	0.70	0/2642
2	B	0.65	0/1934	0.71	0/2618
2	P	0.65	0/1934	0.71	0/2618
3	C	0.65	0/1910	0.72	0/2586
3	Q	0.66	0/1910	0.72	0/2586
4	D	0.66	0/1837	0.70	0/2475
4	R	0.66	0/1837	0.70	0/2475
5	E	0.66	0/1800	0.71	0/2433
5	S	0.66	0/1800	0.71	0/2433
6	F	0.65	0/1932	0.70	0/2609
6	T	0.65	0/1932	0.70	0/2609
7	G	0.64	0/1945	0.69	0/2634
7	U	0.64	0/1945	0.70	0/2634
8	H	0.65	0/1715	0.73	0/2326
8	V	0.65	0/1715	0.74	0/2326
9	I	0.65	0/1611	0.71	0/2174
9	W	0.65	0/1611	0.72	0/2174
10	J	0.63	0/1589	0.70	0/2142
10	X	0.63	0/1589	0.70	0/2142
11	K	0.64	0/1681	0.72	0/2274
11	Y	0.65	0/1681	0.72	0/2274
12	L	0.63	0/1795	0.70	0/2420
12	Z	0.63	0/1795	0.70	0/2420
13	M	0.64	0/1855	0.72	0/2514
13	a	0.64	0/1855	0.73	0/2514
14	N	0.64	0/1541	0.70	0/2087
14	b	0.64	0/1541	0.70	0/2087
15	g	1.17	0/7	1.84	0/8
15	h	1.20	0/7	1.72	0/8
16	e	1.69	0/7	2.52	0/8
16	f	1.11	0/7	1.93	0/8

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
16	i	1.14	0/7	1.92	0/8
16	j	0.93	0/7	1.91	0/8
All	All	0.65	0/50236	0.71	0/67916

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	7	0
2	B	1904	0	1904	8	0
2	P	1904	0	1904	8	0
3	C	1881	0	1895	12	0
3	Q	1881	0	1895	12	0
4	D	1813	0	1797	6	0
4	R	1813	0	1797	5	0
5	E	1773	0	1775	7	0
5	S	1773	0	1775	5	0
6	F	1892	0	1883	4	0
6	T	1892	0	1883	5	0
7	G	1907	0	1901	7	0
7	U	1907	0	1901	10	0
8	H	1684	0	1684	9	0
8	V	1684	0	1684	9	0
9	I	1581	0	1574	13	0
9	W	1581	0	1574	12	0
10	J	1561	0	1569	15	0
10	X	1561	0	1569	14	0
11	K	1644	0	1591	24	0
11	Y	1644	0	1591	21	0
12	L	1757	0	1711	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	Z	1757	0	1711	9	0
13	M	1824	0	1832	7	0
13	a	1824	0	1832	0	0
14	N	1512	0	1477	3	0
14	b	1512	0	1477	0	0
15	g	54	0	14	0	0
15	h	54	0	14	0	0
16	e	54	0	14	0	0
16	f	54	0	14	0	0
16	i	54	0	14	0	0
16	j	54	0	14	0	0
17	G	1	0	0	0	0
17	I	1	0	0	0	0
17	K	1	0	0	0	0
17	N	1	0	0	0	0
17	V	1	0	0	0	0
17	X	1	0	0	0	0
17	Y	1	0	0	0	0
17	Z	1	0	0	0	0
18	G	1	0	0	0	0
18	U	1	0	0	0	0
19	K	12	0	13	1	0
19	Y	12	0	13	1	0
20	A	9	0	0	0	0
20	B	16	0	0	0	0
20	C	5	0	0	0	0
20	D	9	0	0	0	0
20	E	5	0	0	0	0
20	F	4	0	0	0	0
20	G	8	0	0	0	0
20	H	17	0	0	1	0
20	I	7	0	0	0	0
20	J	19	0	0	0	0
20	K	12	0	0	0	0
20	L	21	0	0	0	0
20	M	14	0	0	0	0
20	N	13	0	0	0	0
20	O	2	0	0	0	0
20	P	10	0	0	0	0
20	Q	8	0	0	1	0
20	R	2	0	0	0	0
20	S	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	T	3	0	0	0	0
20	U	11	0	0	0	0
20	V	12	0	0	0	0
20	W	7	0	0	0	0
20	X	14	0	0	0	0
20	Y	12	0	0	0	0
20	Z	11	0	0	0	0
20	a	12	0	0	0	0
20	b	7	0	0	0	0
20	e	2	0	0	0	0
20	f	1	0	0	0	0
20	h	1	0	0	0	0
20	i	2	0	0	0	0
20	j	1	0	0	0	0
All	All	49935	0	49154	203	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 3.

All (203) 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:X:101:ASN:HB3	10:X:133:HIS:CD2	1.80	1.17
10:J:101:ASN:HB3	10:J:133:HIS:CD2	1.82	1.15
10:X:101:ASN:HB3	10:X:133:HIS:HD2	1.35	0.88
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.41	0.84
10:J:101:ASN:HB3	10:J:133:HIS:HD2	1.38	0.82
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.44	0.81
10:X:101:ASN:CB	10:X:133:HIS:CD2	2.66	0.77
10:X:23:ARG:NH2	19:Y:301:MES:O1	2.21	0.73
10:J:101:ASN:CB	10:J:133:HIS:HD2	2.00	0.73
10:X:101:ASN:CB	10:X:133:HIS:HD2	1.99	0.72
10:J:101:ASN:CB	10:J:133:HIS:CD2	2.67	0.71
14:N:157:VAL:HA	14:N:180:MET:HE1	1.74	0.69
11:Y:14:GLN:NE2	11:Y:153:LEU:O	2.28	0.67
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.79	0.65
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.79	0.64
7:U:23:PHE:O	7:U:26:THR:HB	1.99	0.63
7:G:23:PHE:O	7:G:26:THR:HB	1.98	0.63
11:K:14:GLN:NE2	11:K:153:LEU:O	2.31	0.63
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:78:ARG:HG2	11:K:78:ARG:HH11	1.67	0.60
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.50	0.60
11:Y:78:ARG:HG2	11:Y:78:ARG:HH11	1.66	0.60
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.84	0.59
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.67	0.59
6:T:123:ASN:C	6:T:123:ASN:HD22	2.07	0.58
6:F:123:ASN:C	6:F:123:ASN:HD22	2.08	0.56
2:P:6:ASP:OD2	3:Q:4:ARG:HG3	2.05	0.56
9:W:36:SER:HB2	10:X:126:VAL:HG11	1.88	0.55
12:L:8:ASN:HA	12:L:30:ILE:O	2.07	0.55
11:K:61:GLU:OE2	11:K:104:THR:OG1	2.24	0.54
11:K:136:SER:N	19:K:301:MES:O1S	2.41	0.54
6:T:123:ASN:HD22	6:T:124:SER:N	2.06	0.54
1:O:12:PHE:H	2:P:20:GLN:HE22	1.54	0.54
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.89	0.54
8:V:215:THR:HG21	9:W:167:SER:HB3	1.90	0.54
2:B:12:PHE:H	3:C:17:GLN:HE22	1.54	0.54
11:Y:61:GLU:OE2	11:Y:104:THR:OG1	2.24	0.53
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.90	0.53
1:A:12:PHE:H	2:B:20:GLN:HE22	1.57	0.53
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.08	0.53
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.91	0.52
13:M:97:ALA:HA	13:M:130:VAL:HG21	1.91	0.52
6:F:123:ASN:HD22	6:F:124:SER:N	2.07	0.52
1:O:119:GLN:O	1:O:122:THR:HB	2.10	0.51
10:J:174:MET:HA	10:X:174:MET:HA	1.91	0.51
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.92	0.51
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.45	0.51
11:K:9:LEU:HD11	11:K:166:ILE:HG12	1.93	0.51
3:C:38:ASN:C	3:C:38:ASN:HD22	2.14	0.51
11:K:9:LEU:HD22	11:K:9:LEU:O	2.11	0.51
11:Y:9:LEU:HD11	11:Y:166:ILE:HG12	1.93	0.50
11:Y:6:THR:O	11:Y:135:GLY:HA3	2.11	0.50
8:H:55:ALA:CB	9:I:126:ILE:CG2	2.89	0.50
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.46	0.50
13:M:156:ARG:HH11	8:V:170:ASN:HD22	1.59	0.50
5:S:92:ASN:HD21	12:Z:70:ASN:ND2	2.10	0.50
8:V:55:ALA:CB	9:W:126:ILE:CG2	2.90	0.50
8:H:215:THR:HG21	9:I:167:SER:HB3	1.93	0.50
3:C:9:PHE:H	4:D:15:GLN:HE22	1.60	0.50
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.46	0.49
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.95	0.49
7:U:78:ILE:N	7:U:79:PRO:CD	2.75	0.49
10:J:101:ASN:HB3	10:J:133:HIS:NE2	2.25	0.49
10:X:101:ASN:HB3	10:X:133:HIS:NE2	2.24	0.49
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.28	0.49
11:Y:35:THR:OG1	12:Z:132:GLU:OE2	2.30	0.49
10:J:23:ARG:NH1	11:K:123:ASP:OD2	2.47	0.48
1:O:55:LEU:HB3	7:U:159:ALA:O	2.14	0.48
7:G:78:ILE:N	7:G:79:PRO:CD	2.76	0.48
11:K:181:ASN:ND2	11:K:195:ASN:HD22	2.10	0.48
8:H:55:ALA:HB3	9:I:126:ILE:CG2	2.43	0.48
13:M:220:ASP:O	13:M:223:LYS:HG2	2.13	0.48
12:L:147:MET:N	12:L:148:PRO:HD2	2.28	0.48
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.95	0.48
11:Y:9:LEU:HD22	11:Y:9:LEU:O	2.14	0.48
11:Y:21:VAL:HG21	11:Y:39:VAL:HG23	1.95	0.48
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.79	0.48
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.96	0.47
5:E:92:ASN:HD21	12:L:70:ASN:ND2	2.13	0.47
11:K:42:ILE:HG23	11:K:65:GLY:HA2	1.97	0.47
11:K:78:ARG:HH11	11:K:78:ARG:CG	2.28	0.47
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.96	0.47
9:I:37:ASN:ND2	11:Y:214:ASN:O	2.47	0.47
3:Q:38:ASN:C	3:Q:38:ASN:HD22	2.17	0.47
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.97	0.47
11:Y:55:ALA:CB	12:Z:128:VAL:HG23	2.44	0.47
1:A:119:GLN:O	1:A:122:THR:HB	2.14	0.47
11:K:9:LEU:HD22	11:K:9:LEU:C	2.35	0.47
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.97	0.47
10:J:1:MET:O	10:J:2:ASP:HB2	2.15	0.47
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.44	0.47
12:L:49:ASN:HD21	12:L:211:GLY:HA2	1.80	0.47
12:Z:49:ASN:HD21	12:Z:211:GLY:HA2	1.80	0.47
3:C:108:THR:HG21	3:C:146:TYR:HB3	1.97	0.47
11:Y:9:LEU:HD22	11:Y:9:LEU:C	2.36	0.46
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.79	0.46
3:Q:108:THR:HG21	3:Q:146:TYR:HB3	1.96	0.46
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.97	0.46
5:S:77:ALA:N	5:S:78:PRO:CD	2.79	0.46
3:C:201:VAL:HG13	3:C:202:GLN:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.97	0.46
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.43	0.46
11:Y:42:ILE:HB	11:Y:46:LEU:HB3	1.98	0.46
8:H:55:ALA:CB	9:I:126:ILE:HG22	2.45	0.46
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.51	0.46
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.31	0.46
11:Y:78:ARG:HH11	11:Y:78:ARG:CG	2.27	0.46
11:K:21:VAL:HG21	11:K:39:VAL:HG23	1.98	0.45
4:D:113:LEU:HD12	5:E:78:PRO:HB2	1.98	0.45
5:E:77:ALA:N	5:E:78:PRO:CD	2.80	0.45
11:Y:42:ILE:HG23	11:Y:65:GLY:HA2	1.97	0.45
8:H:109:ASP:HB2	8:H:110:PRO:HD2	1.99	0.45
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.65	0.45
10:J:168:LEU:O	10:J:172:MET:HB2	2.16	0.45
11:K:55:ALA:CB	12:L:128:VAL:HG23	2.45	0.45
3:Q:160:GLN:HE21	3:Q:160:GLN:CA	2.20	0.45
1:A:149:GLN:O	1:A:156:TYR:HA	2.17	0.45
11:K:42:ILE:HB	11:K:46:LEU:HB3	1.97	0.45
1:O:149:GLN:O	1:O:156:TYR:HA	2.17	0.45
10:X:1:MET:O	10:X:2:ASP:HB2	2.17	0.45
3:Q:51:LYS:NZ	20:Q:301:HOH:O	2.46	0.44
6:T:155:GLY:HA3	7:U:59:THR:HG21	1.99	0.44
1:A:115:ALA:HB1	1:A:154:GLY:O	2.17	0.44
4:R:99:ILE:HD11	4:R:104:LEU:HB2	1.98	0.44
8:V:53:THR:HB	8:V:56:ASP:HB2	2.00	0.44
8:V:109:ASP:HB2	8:V:110:PRO:HD2	2.00	0.44
11:Y:49:THR:HG21	11:Y:105:MET:HE3	1.99	0.44
8:V:55:ALA:HB3	9:W:126:ILE:CG2	2.47	0.44
2:B:14:PRO:HA	3:C:20:TYR:CE1	2.52	0.44
8:V:55:ALA:CB	9:W:126:ILE:HG22	2.47	0.44
10:J:118:GLN:HG2	10:J:133:HIS:HE1	1.83	0.44
6:F:172:LEU:CD1	6:F:195:ILE:HD13	2.47	0.44
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.99	0.44
11:K:49:THR:HG21	11:K:105:MET:HE3	1.99	0.43
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.99	0.43
4:D:99:ILE:HD11	4:D:104:LEU:HB2	2.00	0.43
10:J:21:VAL:HG11	11:K:127:LEU:HD11	2.00	0.43
11:K:214:ASN:O	9:W:37:ASN:ND2	2.52	0.43
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.66	0.43
11:K:35:THR:OG1	12:L:132:GLU:OE2	2.33	0.43
11:K:88:LEU:CD2	11:K:104:THR:HG21	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:115:ALA:HB1	1:O:154:GLY:O	2.18	0.43
11:Y:181:ASN:ND2	11:Y:195:ASN:HD22	2.17	0.43
5:E:9:THR:HG21	5:E:119:THR:HA	2.01	0.43
11:K:6:THR:HG22	11:K:7:THR:N	2.34	0.43
6:T:172:LEU:CD1	6:T:195:ILE:HD13	2.48	0.43
3:C:201:VAL:O	3:C:202:GLN:CB	2.66	0.43
11:K:6:THR:CG2	11:K:7:THR:N	2.82	0.43
7:U:78:ILE:HG22	7:U:79:PRO:HD3	2.01	0.43
8:H:40:HIS:HB3	8:H:61:THR:HG21	2.00	0.42
5:S:9:THR:HG21	5:S:119:THR:HA	2.01	0.42
9:W:62:LEU:CD1	9:W:104:VAL:HG21	2.49	0.42
10:X:21:VAL:HG11	11:Y:127:LEU:HD11	2.00	0.42
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.54	0.42
7:G:34:LEU:C	7:G:34:LEU:HD23	2.39	0.42
7:U:73:VAL:HG12	7:U:133:THR:HB	2.00	0.42
11:K:25:ALA:HB2	11:K:36:VAL:HG21	2.01	0.42
8:V:40:HIS:HB3	8:V:61:THR:HG21	2.01	0.42
10:X:118:GLN:HG2	10:X:133:HIS:HE1	1.84	0.42
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	2.02	0.42
10:X:168:LEU:O	10:X:172:MET:HB2	2.20	0.42
11:Y:25:ALA:HB2	11:Y:36:VAL:HG21	2.00	0.42
11:Y:88:LEU:CD2	11:Y:104:THR:HG21	2.50	0.42
12:L:18:GLU:O	12:L:119:LYS:HA	2.20	0.42
9:I:7:ASN:HA	9:I:29:GLY:O	2.19	0.41
14:N:53:SER:HB3	14:N:56:ASP:HB2	2.02	0.41
7:U:114:ASN:HD22	7:U:114:ASN:HA	1.67	0.41
2:B:6:ASP:OD2	3:C:4:ARG:HG3	2.19	0.41
2:B:146:GLN:HG2	3:C:57:ILE:HG21	2.01	0.41
2:P:50:LYS:O	2:P:51:VAL:C	2.59	0.41
7:G:78:ILE:HG22	7:G:79:PRO:HD3	2.01	0.41
11:Y:46:LEU:HD23	11:Y:46:LEU:HA	1.86	0.41
7:G:43:VAL:HG11	7:G:194:VAL:HA	2.03	0.41
7:G:114:ASN:HD22	7:G:114:ASN:HA	1.67	0.41
5:E:12:PHE:H	6:F:19:GLN:HE22	1.68	0.41
12:L:4:PRO:O	13:M:104:ARG:NH1	2.44	0.41
2:P:93:HIS:HB3	2:P:113:ARG:HH21	1.86	0.41
2:P:134:PHE:O	2:P:149:THR:HA	2.21	0.41
9:W:7:ASN:HA	9:W:29:GLY:O	2.21	0.41
4:D:24:LYS:O	4:D:166:SER:HA	2.21	0.41
7:G:73:VAL:HG12	7:G:133:THR:HB	2.02	0.41
10:J:118:GLN:CG	10:J:133:HIS:CE1	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.20	0.41
7:U:34:LEU:C	7:U:34:LEU:HD23	2.41	0.41
8:H:14:ASN:HB3	20:H:305:HOH:O	2.22	0.40
9:I:62:LEU:CD1	9:I:104:VAL:HG21	2.50	0.40
13:M:26:ASN:HA	13:M:39:VAL:O	2.20	0.40
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.03	0.40
4:R:24:LYS:O	4:R:166:SER:HA	2.21	0.40
13:M:96:LEU:O	13:M:100:MET:HG2	2.22	0.40
2:P:1:GLY:HA3	5:S:122:TYR:CE1	2.57	0.40
7:U:43:VAL:HG11	7:U:194:VAL:HA	2.02	0.40
11:Y:9:LEU:HD13	11:Y:166:ILE:HD11	2.03	0.40
8:H:53:THR:HB	8:H:56:ASP:HB2	2.02	0.40
11:K:46:LEU:HD23	11:K:46:LEU:HA	1.86	0.40
8:V:55:ALA:HB2	9:W:128:CYS:HB2	2.03	0.40
8:H:40:HIS:CB	8:H:61:THR:HG21	2.51	0.40
11:K:9:LEU:HD13	11:K:166:ILE:HD11	2.04	0.40
14:N:19:LEU:O	14:N:180:MET:HA	2.22	0.40
5:E:65:CYS:SG	5:E:71:LEU:CD1	3.10	0.40
9:I:126:ILE:HD12	9:I:126:ILE:HA	1.79	0.40
6:T:78:ILE:N	6:T:79:PRO:CD	2.84	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%)	238 (96%)	10 (4%)	0	100	100
1	O	248/250 (99%)	238 (96%)	10 (4%)	0	100	100
2	B	242/258 (94%)	233 (96%)	8 (3%)	1 (0%)	34	66
2	P	242/258 (94%)	233 (96%)	8 (3%)	1 (0%)	34	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	238/254 (94%)	229 (96%)	6 (2%)	3 (1%)	12	36
3	Q	238/254 (94%)	229 (96%)	6 (2%)	3 (1%)	12	36
4	D	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
4	R	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
5	E	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
5	S	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
6	F	241/288 (84%)	233 (97%)	8 (3%)	0	100	100
6	T	241/288 (84%)	233 (97%)	8 (3%)	0	100	100
7	G	239/252 (95%)	232 (97%)	7 (3%)	0	100	100
7	U	239/252 (95%)	231 (97%)	8 (3%)	0	100	100
8	H	220/232 (95%)	216 (98%)	4 (2%)	0	100	100
8	V	220/232 (95%)	217 (99%)	3 (1%)	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%)	29	61
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	29	61
11	K	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
11	Y	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
12	L	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
12	Z	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
13	M	231/246 (94%)	224 (97%)	7 (3%)	0	100	100
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	g	1/5 (20%)	1 (100%)	0	0	100	100
15	h	1/5 (20%)	1 (100%)	0	0	100	100
16	e	1/5 (20%)	1 (100%)	0	0	100	100
16	f	1/5 (20%)	1 (100%)	0	0	100	100
16	i	1/5 (20%)	1 (100%)	0	0	100	100
16	j	1/5 (20%)	1 (100%)	0	0	100	100
All	All	6282/6644 (95%)	6102 (97%)	170 (3%)	10 (0%)	47	78

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
3	C	202	GLN
2	P	51	VAL
3	Q	202	GLN
10	J	2	ASP
10	X	2	ASP
3	C	205	ALA
3	C	239	GLN
3	Q	205	ALA
3	Q	239	GLN

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	90
1	O	209/209 (100%)	206 (99%)	3 (1%)	67	90
2	B	203/216 (94%)	195 (96%)	8 (4%)	32	66
2	P	203/216 (94%)	195 (96%)	8 (4%)	32	66
3	C	212/226 (94%)	204 (96%)	8 (4%)	33	67
3	Q	212/226 (94%)	204 (96%)	8 (4%)	33	67
4	D	194/215 (90%)	186 (96%)	8 (4%)	30	64
4	R	194/215 (90%)	186 (96%)	8 (4%)	30	64
5	E	190/193 (98%)	182 (96%)	8 (4%)	30	63
5	S	190/193 (98%)	182 (96%)	8 (4%)	30	63
6	F	201/239 (84%)	190 (94%)	11 (6%)	21	52
6	T	201/239 (84%)	190 (94%)	11 (6%)	21	52
7	G	206/210 (98%)	198 (96%)	8 (4%)	32	66
7	U	206/210 (98%)	198 (96%)	8 (4%)	32	66
8	H	181/190 (95%)	170 (94%)	11 (6%)	18	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	V	181/190 (95%)	170 (94%)	11 (6%)	18 48
9	I	172/173 (99%)	167 (97%)	5 (3%)	42 76
9	W	172/173 (99%)	167 (97%)	5 (3%)	42 76
10	J	173/175 (99%)	166 (96%)	7 (4%)	31 65
10	X	173/175 (99%)	166 (96%)	7 (4%)	31 65
11	K	169/169 (100%)	162 (96%)	7 (4%)	30 64
11	Y	169/169 (100%)	162 (96%)	7 (4%)	30 64
12	L	185/185 (100%)	179 (97%)	6 (3%)	39 73
12	Z	185/185 (100%)	179 (97%)	6 (3%)	39 73
13	M	199/208 (96%)	193 (97%)	6 (3%)	41 75
13	a	199/208 (96%)	193 (97%)	6 (3%)	41 75
14	N	162/162 (100%)	158 (98%)	4 (2%)	47 80
14	b	162/162 (100%)	159 (98%)	3 (2%)	57 85
15	g	1/1 (100%)	1 (100%)	0	100 100
15	h	1/1 (100%)	1 (100%)	0	100 100
16	e	1/1 (100%)	1 (100%)	0	100 100
16	f	1/1 (100%)	0	1 (100%)	0 0
16	i	1/1 (100%)	1 (100%)	0	100 100
16	j	1/1 (100%)	1 (100%)	0	100 100
All	All	5318/5546 (96%)	5118 (96%)	200 (4%)	33 67

All (200) 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	55	LEU
2	B	58	GLN
2	B	79	LEU
2	B	114	LEU
2	B	184	LYS
2	B	191	LEU

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Mol	Chain	Res	Type
3	C	4	ARG
3	C	38	ASN
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	99	ILE
4	D	125	LEU
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	224	ASP
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	54	GLU
5	E	71	LEU
5	E	116	GLN
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
6	F	14	ASP
6	F	94	SER
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	172	LEU
6	F	181	GLU
6	F	203	ASN
6	F	206	LYS
6	F	214	TRP
6	F	221	ASN
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	125	MET
7	G	166	GLN
7	G	181	LYS
7	G	235	ARG

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Mol	Chain	Res	Type
7	G	236	LEU
8	H	14	ASN
8	H	27	GLN
8	H	35	ASN
8	H	36	CYS
8	H	39	LEU
8	H	43	SER
8	H	61	THR
8	H	89	LYS
8	H	118	ILE
8	H	132	LEU
8	H	201	ARG
9	I	37	ASN
9	I	97	ARG
9	I	126	ILE
9	I	171	LEU
9	I	182	TRP
10	J	23	ARG
10	J	35	THR
10	J	75	LEU
10	J	78	GLN
10	J	133	HIS
10	J	144	LEU
10	J	174	MET
11	K	9	LEU
11	K	14	GLN
11	K	40	ILE
11	K	46	LEU
11	K	104	THR
11	K	111	ARG
11	K	123	ASP
12	L	1	GLN
12	L	23	LEU
12	L	49	ASN
12	L	126	ASP
12	L	136	CYS
12	L	167	LYS
13	M	43	ILE
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG

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Mol	Chain	Res	Type
13	M	187	ARG
14	N	14	LYS
14	N	41	ARG
14	N	99	THR
14	N	109	ASP
1	O	17	LYS
1	O	61	LEU
1	O	157	PHE
2	P	50	LYS
2	P	52	THR
2	P	55	LEU
2	P	58	GLN
2	P	79	LEU
2	P	114	LEU
2	P	184	LYS
2	P	191	LEU
3	Q	4	ARG
3	Q	38	ASN
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	99	ILE
4	R	125	LEU
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	224	ASP
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	54	GLU
5	S	71	LEU
5	S	116	GLN
5	S	184	ASN
5	S	188	LEU
5	S	202	ASP
6	T	14	ASP
6	T	94	SER

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Mol	Chain	Res	Type
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	117	GLN
7	U	125	MET
7	U	166	GLN
7	U	181	LYS
7	U	235	ARG
7	U	236	LEU
8	V	14	ASN
8	V	27	GLN
8	V	35	ASN
8	V	36	CYS
8	V	39	LEU
8	V	43	SER
8	V	61	THR
8	V	89	LYS
8	V	118	ILE
8	V	132	LEU
8	V	201	ARG
9	W	37	ASN
9	W	97	ARG
9	W	126	ILE
9	W	171	LEU
9	W	182	TRP
10	X	23	ARG
10	X	35	THR
10	X	75	LEU
10	X	78	GLN
10	X	133	HIS
10	X	144	LEU
10	X	174	MET
11	Y	9	LEU
11	Y	14	GLN

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Mol	Chain	Res	Type
11	Y	40	ILE
11	Y	46	LEU
11	Y	104	THR
11	Y	111	ARG
11	Y	123	ASP
12	Z	1	GLN
12	Z	23	LEU
12	Z	49	ASN
12	Z	126	ASP
12	Z	136	CYS
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
14	b	14	LYS
14	b	41	ARG
14	b	109	ASP
16	f	3	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (127) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
3	C	17	GLN
3	C	38	ASN
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
4	D	146	GLN
4	D	160	ASN
4	D	198	GLN

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Mol	Chain	Res	Type
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	147	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	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	175	ASN
8	H	14	ASN
8	H	35	ASN
8	H	71	HIS
8	H	170	ASN
8	H	177	ASN
8	H	194	ASN
9	I	88	GLN
10	J	55	GLN
10	J	118	GLN
10	J	191	GLN
11	K	90	ASN
11	K	181	ASN
12	L	1	GLN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	79	HIS
12	L	158	ASN
12	L	165	ASN
13	M	18	ASN
13	M	48	ASN

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Mol	Chain	Res	Type
13	M	102	GLN
13	M	108	ASN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	166	GLN
2	P	20	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	176	GLN
3	Q	17	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS
4	R	146	GLN
4	R	160	ASN
4	R	198	GLN
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	147	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	175	ASN
8	V	14	ASN

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Mol	Chain	Res	Type
8	V	35	ASN
8	V	170	ASN
8	V	194	ASN
9	W	88	GLN
10	X	55	GLN
10	X	118	GLN
10	X	133	HIS
10	X	191	GLN
11	Y	90	ASN
11	Y	138	GLN
11	Y	181	ASN
12	Z	1	GLN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	80	ASN
12	Z	158	ASN
12	Z	165	ASN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN
14	b	166	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

12 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	$\#\|Z\| > 2$
16	A1H2I	e	4	16	14,17,18	4.10	7 (50%)	16,24,26	2.99	2 (12%)
16	A1H2I	j	4	16	14,17,18	4.08	7 (50%)	16,24,26	2.93	4 (25%)
16	A1H2I	i	4	16	14,17,18	3.83	6 (42%)	16,24,26	2.68	3 (18%)
16	A1H2I	f	4	16	14,17,18	3.98	7 (50%)	16,24,26	2.77	4 (25%)
16	A1H2H	e	2	16	13,15,16	3.68	4 (30%)	13,20,22	2.07	2 (15%)
15	A1H2H	g	2	15	13,15,16	3.98	4 (30%)	13,20,22	1.97	4 (30%)
16	A1H2H	j	2	16	13,15,16	4.78	3 (23%)	13,20,22	1.63	2 (15%)
15	A1H45	g	4	15	14,17,18	4.72	7 (50%)	16,24,26	3.63	3 (18%)
15	A1H45	h	4	15	14,17,18	4.28	7 (50%)	16,24,26	2.80	4 (25%)
15	A1H2H	h	2	15	13,15,16	4.08	5 (38%)	13,20,22	2.42	4 (30%)
16	A1H2H	i	2	16	13,15,16	3.29	4 (30%)	13,20,22	1.94	2 (15%)
16	A1H2H	f	2	16	13,15,16	2.92	4 (30%)	13,20,22	2.00	3 (23%)

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
16	A1H2I	e	4	16	-	1/5/18/20	0/2/2/2
16	A1H2I	j	4	16	-	2/5/18/20	0/2/2/2
16	A1H2I	i	4	16	-	1/5/18/20	0/2/2/2
16	A1H2I	f	4	16	-	1/5/18/20	0/2/2/2
16	A1H2H	e	2	16	-	2/7/10/12	0/1/1/1
15	A1H2H	g	2	15	-	3/7/10/12	0/1/1/1
16	A1H2H	j	2	16	-	4/7/10/12	0/1/1/1
15	A1H45	g	4	15	-	1/5/18/20	0/2/2/2
15	A1H45	h	4	15	-	1/5/18/20	0/2/2/2
15	A1H2H	h	2	15	-	2/7/10/12	0/1/1/1
16	A1H2H	i	2	16	-	6/7/10/12	0/1/1/1
16	A1H2H	f	2	16	-	2/7/10/12	0/1/1/1

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	j	2	A1H2H	O34-N33	14.75	1.47	1.22
15	g	2	A1H2H	F19-CE2	-10.86	1.07	1.35
15	g	4	A1H45	CE2-CD2	-9.46	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	g	4	A1H45	CD2-CG	-9.08	1.35	1.51
15	h	4	A1H45	CE2-CD2	-8.98	1.31	1.39
15	h	2	A1H2H	F19-CE2	-8.76	1.13	1.35
16	e	4	A1H2I	CD2-CG	-8.62	1.36	1.51
16	j	4	A1H2I	CD2-CG	-8.50	1.36	1.51
16	i	4	A1H2I	CD2-CG	-8.13	1.37	1.51
15	h	2	A1H2H	CZ-N33	-8.03	1.31	1.45
16	f	4	A1H2I	CE2-CD2	-7.96	1.32	1.39
16	f	4	A1H2I	CD2-CG	-7.86	1.37	1.51
16	i	4	A1H2I	CE2-CD2	-7.81	1.33	1.39
16	j	4	A1H2I	CE2-CD2	-7.75	1.33	1.39
15	h	4	A1H45	CD2-CG	-7.75	1.37	1.51
16	e	4	A1H2I	CE2-CD2	-7.61	1.33	1.39
16	e	2	A1H2H	CZ-N33	-7.45	1.32	1.45
16	i	2	A1H2H	O34-N33	7.42	1.35	1.22
16	f	2	A1H2H	CZ-N33	-7.23	1.32	1.45
16	j	2	A1H2H	CZ-N33	-6.96	1.33	1.45
16	e	2	A1H2H	F19-CE2	-6.62	1.18	1.35
16	i	2	A1H2H	CZ-N33	-6.44	1.34	1.45
15	g	4	A1H45	CD1-NE1	-6.33	1.30	1.35
15	h	4	A1H45	CD1-NE1	-6.31	1.30	1.35
16	e	2	A1H2H	CB-CG	-6.15	1.36	1.51
15	g	2	A1H2H	CZ-N33	-6.06	1.34	1.45
15	h	2	A1H2H	CB-CG	-6.00	1.36	1.51
16	e	2	A1H2H	O34-N33	5.77	1.32	1.22
16	f	4	A1H2I	CD1-NE1	-5.70	1.31	1.35
15	h	2	A1H2H	O34-N33	5.67	1.32	1.22
16	e	4	A1H2I	CD1-NE1	-5.66	1.31	1.35
16	f	2	A1H2H	CB-CG	-5.62	1.37	1.51
15	g	4	A1H45	CB-CG	-5.45	1.48	1.54
15	g	4	A1H45	CE3-CD2	-5.31	1.30	1.39
16	j	4	A1H2I	CD1-NE1	-5.04	1.31	1.35
16	j	2	A1H2H	CB-CG	-5.02	1.39	1.51
15	g	2	A1H2H	CB-CG	-4.92	1.39	1.51
16	j	4	A1H2I	CZ2-CE2	-4.85	1.31	1.39
15	g	2	A1H2H	O34-N33	4.83	1.31	1.22
16	i	2	A1H2H	CB-CG	-4.81	1.39	1.51
16	i	4	A1H2I	CE3-CD2	-4.78	1.31	1.39
16	j	4	A1H2I	CE3-CD2	-4.76	1.31	1.39
16	i	4	A1H2I	CD1-NE1	-4.67	1.32	1.35
15	g	4	A1H45	CZ2-CE2	-4.61	1.31	1.39
15	h	4	A1H45	CZ2-CE2	-4.50	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	e	4	A1H2I	CE3-CD2	-4.49	1.32	1.39
15	h	4	A1H45	CE3-CD2	-4.46	1.32	1.39
16	i	2	A1H2H	F19-CE2	-4.38	1.24	1.35
16	f	4	A1H2I	CE3-CD2	-4.30	1.32	1.39
16	i	4	A1H2I	CZ2-CE2	-4.29	1.32	1.39
16	e	4	A1H2I	CZ2-CE2	-4.13	1.32	1.39
16	j	4	A1H2I	CE2-NE1	-4.11	1.31	1.38
16	f	4	A1H2I	CZ2-CE2	-4.03	1.32	1.39
16	e	4	A1H2I	CE2-NE1	-4.02	1.31	1.38
15	h	4	A1H45	CE2-NE1	-4.01	1.31	1.38
15	g	4	A1H45	CE2-NE1	-3.76	1.31	1.38
15	h	4	A1H45	CB-CG	-3.75	1.50	1.54
16	f	4	A1H2I	CE2-NE1	-3.64	1.32	1.38
16	f	2	A1H2H	F19-CE2	-3.62	1.26	1.35
16	e	4	A1H2I	CB-CG	-3.44	1.50	1.54
16	i	4	A1H2I	CE2-NE1	-3.35	1.32	1.38
16	f	4	A1H2I	CB-CG	-3.31	1.50	1.54
16	j	4	A1H2I	CB-CG	-2.93	1.51	1.54
16	f	2	A1H2H	O34-N33	2.93	1.27	1.22
15	h	2	A1H2H	CB-CA	-2.05	1.49	1.53

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	e	4	A1H2I	CE2-NE1-CD1	-10.90	105.91	111.85
16	j	4	A1H2I	CE2-NE1-CD1	-10.00	106.40	111.85
15	g	4	A1H45	CD2-CG-CD1	9.79	105.67	102.40
15	g	4	A1H45	CE2-NE1-CD1	-9.72	106.55	111.85
16	f	4	A1H2I	CE2-NE1-CD1	-9.33	106.77	111.85
15	h	4	A1H45	CE2-NE1-CD1	-8.42	107.26	111.85
16	i	4	A1H2I	CD2-CG-CD1	7.17	104.80	102.40
16	i	4	A1H2I	CE2-NE1-CD1	-6.95	108.06	111.85
16	i	2	A1H2H	CE1-CZ-N33	5.85	122.72	116.47
15	h	4	A1H45	CD2-CG-CD1	5.75	104.32	102.40
15	h	2	A1H2H	CB-CA-C	-5.61	100.95	111.47
16	e	2	A1H2H	CB-CA-C	-5.38	101.38	111.47
15	g	2	A1H2H	CE1-CZ-N33	5.37	122.21	116.47
16	f	2	A1H2H	CE1-CZ-N33	4.68	121.47	116.47
15	h	2	A1H2H	CE1-CZ-N33	4.63	121.42	116.47
16	j	2	A1H2H	CE1-CZ-N33	4.41	121.19	116.47
16	e	2	A1H2H	CE1-CZ-N33	3.63	120.35	116.47
16	f	4	A1H2I	CB-CG-CD1	-3.35	105.76	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	j	4	A1H2I	CB-CA-N	3.25	117.56	110.32
16	f	2	A1H2H	CG-CD2-CE2	3.25	121.47	119.37
16	j	4	A1H2I	CD2-CG-CD1	3.21	103.47	102.40
16	f	2	A1H2H	CB-CA-C	-3.04	105.77	111.47
16	f	4	A1H2I	CB-CG-CD2	-2.90	108.53	114.53
15	h	2	A1H2H	F19-CE2-CZ	2.85	123.32	118.39
16	f	4	A1H2I	CD2-CE2-NE1	-2.85	107.99	109.31
15	g	4	A1H45	CB-CG-CD2	2.80	120.33	114.53
15	h	4	A1H45	CZ2-CH2-CZ3	-2.66	116.96	119.88
15	h	4	A1H45	CB-CG-CD2	2.54	119.79	114.53
16	j	2	A1H2H	CG-CB-CA	-2.47	109.11	114.10
15	g	2	A1H2H	F19-CE2-CZ	2.44	122.62	118.39
15	h	2	A1H2H	CB-CG-CD2	-2.44	116.24	120.44
15	g	2	A1H2H	CG-CD2-CE2	2.43	120.94	119.37
16	j	4	A1H2I	CB-CG-CD1	-2.39	108.02	113.69
16	i	4	A1H2I	CB-CA-N	2.16	115.12	110.32
16	e	4	A1H2I	CB-CG-CD2	-2.14	110.11	114.53
16	i	2	A1H2H	CG-CD2-CE2	2.13	120.75	119.37
15	g	2	A1H2H	CB-CA-C	-2.13	107.48	111.47

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	g	2	A1H2H	O-C-CA-CB
15	g	4	A1H45	CA-CB-CG-CD1
15	h	4	A1H45	CA-CB-CG-CD1
16	i	2	A1H2H	C-CA-CB-CG
16	i	2	A1H2H	N-CA-CB-CG
16	i	2	A1H2H	CE1-CZ-N33-O34
16	i	2	A1H2H	CE2-CZ-N33-O34
16	j	2	A1H2H	C-CA-CB-CG
16	j	2	A1H2H	N-CA-CB-CG
16	e	4	A1H2I	N-CA-CB-CG
16	f	4	A1H2I	N-CA-CB-CG
16	j	4	A1H2I	CA-CB-CG-CD1
15	g	2	A1H2H	CE1-CZ-N33-O34
15	h	2	A1H2H	CE1-CZ-N33-O34
16	e	2	A1H2H	CA-CB-CG-CD2
16	e	2	A1H2H	CA-CB-CG-CD1
16	j	2	A1H2H	CA-CB-CG-CD1
16	j	2	A1H2H	CA-CB-CG-CD2

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Mol	Chain	Res	Type	Atoms
16	f	2	A1H2H	CA-CB-CG-CD2
16	f	2	A1H2H	CA-CB-CG-CD1
16	i	2	A1H2H	CA-CB-CG-CD2
16	i	2	A1H2H	CA-CB-CG-CD1
16	j	4	A1H2I	CA-CB-CG-CD2
16	i	4	A1H2I	CA-CB-CG-CD1
15	g	2	A1H2H	CE2-CZ-N33-O34
15	h	2	A1H2H	CE2-CZ-N33-O34

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 10 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
19	MES	K	301	-	12,12,12	0.76	0	14,16,16	0.50	0
19	MES	Y	301	-	12,12,12	0.70	0	14,16,16	0.50	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	MES	K	301	-	-	2/6/14/14	0/1/1/1
19	MES	Y	301	-	-	3/6/14/14	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	K	301	MES	C8-C7-N4-C3
19	K	301	MES	C8-C7-N4-C5
19	Y	301	MES	C7-C8-S-O3S
19	Y	301	MES	C7-C8-S-O2S
19	Y	301	MES	C7-C8-S-O1S

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	K	301	MES	1	0
19	Y	301	MES	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.30	2 (0%)	86	81	54, 68, 103, 161	0
1	O	250/250 (100%)	-0.18	8 (3%)	47	37	57, 78, 114, 164	0
2	B	244/258 (94%)	-0.18	5 (2%)	65	56	55, 73, 126, 163	0
2	P	244/258 (94%)	-0.13	10 (4%)	37	27	60, 78, 133, 155	0
3	C	240/254 (94%)	-0.19	8 (3%)	46	36	54, 77, 127, 148	0
3	Q	240/254 (94%)	0.07	13 (5%)	25	17	62, 95, 156, 175	0
4	D	235/260 (90%)	-0.37	2 (0%)	84	80	57, 77, 104, 146	0
4	R	235/260 (90%)	-0.24	2 (0%)	84	80	58, 85, 119, 151	0
5	E	231/234 (98%)	-0.22	3 (1%)	77	72	59, 81, 113, 128	0
5	S	231/234 (98%)	-0.08	5 (2%)	62	52	62, 94, 130, 150	0
6	F	243/288 (84%)	-0.29	2 (0%)	86	81	54, 77, 116, 145	0
6	T	243/288 (84%)	-0.13	7 (2%)	51	41	61, 87, 129, 147	0
7	G	241/252 (95%)	-0.37	2 (0%)	86	81	52, 70, 103, 146	0
7	U	241/252 (95%)	-0.40	2 (0%)	86	81	58, 73, 107, 134	0
8	H	222/232 (95%)	-0.39	2 (0%)	84	80	53, 65, 93, 123	0
8	V	222/232 (95%)	-0.34	2 (0%)	84	80	55, 69, 91, 128	0
9	I	204/205 (99%)	-0.46	1 (0%)	91	88	48, 65, 90, 118	0
9	W	204/205 (99%)	-0.45	1 (0%)	91	88	48, 65, 88, 117	0
10	J	195/198 (98%)	-0.35	1 (0%)	91	88	49, 66, 90, 122	0
10	X	195/198 (98%)	-0.44	3 (1%)	73	68	55, 69, 91, 134	0
11	K	212/212 (100%)	-0.35	1 (0%)	91	88	51, 64, 88, 120	0
11	Y	212/212 (100%)	-0.36	1 (0%)	91	88	57, 68, 92, 112	0
12	L	222/222 (100%)	-0.44	0	100	100	50, 67, 90, 105	0
12	Z	222/222 (100%)	-0.43	0	100	100	50, 69, 96, 104	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	M	233/246 (94%)	-0.52	1 (0%)	92	91	50, 66, 87, 103	0
13	a	233/246 (94%)	-0.49	1 (0%)	92	91	50, 66, 85, 94	0
14	N	196/196 (100%)	-0.41	1 (0%)	91	88	51, 62, 91, 112	0
14	b	196/196 (100%)	-0.35	1 (0%)	91	88	52, 64, 92, 115	0
15	g	1/5 (20%)	-0.46	0	100	100	66, 66, 66, 66	0
15	h	1/5 (20%)	-1.08	0	100	100	68, 68, 68, 68	0
16	e	1/5 (20%)	-1.09	0	100	100	60, 60, 60, 60	0
16	f	1/5 (20%)	-0.73	0	100	100	67, 67, 67, 67	0
16	i	1/5 (20%)	-0.86	0	100	100	73, 73, 73, 73	0
16	j	1/5 (20%)	-1.07	0	100	100	71, 71, 71, 71	0
All	All	6342/6644 (95%)	-0.31	87 (1%)	75	70	48, 72, 117, 175	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	49	THR	7.7
1	A	1	MET	7.0
3	Q	50	LEU	6.4
3	Q	48	SER	5.3
3	Q	206	LYS	5.3
2	B	220	ASN	4.9
3	Q	204	GLY	4.9
9	I	1	SER	4.6
1	O	1	MET	4.5
5	S	202	ASP	4.4
5	S	233	ILE	4.3
5	E	202	ASP	4.2
6	T	2	THR	3.8
13	M	1	THR	3.8
3	C	49	THR	3.7
10	X	1	MET	3.7
8	V	227	ASP	3.6
6	T	53	LYS	3.5
9	W	191	LYS	3.3
11	K	217	GLY	3.3
3	C	206	LYS	3.3
3	C	202	GLN	3.3
3	C	50	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
10	X	194	ASP	3.3
1	O	249	ALA	3.2
3	Q	205	ALA	3.2
2	P	219	ALA	3.1
14	N	200	GLN	3.1
4	R	241	ALA	3.1
5	E	233	ILE	3.1
3	Q	180	LYS	3.1
3	Q	235	GLU	3.1
8	V	226	CYS	3.1
8	H	227	ASP	3.0
2	B	219	ALA	3.0
3	C	205	ALA	3.0
7	U	2	GLY	3.0
2	P	220	ASN	3.0
11	Y	217	GLY	2.9
2	B	221	ASP	2.9
14	b	200	GLN	2.9
2	P	244	THR	2.8
8	H	226	CYS	2.8
1	O	52	SER	2.8
6	T	241	LYS	2.7
5	S	204	SER	2.7
6	T	180	PRO	2.7
3	C	48	SER	2.7
10	J	1	MET	2.7
1	O	250	LEU	2.7
13	a	1	THR	2.7
3	Q	203	THR	2.6
2	P	52	THR	2.6
3	Q	236	GLN	2.6
2	P	59	ASP	2.6
2	B	244	THR	2.6
1	A	2	THR	2.5
3	Q	51	LYS	2.5
2	B	240	LYS	2.5
1	O	201	GLU	2.5
3	Q	47	ARG	2.5
1	O	231	LYS	2.5
5	S	207	VAL	2.4
3	Q	202	GLN	2.4
6	F	2	THR	2.4

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Mol	Chain	Res	Type	RSRZ
2	P	221	ASP	2.4
6	F	205	GLU	2.3
2	P	243	ILE	2.3
1	O	230	ASP	2.2
7	G	179	LYS	2.2
6	T	181	GLU	2.2
2	P	51	VAL	2.2
5	S	173	ARG	2.1
3	C	51	LYS	2.1
4	D	241	ALA	2.1
1	O	2	THR	2.1
7	U	241	GLU	2.1
2	P	223	GLU	2.1
2	P	1	GLY	2.1
5	E	207	VAL	2.1
10	X	193	ASP	2.1
7	G	180	SER	2.1
4	R	177	ASN	2.0
6	T	243	ILE	2.0
3	C	238	LYS	2.0
4	D	10	GLU	2.0
6	T	237	ASP	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
16	A1H2H	j	2	15/16	0.75	0.51	83,111,129,133	0
16	A1H2H	i	2	15/16	0.77	0.50	87,117,142,142	0
16	A1H2I	i	4	16/17	0.83	0.23	59,86,89,94	0
15	A1H2H	h	2	15/16	0.90	0.36	75,93,112,113	0
15	A1H2H	g	2	15/16	0.90	0.40	73,95,105,109	0
16	A1H2H	e	2	15/16	0.91	0.29	64,81,102,111	0
15	A1H45	h	4	16/17	0.91	0.21	59,73,76,82	0
16	A1H2I	j	4	16/17	0.91	0.23	62,84,90,92	0
15	A1H45	g	4	16/17	0.92	0.18	57,72,75,81	0
16	A1H2I	e	4	16/17	0.92	0.22	59,77,81,82	0
16	A1H2I	f	4	16/17	0.94	0.23	61,79,85,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
16	A1H2H	f	2	15/16	0.94	0.25	68,80,103,108	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	MG	Z	301	1/1	0.87	0.19	89,89,89,89	0
17	MG	V	301	1/1	0.95	0.26	107,107,107,107	0
17	MG	G	301	1/1	0.97	0.19	81,81,81,81	0
17	MG	N	301	1/1	0.97	0.12	65,65,65,65	0
18	CL	U	301	1/1	0.97	0.06	65,65,65,65	0
19	MES	K	301	12/12	0.97	0.20	48,52,71,82	0
18	CL	G	302	1/1	0.98	0.07	60,60,60,60	0
17	MG	K	302	1/1	0.98	0.13	72,72,72,72	0
17	MG	I	301	1/1	0.98	0.13	76,76,76,76	0
19	MES	Y	301	12/12	0.98	0.17	50,54,67,72	0
17	MG	Y	302	1/1	0.99	0.09	73,73,73,73	0
17	MG	X	201	1/1	0.99	0.32	48,48,48,48	0

6.5 Other polymers (i)

There are no such residues in this entry.