Full wwPDB X-ray Structure Validation Report (i)

Dec 6, 2016 – 03:13 AM EST

PDB ID	:	5L5A
Title	:	Yeast 20S proteasome with human beta5i (1-138; R57T)
Authors	:	Groll, M.; Huber, E.M.
Deposited on	:	2016-05-28
Resolution	:	2.40 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:

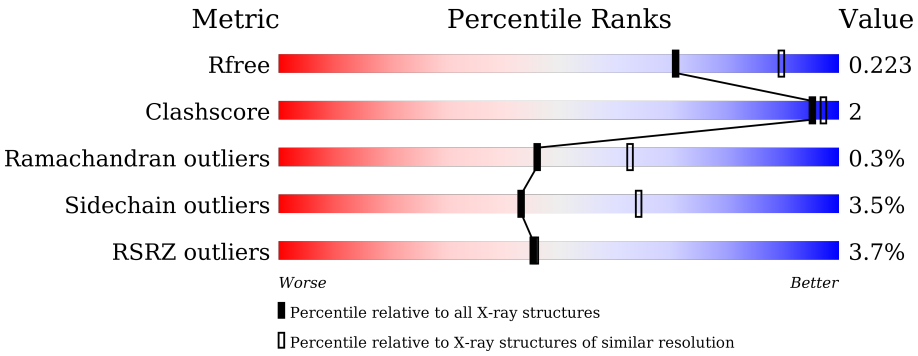
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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% 98% ·
1	O	250	4% 96% ·
2	B	258	6% 86% 8% · 5%
2	P	258	5% 86% 7% · 5%
3	C	254	9% 86% 7% · 6%
3	Q	254	12% 87% 7% · 6%

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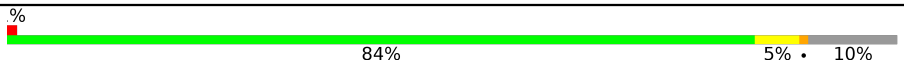
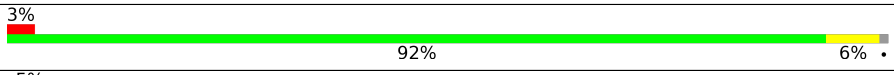
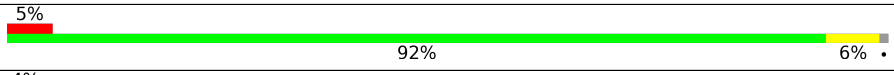
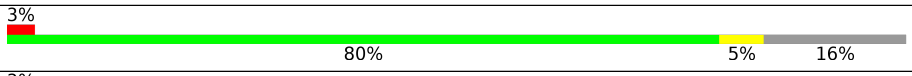
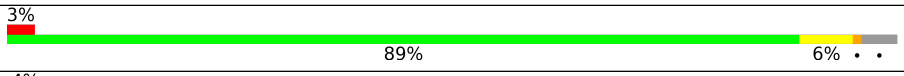
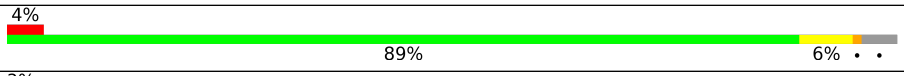
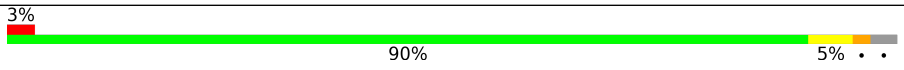
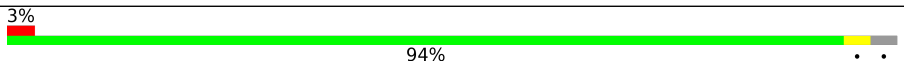
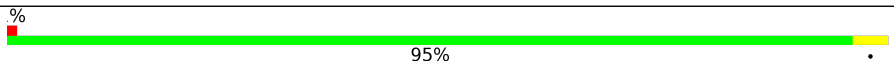
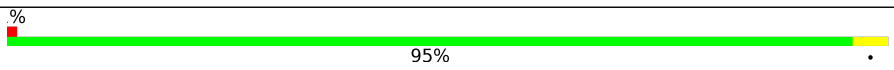
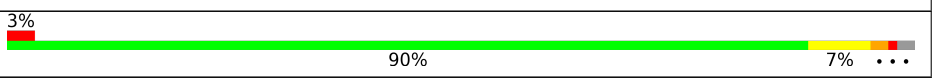
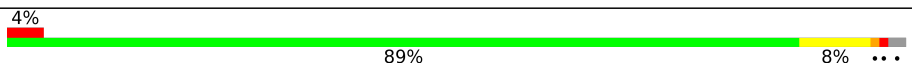
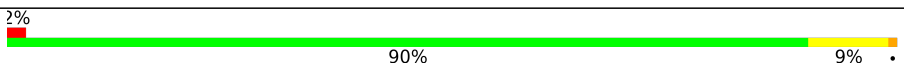
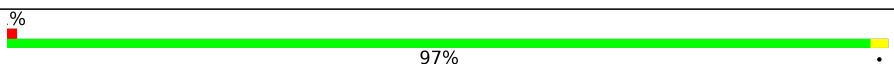
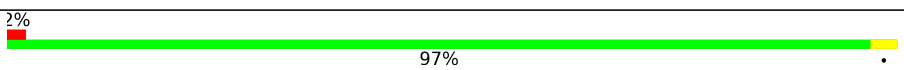
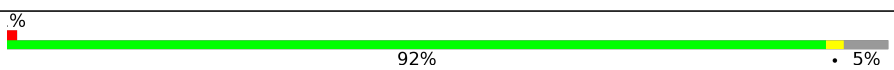
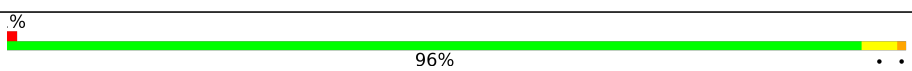
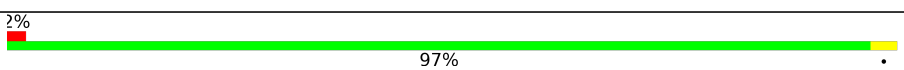
Mol	Chain	Length	Quality of chain
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	211	
11	Y	211	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 50851 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	226	Total	C	N	O	S	0	1	0
			1726	1087	300	332	7			
8	V	226	Total	C	N	O	S	0	0	0
			1719	1082	298	332	7			

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

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

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

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

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

- Molecule 11 is a protein called Proteasome subunit beta type-8,Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	211	Total	C	N	O	S	0	0	0
			1636	1033	279	312	12			
11	Y	211	Total	C	N	O	S	0	0	0
			1636	1033	279	312	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	57	THR	ARG	engineered mutation	UNP P28062
Y	57	THR	ARG	engineered mutation	UNP P28062

- 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	1	0
			1832	1159	315	351	7			
13	a	233	Total	C	N	O	S	0	1	0
			1835	1160	316	352	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 MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 16 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	68	Total O 68 68	0	0
17	B	44	Total O 44 44	0	0
17	C	39	Total O 39 39	0	0
17	D	35	Total O 35 35	0	0
17	E	25	Total O 25 25	0	0
17	F	49	Total O 49 49	0	0
17	G	66	Total O 66 66	0	0

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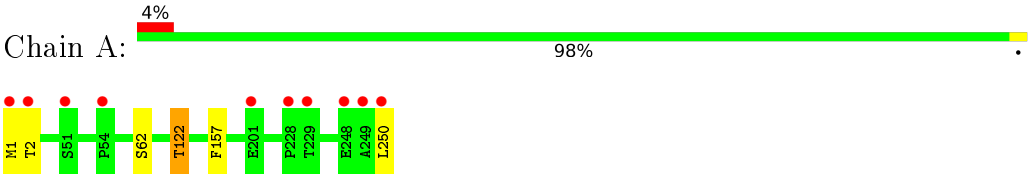
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	H	60	Total O 60 60	0	0
17	I	67	Total O 67 67	0	0
17	J	55	Total O 55 55	0	0
17	K	39	Total O 39 39	0	0
17	L	68	Total O 68 68	0	0
17	M	86	Total O 86 86	0	0
17	N	58	Total O 58 58	0	0
17	O	35	Total O 35 35	0	0
17	P	33	Total O 33 33	0	0
17	Q	24	Total O 24 24	0	0
17	R	30	Total O 30 30	0	0
17	S	27	Total O 27 27	0	0
17	T	38	Total O 38 38	0	0
17	U	75	Total O 75 75	0	0
17	V	55	Total O 55 55	0	0
17	W	71	Total O 71 71	0	0
17	X	54	Total O 54 54	0	0
17	Y	45	Total O 45 45	0	0
17	Z	72	Total O 72 72	0	0
17	a	81	Total O 81 81	0	0
17	b	64	Total O 64 64	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.

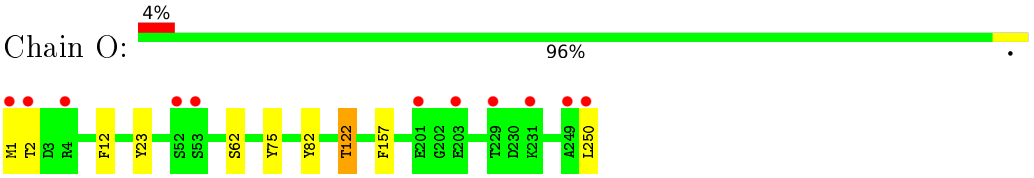
- Molecule 1: Proteasome subunit alpha type-2

Chain A:



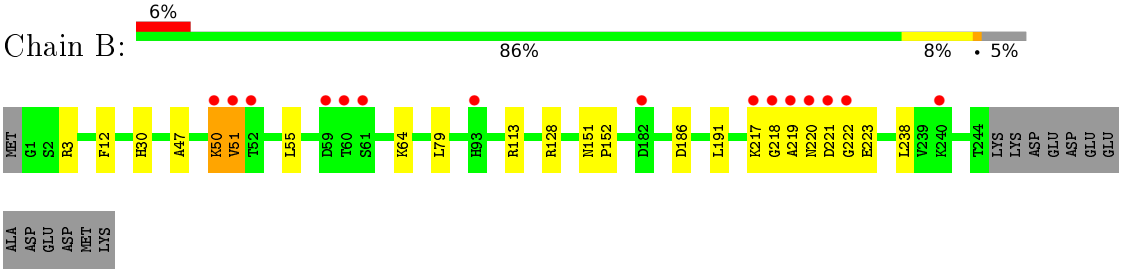
- Molecule 1: Proteasome subunit alpha type-2

Chain O:



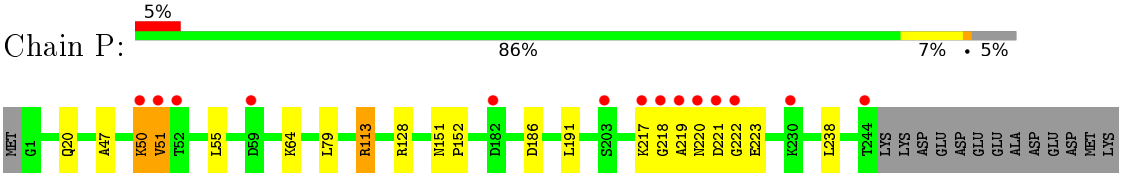
- Molecule 2: Proteasome subunit alpha type-3

Chain B:



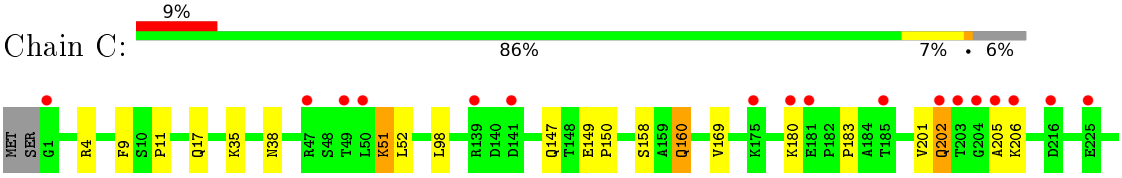
- Molecule 2: Proteasome subunit alpha type-3

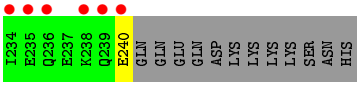
Chain P:



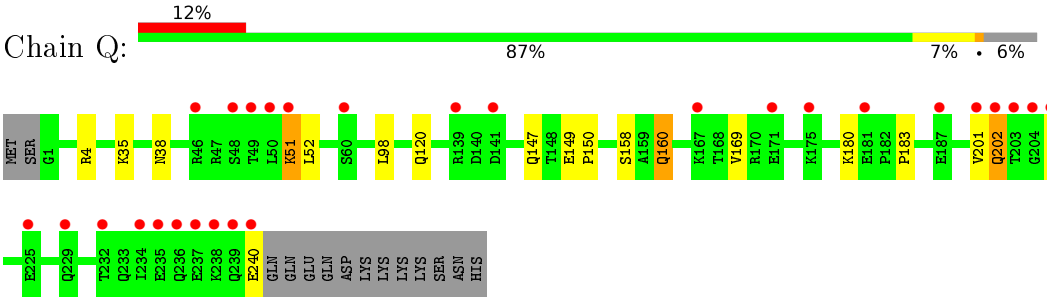
- Molecule 3: Proteasome subunit alpha type-4

Chain C:

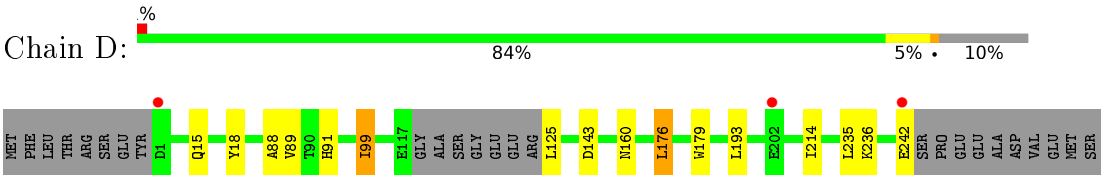




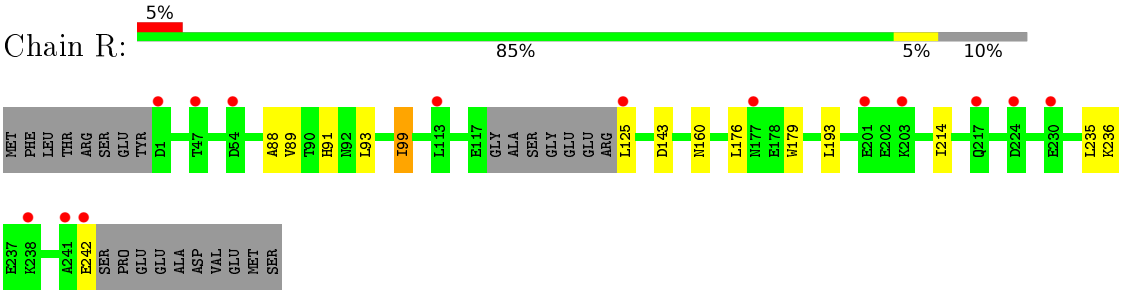
• Molecule 3: Proteasome subunit alpha type-4



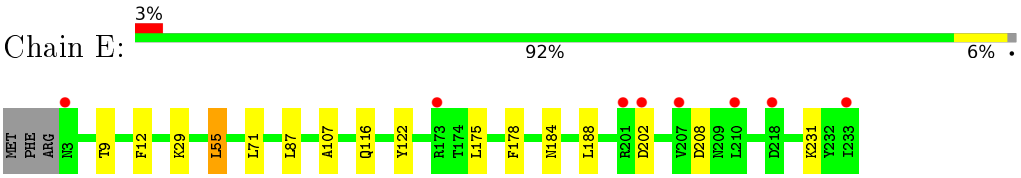
• Molecule 4: Proteasome subunit alpha type-5



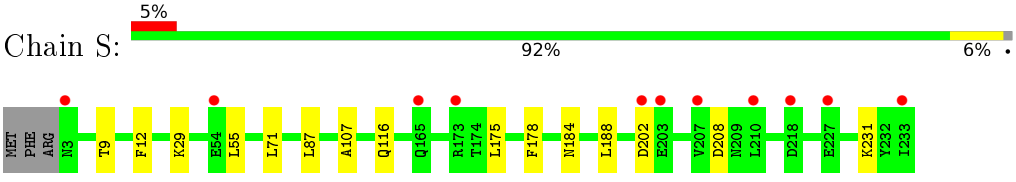
• Molecule 4: Proteasome subunit alpha type-5



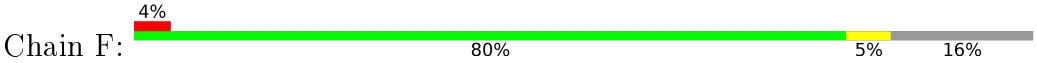
• Molecule 5: Proteasome subunit alpha type-6

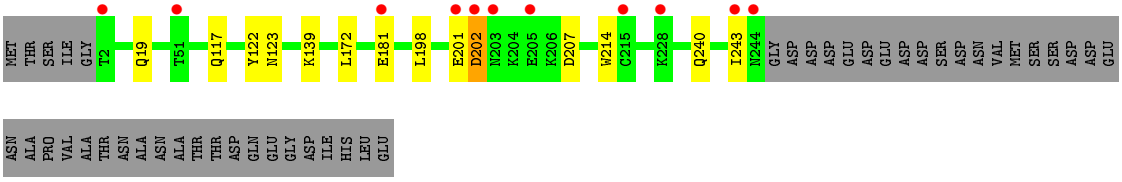


• Molecule 5: Proteasome subunit alpha type-6

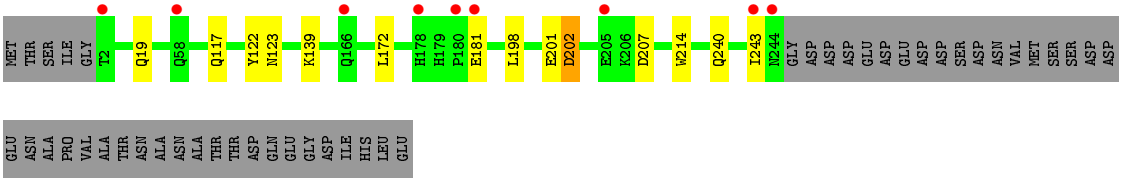


• Molecule 6: Probable proteasome subunit alpha type-7

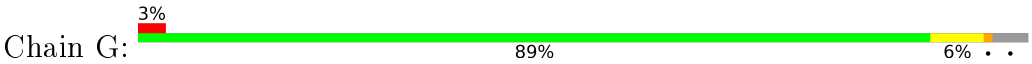


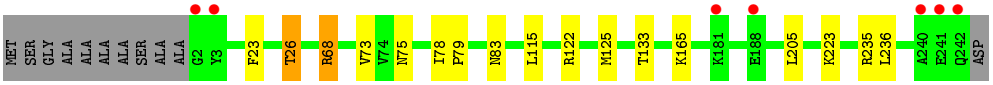


• Molecule 6: Probable proteasome subunit alpha type-7

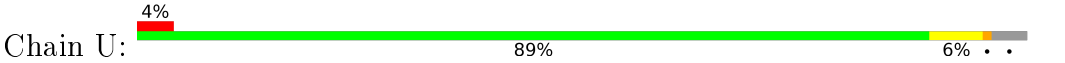


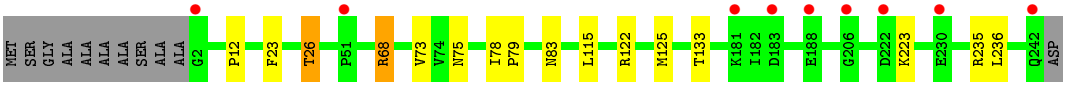
• Molecule 7: Proteasome subunit alpha type-1



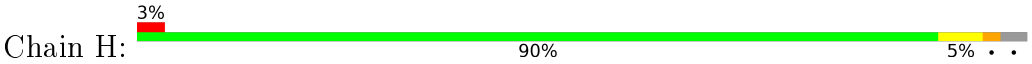


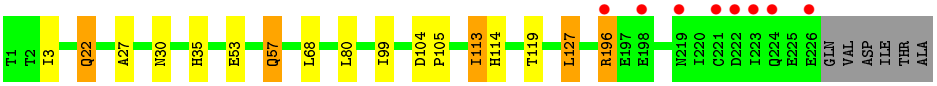
• Molecule 7: Proteasome subunit alpha type-1



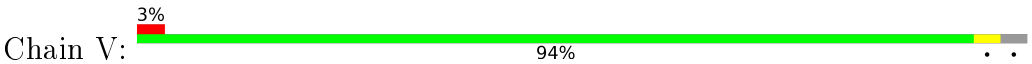


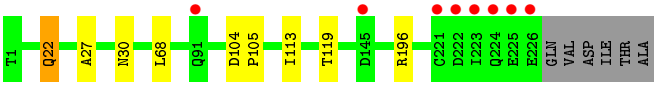
• Molecule 8: Proteasome subunit beta type-2



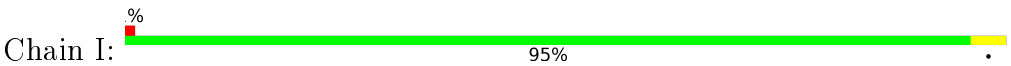


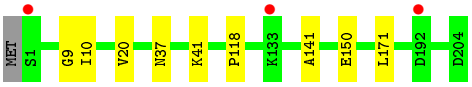
• Molecule 8: Proteasome subunit beta type-2



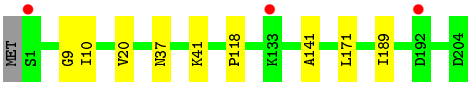


• Molecule 9: Proteasome subunit beta type-3

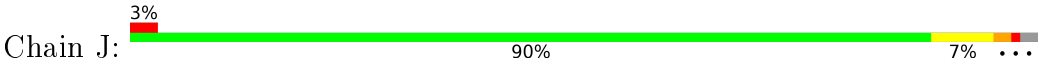


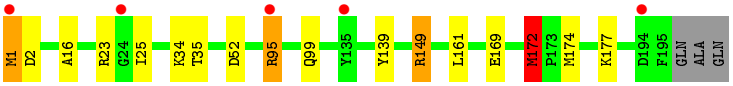


• Molecule 9: Proteasome subunit beta type-3

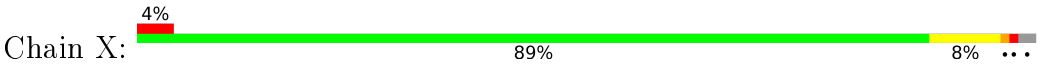


• Molecule 10: Proteasome subunit beta type-4

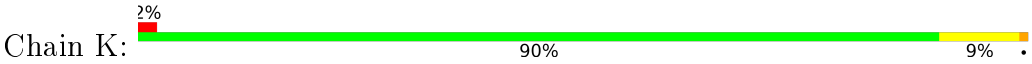




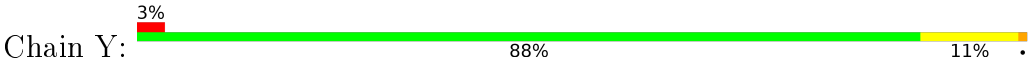
• Molecule 10: Proteasome subunit beta type-4

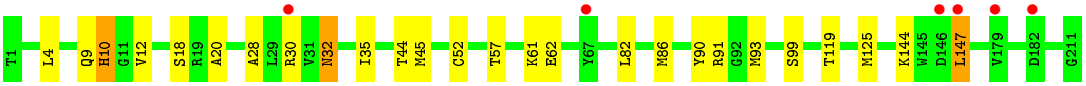


• Molecule 11: Proteasome subunit beta type-8,Proteasome subunit beta type-5

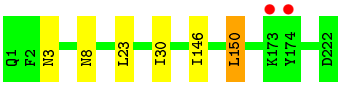


• Molecule 11: Proteasome subunit beta type-8,Proteasome subunit beta type-5

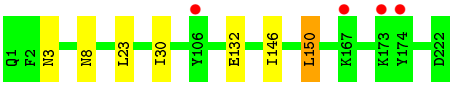




• Molecule 12: Proteasome subunit beta type-6

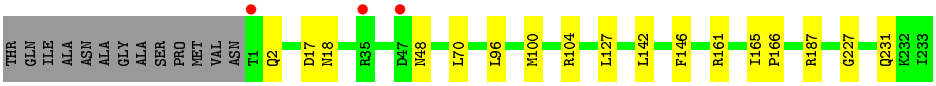


• Molecule 12: Proteasome subunit beta type-6



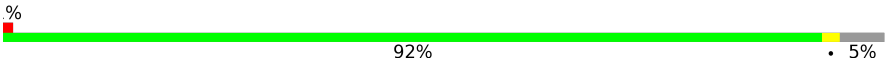
• Molecule 13: Proteasome subunit beta type-7

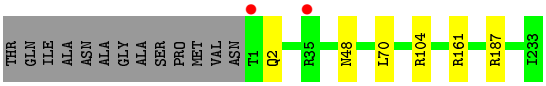
Chain M:



• Molecule 13: Proteasome subunit beta type-7

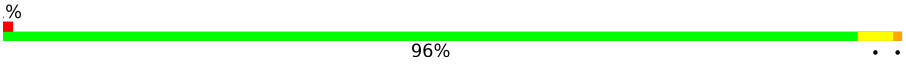
Chain a:

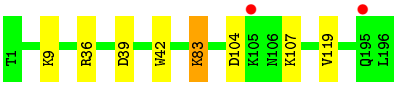




• Molecule 14: Proteasome subunit beta type-1

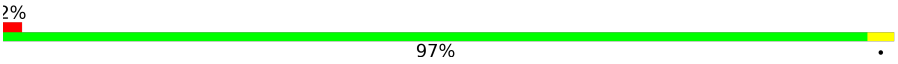
Chain N:

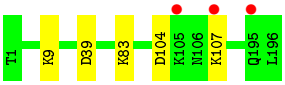




• Molecule 14: Proteasome subunit beta type-1

Chain b:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	135.14Å 301.15Å 145.06Å 90.00° 112.57° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40 15.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (15.00-2.40) 99.2 (15.00-2.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.05 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.200 , 0.219 0.204 , 0.223	Depositor DCC
R_{free} test set	20515 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	46.9	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 38.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	50851	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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: MG, CL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.27	0/1952	0.46	0/2642
1	O	0.27	0/1952	0.46	0/2642
2	B	0.27	0/1934	0.49	0/2618
2	P	0.27	0/1934	0.49	0/2618
3	C	0.27	0/1910	0.51	0/2586
3	Q	0.28	0/1910	0.51	0/2586
4	D	0.27	0/1837	0.47	0/2475
4	R	0.27	0/1837	0.47	0/2475
5	E	0.27	0/1800	0.47	0/2433
5	S	0.27	0/1800	0.47	0/2433
6	F	0.27	0/1932	0.45	0/2609
6	T	0.27	0/1932	0.45	0/2609
7	G	0.28	0/1945	0.48	0/2634
7	U	0.28	0/1945	0.47	0/2634
8	H	0.40	2/1761 (0.1%)	0.56	2/2388 (0.1%)
8	V	0.30	0/1750	0.47	0/2373
9	I	0.28	0/1611	0.49	0/2174
9	W	0.28	0/1611	0.49	0/2174
10	J	0.38	0/1589	1.01	8/2142 (0.4%)
10	X	0.34	0/1589	0.97	6/2142 (0.3%)
11	K	0.35	0/1673	0.52	0/2259
11	Y	0.38	0/1673	0.54	0/2259
12	L	0.29	0/1795	0.47	0/2420
12	Z	0.35	0/1795	0.48	0/2420
13	M	0.38	0/1866	0.55	0/2528
13	a	0.27	0/1866	0.51	0/2528
14	N	0.28	0/1541	0.48	0/2087
14	b	0.27	0/1541	0.48	0/2087
All	All	0.30	2/50281 (0.0%)	0.53	16/67975 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying

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

Mol	Chain	#Chirality outliers	#Planarity outliers
10	J	0	2
10	X	0	2
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	114[A]	HIS	CA-C	5.99	1.68	1.52
8	H	114[B]	HIS	CA-C	5.99	1.68	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	J	149	ARG	NE-CZ-NH1	-21.12	109.74	120.30
10	J	95	ARG	NE-CZ-NH2	-20.61	110.00	120.30
10	X	149	ARG	NE-CZ-NH2	-20.09	110.25	120.30
10	X	95	ARG	NE-CZ-NH1	-19.31	110.65	120.30
10	X	95	ARG	NE-CZ-NH2	16.04	128.32	120.30
10	J	149	ARG	NE-CZ-NH2	15.71	128.16	120.30
10	X	149	ARG	NE-CZ-NH1	15.06	127.83	120.30
10	J	95	ARG	NE-CZ-NH1	13.78	127.19	120.30
10	J	149	ARG	CD-NE-CZ	10.86	138.81	123.60
10	J	95	ARG	CD-NE-CZ	10.62	138.47	123.60
10	X	149	ARG	CD-NE-CZ	9.42	136.78	123.60
10	X	95	ARG	CD-NE-CZ	9.18	136.46	123.60
10	J	172	MET	C-N-CD	5.95	140.89	128.40
10	J	149	ARG	CG-CD-NE	-5.89	99.42	111.80
8	H	114[A]	HIS	CA-C-O	5.52	131.69	120.10
8	H	114[B]	HIS	CA-C-O	5.52	131.69	120.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	J	149	ARG	Sidechain
10	J	95	ARG	Sidechain
10	X	149	ARG	Sidechain
10	X	95	ARG	Sidechain

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	2	0
1	O	1915	0	1929	5	0
2	B	1904	0	1904	11	0
2	P	1904	0	1904	9	0
3	C	1881	0	1895	8	0
3	Q	1881	0	1895	6	0
4	D	1813	0	1797	9	0
4	R	1813	0	1797	7	0
5	E	1773	0	1775	5	0
5	S	1773	0	1775	3	0
6	F	1892	0	1883	4	0
6	T	1892	0	1883	4	0
7	G	1907	0	1901	5	0
7	U	1907	0	1901	6	0
8	H	1726	0	1726	13	0
8	V	1719	0	1719	4	0
9	I	1581	0	1574	4	0
9	W	1581	0	1574	4	0
10	J	1561	0	1569	11	0
10	X	1561	0	1569	14	0
11	K	1636	0	1575	14	0
11	Y	1636	0	1575	18	0
12	L	1757	0	1711	2	0
12	Z	1757	0	1711	3	0
13	M	1832	0	1845	5	0
13	a	1835	0	1844	0	0
14	N	1512	0	1481	2	0
14	b	1512	0	1481	0	0
15	G	1	0	0	0	0
15	H	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	K	2	0	0	0	0
15	L	1	0	0	0	0
15	N	1	0	0	0	0
15	Z	1	0	0	0	0
16	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	U	1	0	0	0	0
17	A	68	0	0	0	0
17	B	44	0	0	0	0
17	C	39	0	0	0	0
17	D	35	0	0	0	0
17	E	25	0	0	0	0
17	F	49	0	0	0	0
17	G	66	0	0	0	0
17	H	60	0	0	0	0
17	I	67	0	0	0	0
17	J	55	0	0	0	0
17	K	39	0	0	0	0
17	L	68	0	0	0	0
17	M	86	0	0	0	0
17	N	58	0	0	0	0
17	O	35	0	0	0	0
17	P	33	0	0	1	0
17	Q	24	0	0	0	0
17	R	30	0	0	1	0
17	S	27	0	0	0	0
17	T	38	0	0	0	0
17	U	75	0	0	0	0
17	V	55	0	0	0	0
17	W	71	0	0	0	0
17	X	54	0	0	0	0
17	Y	45	0	0	0	0
17	Z	72	0	0	0	0
17	a	81	0	0	0	0
17	b	64	0	0	0	0
All	All	50851	0	49122	149	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (149) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:18:SER:OG	11:Y:30:ARG:HA	1.73	0.88
8:H:53:GLU:O	8:H:57:GLN:HG2	1.79	0.82
10:J:23:ARG:NH2	11:K:119:THR:OG1	2.15	0.80
10:J:174:MET:SD	10:X:174:MET:SD	2.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:89:VAL:HG12	11:Y:61:LYS:HG3	1.65	0.78
4:D:89:VAL:HG12	11:K:61:LYS:HG3	1.66	0.78
10:X:23:ARG:NH2	11:Y:119:THR:OG1	2.17	0.76
11:K:86:MET:HA	11:K:89:GLN:HE21	1.53	0.71
10:X:1:MET:HA	10:X:34:LYS:HE3	1.75	0.68
10:J:1:MET:HA	10:J:34:LYS:CE	2.27	0.64
10:X:1:MET:HA	10:X:34:LYS:CE	2.27	0.64
10:X:52:ASP:OD1	11:Y:91:ARG:NH1	2.30	0.63
10:J:1:MET:HA	10:J:34:LYS:HE3	1.80	0.62
8:H:80:LEU:HD12	8:H:113:ILE:CD1	2.30	0.62
8:H:53:GLU:O	8:H:57:GLN:CG	2.47	0.62
11:K:9:GLN:HB3	11:K:10:HIS:CD2	2.35	0.62
10:J:25:ILE:O	10:X:139:TYR:OH	2.17	0.62
11:Y:18:SER:HG	11:Y:30:ARG:HA	1.66	0.61
10:J:139:TYR:OH	10:X:25:ILE:O	2.18	0.60
11:Y:9:GLN:HB3	11:Y:10:HIS:CD2	2.36	0.59
8:H:80:LEU:HD12	8:H:113:ILE:HD13	1.85	0.58
4:R:89:VAL:CG1	11:Y:61:LYS:HG3	2.35	0.57
10:X:1:MET:HG3	10:X:1:MET:O	2.04	0.56
10:J:52:ASP:OD1	11:K:91:ARG:NH1	2.39	0.54
2:P:217:LYS:C	2:P:219:ALA:H	2.13	0.52
8:H:113:ILE:HG23	8:H:119:THR:HG22	1.92	0.52
11:K:9:GLN:HB3	11:K:10:HIS:HD2	1.74	0.52
4:D:89:VAL:CG1	11:K:61:LYS:HG3	2.38	0.52
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.40	0.51
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.76	0.51
2:P:113:ARG:NE	17:P:301:HOH:O	2.42	0.51
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.10	0.51
10:X:3:ILE:HD13	10:X:3:ILE:C	2.31	0.51
5:S:12:PHE:H	6:T:19:GLN:HE22	1.59	0.51
2:P:221:ASP:O	2:P:223:GLU:N	2.44	0.51
2:B:217:LYS:C	2:B:219:ALA:H	2.13	0.51
2:B:221:ASP:O	2:B:223:GLU:N	2.44	0.51
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.93	0.50
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.58	0.50
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.93	0.50
3:C:201:VAL:O	3:C:202:GLN:CB	2.58	0.50
11:Y:90:TYR:O	11:Y:93:MET:HB2	2.11	0.50
7:G:23:PHE:O	7:G:26:THR:HB	2.12	0.50
11:Y:45:MET:HG2	11:Y:52:CYS:HB3	1.93	0.50
11:K:86:MET:HA	11:K:89:GLN:NE2	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:51:LYS:O	3:C:52:LEU:HB2	2.10	0.50
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.76	0.49
11:Y:9:GLN:HB3	11:Y:10:HIS:HD2	1.76	0.49
11:Y:32:ASN:N	12:Z:132:GLU:OE2	2.38	0.49
7:U:23:PHE:O	7:U:26:THR:HB	2.13	0.49
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.95	0.49
8:H:80:LEU:CD1	8:H:113:ILE:HD13	2.43	0.48
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.95	0.48
8:H:35:HIS:CE1	8:H:53:GLU:HG2	2.49	0.48
3:Q:120:GLN:NE2	17:R:301:HOH:O	2.46	0.48
4:D:91:HIS:HB3	4:D:99:ILE:HG22	1.96	0.48
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.96	0.48
4:R:91:HIS:HB3	4:R:99:ILE:HG22	1.96	0.48
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.96	0.47
11:Y:82:LEU:O	11:Y:86:MET:HG3	2.15	0.47
1:O:1:MET:HG3	6:T:122:TYR:CZ	2.50	0.47
1:A:1:MET:HG3	6:F:122:TYR:CZ	2.50	0.47
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.45	0.47
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.96	0.47
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.96	0.47
2:B:3:ARG:HB3	5:E:122:TYR:OH	2.15	0.46
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.45	0.46
11:K:82:LEU:O	11:K:86:MET:HG3	2.15	0.46
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.16	0.46
10:X:148:TYR:O	10:X:149:ARG:HD3	2.15	0.46
11:K:10:HIS:CD2	11:K:10:HIS:N	2.84	0.46
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.50	0.46
3:C:35:LYS:HG2	3:C:158:SER:O	2.15	0.46
2:B:12:PHE:H	3:C:17:GLN:HE22	1.63	0.46
7:G:68:ARG:O	7:G:223:LYS:HA	2.16	0.45
8:H:3:ILE:HG13	8:H:99:ILE:HD12	1.98	0.45
11:K:20:ALA:HB3	11:K:28:ALA:HB3	1.98	0.45
11:Y:10:HIS:CD2	11:Y:10:HIS:N	2.84	0.45
3:C:149:GLU:HB2	3:C:150:PRO:HD2	1.99	0.45
2:B:50:LYS:HD3	2:B:50:LYS:HA	1.86	0.45
8:H:22:GLN:HG2	8:H:27:ALA:HB2	1.99	0.44
11:K:44:THR:C	11:K:45:MET:HG3	2.38	0.44
5:E:12:PHE:H	6:F:19:GLN:HE22	1.66	0.44
8:H:196:ARG:NH2	9:I:150:GLU:O	2.51	0.44
11:Y:20:ALA:HB3	11:Y:28:ALA:HB3	1.98	0.44
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:68:ARG:O	7:U:223:LYS:HA	2.18	0.44
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.00	0.44
11:K:44:THR:O	11:K:99:SER:HB2	2.18	0.43
8:V:104:ASP:HB2	8:V:105:PRO:HD2	2.00	0.43
12:L:8:ASN:HA	12:L:30:ILE:O	2.18	0.43
11:Y:44:THR:O	11:Y:99:SER:HB2	2.18	0.43
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.48	0.43
8:H:99:ILE:HG13	8:H:127:LEU:HD22	2.00	0.43
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.01	0.43
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.18	0.43
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.83	0.43
2:B:50:LYS:O	2:B:51:VAL:C	2.57	0.43
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.53	0.43
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.48	0.43
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	0.43
10:X:1:MET:CA	10:X:34:LYS:HE3	2.47	0.42
2:P:50:LYS:O	2:P:51:VAL:C	2.57	0.42
3:C:9:PHE:H	4:D:15:GLN:HE22	1.67	0.42
5:S:87:LEU:HD21	5:S:107:ALA:HB1	2.00	0.42
7:U:68:ARG:HG2	7:U:68:ARG:HH21	1.84	0.42
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.02	0.42
8:H:104:ASP:HB2	8:H:105:PRO:HD2	2.00	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.42
8:V:113:ILE:HG12	8:V:119:THR:HG22	2.02	0.42
11:Y:144:LYS:HB2	11:Y:147:LEU:HD13	2.01	0.41
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.85	0.41
5:E:87:LEU:HD21	5:E:107:ALA:HB1	2.00	0.41
1:O:12:PHE:H	2:P:20:GLN:HE22	1.68	0.41
6:T:198:LEU:HD12	6:T:243:ILE:HG22	2.01	0.41
11:Y:44:THR:C	11:Y:45:MET:HG3	2.41	0.41
9:W:20:VAL:HG23	9:W:189:ILE:HB	2.02	0.41
11:K:144:LYS:HB2	11:K:147:LEU:HD13	2.01	0.41
13:M:96:LEU:O	13:M:100:MET:HG2	2.21	0.41
2:B:151:ASN:HB2	2:B:152:PRO:HD2	2.02	0.41
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.02	0.41
12:Z:146:ILE:HG22	12:Z:150:LEU:HD22	2.02	0.41
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.51	0.41
10:J:177:LYS:NZ	10:X:169:GLU:O	2.53	0.41
6:F:202:ASP:OD1	6:F:202:ASP:N	2.53	0.41
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.56	0.41
10:J:169:GLU:O	10:X:177:LYS:NZ	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.56	0.41
4:R:93:LEU:CD1	11:Y:57:THR:HG22	2.50	0.41
6:T:202:ASP:N	6:T:202:ASP:OD1	2.54	0.41
4:D:176:LEU:HD22	5:E:55:LEU:CD2	2.51	0.41
6:F:198:LEU:HD12	6:F:243:ILE:HG22	2.01	0.41
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.03	0.40
13:M:17:ASP:OD1	13:M:18:ASN:N	2.54	0.40
7:U:73:VAL:HG12	7:U:133:THR:HB	2.02	0.40
2:B:30:HIS:O	2:B:50:LYS:NZ	2.55	0.40
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.56	0.40
7:G:165:LYS:HD2	7:G:205:LEU:HD22	2.03	0.40
7:G:73:VAL:HG12	7:G:133:THR:HB	2.02	0.40
12:L:146:ILE:HG22	12:L:150:LEU:HD22	2.02	0.40
13:M:227:GLY:HA3	13:M:231:GLN:HB3	2.04	0.40
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.02	0.40
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.51	0.40
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.04	0.40
1:O:75:TYR:HB3	1:O:82:TYR:CD1	2.56	0.40
8:V:22:GLN:HG2	8:V:27:ALA:HB2	2.03	0.40
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.56	0.40
3:C:11:PRO:HA	4:D:18:TYR:CD1	2.56	0.40
10:J:139:TYR:CE2	10:J:172:MET:HG3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	39	56
1	O	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	39	56
2	B	242/258 (94%)	234 (97%)	4 (2%)	4 (2%)	11	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P	242/258 (94%)	234 (97%)	4 (2%)	4 (2%)	11	14
3	C	238/254 (94%)	232 (98%)	3 (1%)	3 (1%)	15	21
3	Q	238/254 (94%)	232 (98%)	3 (1%)	3 (1%)	15	21
4	D	231/260 (89%)	228 (99%)	3 (1%)	0	100	100
4	R	231/260 (89%)	228 (99%)	3 (1%)	0	100	100
5	E	229/234 (98%)	224 (98%)	5 (2%)	0	100	100
5	S	229/234 (98%)	224 (98%)	5 (2%)	0	100	100
6	F	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
6	T	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
7	G	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
7	U	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
8	H	225/232 (97%)	220 (98%)	5 (2%)	0	100	100
8	V	224/232 (97%)	219 (98%)	5 (2%)	0	100	100
9	I	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
9	W	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
10	J	193/198 (98%)	191 (99%)	2 (1%)	0	100	100
10	X	193/198 (98%)	191 (99%)	2 (1%)	0	100	100
11	K	209/211 (99%)	201 (96%)	8 (4%)	0	100	100
11	Y	209/211 (99%)	201 (96%)	8 (4%)	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	232/246 (94%)	225 (97%)	7 (3%)	0	100	100
13	a	232/246 (94%)	225 (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
All	All	6285/6612 (95%)	6134 (98%)	135 (2%)	16 (0%)	46	63

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
2	B	222	GLY
3	C	202	GLN

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Mol	Chain	Res	Type
2	P	51	VAL
2	P	222	GLY
3	Q	202	GLN
1	A	2	THR
1	O	2	THR
2	B	218	GLY
2	P	218	GLY
2	B	220	ASN
3	C	205	ALA
2	P	220	ASN
3	Q	205	ALA
3	C	183	PRO
3	Q	183	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	205 (98%)	4 (2%)	65	83
1	O	209/209 (100%)	205 (98%)	4 (2%)	65	83
2	B	203/216 (94%)	196 (97%)	7 (3%)	44	65
2	P	203/216 (94%)	196 (97%)	7 (3%)	44	65
3	C	212/226 (94%)	202 (95%)	10 (5%)	32	50
3	Q	212/226 (94%)	202 (95%)	10 (5%)	32	50
4	D	194/215 (90%)	185 (95%)	9 (5%)	33	51
4	R	194/215 (90%)	185 (95%)	9 (5%)	33	51
5	E	190/193 (98%)	180 (95%)	10 (5%)	28	44
5	S	190/193 (98%)	180 (95%)	10 (5%)	28	44
6	F	201/239 (84%)	191 (95%)	10 (5%)	30	48
6	T	201/239 (84%)	191 (95%)	10 (5%)	30	48
7	G	206/210 (98%)	197 (96%)	9 (4%)	35	53
7	U	206/210 (98%)	197 (96%)	9 (4%)	35	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	H	186/190 (98%)	179 (96%)	7 (4%)	40 60
8	V	185/190 (97%)	181 (98%)	4 (2%)	60 79
9	I	172/173 (99%)	170 (99%)	2 (1%)	78 90
9	W	172/173 (99%)	170 (99%)	2 (1%)	78 90
10	J	173/175 (99%)	168 (97%)	5 (3%)	50 71
10	X	173/175 (99%)	169 (98%)	4 (2%)	58 78
11	K	170/170 (100%)	162 (95%)	8 (5%)	32 50
11	Y	170/170 (100%)	162 (95%)	8 (5%)	32 50
12	L	185/185 (100%)	182 (98%)	3 (2%)	70 86
12	Z	185/185 (100%)	182 (98%)	3 (2%)	70 86
13	M	200/208 (96%)	193 (96%)	7 (4%)	43 64
13	a	200/208 (96%)	194 (97%)	6 (3%)	48 70
14	N	162/162 (100%)	157 (97%)	5 (3%)	47 69
14	b	162/162 (100%)	157 (97%)	5 (3%)	47 69
All	All	5325/5542 (96%)	5138 (96%)	187 (4%)	43 64

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	SER
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	50	LYS
2	B	55	LEU
2	B	79	LEU
2	B	113	ARG
2	B	186	ASP
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	51	LYS
3	C	98	LEU
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL

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Mol	Chain	Res	Type
3	C	180	LYS
3	C	206	LYS
3	C	240	GLU
4	D	99	ILE
4	D	125	LEU
4	D	143	ASP
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	55	LEU
5	E	71	LEU
5	E	116	GLN
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
5	E	208	ASP
5	E	231	LYS
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	172	LEU
6	F	181	GLU
6	F	201	GLU
6	F	202	ASP
6	F	207	ASP
6	F	214	TRP
6	F	240	GLN
7	G	26	THR
7	G	68	ARG
7	G	75	ASN
7	G	83	ASN
7	G	115	LEU
7	G	122	ARG
7	G	125	MET
7	G	235	ARG
7	G	236	LEU
8	H	22	GLN

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Mol	Chain	Res	Type
8	H	30	ASN
8	H	57	GLN
8	H	68	LEU
8	H	113	ILE
8	H	127	LEU
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
10	J	1	MET
10	J	2	ASP
10	J	35	THR
10	J	99	GLN
10	J	172	MET
11	K	4	LEU
11	K	10	HIS
11	K	12	VAL
11	K	30	ARG
11	K	35	ILE
11	K	62	GLU
11	K	125	MET
11	K	147	LEU
12	L	3	ASN
12	L	23	LEU
12	L	150	LEU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	146	PHE
13	M	161	ARG
13	M	187	ARG
14	N	9	LYS
14	N	39	ASP
14	N	83	LYS
14	N	104	ASP
14	N	107	LYS
1	O	62	SER
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	50	LYS
2	P	55	LEU

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Mol	Chain	Res	Type
2	P	79	LEU
2	P	113	ARG
2	P	186	ASP
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	51	LYS
3	Q	98	LEU
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	206	LYS
3	Q	240	GLU
4	R	99	ILE
4	R	125	LEU
4	R	143	ASP
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	55	LEU
5	S	71	LEU
5	S	116	GLN
5	S	184	ASN
5	S	188	LEU
5	S	202	ASP
5	S	208	ASP
5	S	231	LYS
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	172	LEU
6	T	181	GLU
6	T	201	GLU
6	T	202	ASP
6	T	207	ASP

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Mol	Chain	Res	Type
6	T	214	TRP
6	T	240	GLN
7	U	26	THR
7	U	68	ARG
7	U	75	ASN
7	U	83	ASN
7	U	115	LEU
7	U	122	ARG
7	U	125	MET
7	U	235	ARG
7	U	236	LEU
8	V	22	GLN
8	V	30	ASN
8	V	68	LEU
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
10	X	2	ASP
10	X	3	ILE
10	X	35	THR
10	X	99	GLN
11	Y	4	LEU
11	Y	10	HIS
11	Y	12	VAL
11	Y	32	ASN
11	Y	35	ILE
11	Y	62	GLU
11	Y	125	MET
11	Y	147	LEU
12	Z	3	ASN
12	Z	23	LEU
12	Z	150	LEU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
14	b	9	LYS
14	b	39	ASP
14	b	83	LYS
14	b	104	ASP

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Mol	Chain	Res	Type
14	b	107	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (104) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
3	C	17	GLN
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	210	GLN
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	151	ASN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
6	F	240	GLN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
8	H	66	HIS
9	I	37	ASN

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Mol	Chain	Res	Type
10	J	55	GLN
10	J	146	HIS
11	K	10	HIS
11	K	85	ASN
11	K	89	GLN
11	K	175	ASN
11	K	207	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	95	HIS
12	L	158	ASN
13	M	48	ASN
13	M	102	GLN
13	M	194	ASN
13	M	213	GLN
14	N	161	GLN
1	O	94	HIS
2	P	20	GLN
2	P	58	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
3	Q	17	GLN
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	100	ASN
4	R	146	GLN
4	R	225	ASN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	151	ASN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN

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Mol	Chain	Res	Type
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	166	GLN
8	V	22	GLN
9	W	37	ASN
10	X	55	GLN
10	X	86	GLN
11	Y	10	HIS
11	Y	32	ASN
11	Y	175	ASN
11	Y	207	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	95	HIS
12	Z	158	ASN
13	a	48	ASN
13	a	102	GLN
13	a	194	ASN
13	a	213	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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%)	-0.23	10 (4%) 42 43	31, 45, 82, 119	0
1	O	250/250 (100%)	-0.12	11 (4%) 38 39	37, 53, 97, 128	0
2	B	244/258 (94%)	-0.00	15 (6%) 25 25	32, 51, 94, 140	0
2	P	244/258 (94%)	0.01	14 (5%) 27 27	36, 54, 96, 141	0
3	C	240/254 (94%)	0.33	23 (9%) 10 10	32, 58, 125, 163	0
3	Q	240/254 (94%)	0.42	30 (12%) 5 5	28, 64, 146, 188	0
4	D	235/260 (90%)	-0.14	3 (1%) 79 79	39, 55, 88, 131	0
4	R	235/260 (90%)	0.01	14 (5%) 25 25	43, 61, 98, 134	0
5	E	231/234 (98%)	-0.12	8 (3%) 48 48	37, 55, 94, 144	0
5	S	231/234 (98%)	0.04	11 (4%) 34 35	42, 64, 102, 143	0
6	F	243/288 (84%)	-0.20	11 (4%) 37 38	31, 49, 98, 126	0
6	T	243/288 (84%)	-0.11	9 (3%) 45 46	34, 58, 111, 141	0
7	G	241/252 (95%)	-0.31	7 (2%) 55 54	25, 45, 80, 132	0
7	U	241/252 (95%)	-0.13	9 (3%) 45 46	35, 50, 82, 121	0
8	H	226/232 (97%)	-0.18	8 (3%) 48 48	29, 45, 77, 137	0
8	V	226/232 (97%)	-0.12	8 (3%) 48 48	32, 47, 78, 146	0
9	I	204/205 (99%)	-0.47	3 (1%) 76 75	29, 41, 70, 92	0
9	W	204/205 (99%)	-0.45	3 (1%) 76 75	31, 43, 73, 95	0
10	J	195/198 (98%)	-0.25	5 (2%) 59 58	25, 45, 69, 121	0
10	X	195/198 (98%)	-0.25	7 (3%) 46 47	29, 46, 72, 131	0
11	K	211/211 (100%)	0.06	4 (1%) 70 69	36, 54, 86, 108	0
11	Y	211/211 (100%)	0.09	6 (2%) 56 55	37, 57, 89, 116	0
12	L	222/222 (100%)	-0.32	2 (0%) 85 85	31, 45, 78, 114	0
12	Z	222/222 (100%)	-0.29	4 (1%) 71 71	28, 48, 81, 120	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	233/246 (94%)	-0.49	3 (1%) 79 79	28, 43, 64, 81	0
13	a	233/246 (94%)	-0.40	2 (0%) 85 85	29, 45, 65, 82	0
14	N	196/196 (100%)	-0.44	2 (1%) 84 83	24, 40, 66, 96	0
14	b	196/196 (100%)	-0.40	3 (1%) 76 75	31, 41, 67, 101	0
All	All	6342/6612 (95%)	-0.15	235 (3%) 45 46	24, 50, 92, 188	0

All (235) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	219	ALA	10.5
8	V	224	GLN	9.3
2	P	51	VAL	8.3
12	L	174	TYR	7.8
9	I	1	SER	7.5
2	B	218	GLY	7.2
2	B	221	ASP	7.1
2	P	220	ASN	6.6
9	W	1	SER	6.6
2	P	222	GLY	6.5
2	B	219	ALA	6.5
3	C	202	GLN	6.4
3	Q	236	GLN	6.3
3	Q	206	LYS	6.3
3	Q	202	GLN	6.2
8	V	223	ILE	5.8
1	O	2	THR	5.8
10	J	1	MET	5.7
10	X	194	ASP	5.7
3	Q	50	LEU	5.7
3	C	206	LYS	5.7
2	B	51	VAL	5.7
12	Z	174	TYR	5.6
3	Q	238	LYS	5.5
5	S	202	ASP	5.5
3	Q	240	GLU	5.5
1	A	2	THR	5.4
3	Q	239	GLN	5.4
1	O	1	MET	5.4
8	H	226	GLU	5.3
8	V	226	GLU	5.3
1	A	1	MET	5.2

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Mol	Chain	Res	Type	RSRZ
14	b	195	GLN	5.1
5	E	202	ASP	4.9
2	P	221	ASP	4.8
3	Q	48	SER	4.8
3	C	49	THR	4.8
6	F	205	GLU	4.8
3	C	239	GLN	4.7
6	T	243	ILE	4.7
8	H	221	CYS	4.6
10	J	194	ASP	4.6
8	V	222	ASP	4.4
2	P	52	THR	4.4
3	Q	49	THR	4.4
3	Q	234	ILE	4.4
4	R	241	ALA	4.4
7	U	2	GLY	4.3
8	H	222	ASP	4.3
3	C	238	LYS	4.3
3	Q	205	ALA	4.2
8	V	221	CYS	4.1
14	b	105	LYS	4.1
2	P	59	ASP	4.1
7	U	51	PRO	4.0
1	O	52	SER	4.0
2	P	218	GLY	4.0
10	X	193	ASP	3.9
3	C	175	LYS	3.9
4	R	113	LEU	3.9
14	N	195	GLN	3.8
4	R	217	GLN	3.8
3	C	205	ALA	3.8
6	T	244	ASN	3.8
3	C	50	LEU	3.8
7	U	242	GLN	3.8
8	H	224	GLN	3.7
6	F	181	GLU	3.7
6	F	244	ASN	3.6
4	R	125	LEU	3.5
3	C	240	GLU	3.5
8	H	223	ILE	3.5
3	Q	225	GLU	3.4
2	B	182	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	59	ASP	3.4
6	F	2	THR	3.4
3	C	225	GLU	3.4
1	A	228	PRO	3.4
1	A	249	ALA	3.4
12	Z	167	LYS	3.3
3	C	235	GLU	3.3
6	F	215	CYS	3.3
7	U	181	LYS	3.3
14	N	105	LYS	3.3
1	O	249	ALA	3.3
3	C	236	GLN	3.3
6	F	202	ASP	3.2
7	G	242	GLN	3.2
7	U	222	ASP	3.2
10	J	135	TYR	3.2
5	S	3	ASN	3.1
4	D	242	GLU	3.1
3	Q	141	ASP	3.1
3	Q	203	THR	3.1
3	Q	181	GLU	3.0
5	S	54	GLU	3.0
13	a	1	THR	3.0
10	X	1	MET	3.0
5	S	173	ARG	2.9
8	V	225	GLU	2.9
2	P	244	THR	2.9
3	Q	232	THR	2.9
2	B	217	LYS	2.9
2	P	203	SER	2.8
3	Q	175	LYS	2.8
5	E	233	ILE	2.8
6	T	205	GLU	2.8
7	G	241	GLU	2.8
3	C	180	LYS	2.8
7	G	3	TYR	2.8
2	B	60	THR	2.8
1	A	201	GLU	2.8
5	S	210	LEU	2.8
3	Q	229	GLN	2.8
3	Q	187	GLU	2.7
1	O	53	SER	2.7

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Mol	Chain	Res	Type	RSRZ
6	F	203	ASN	2.7
2	P	182	ASP	2.7
5	E	207	VAL	2.7
7	G	2	GLY	2.7
11	Y	147	LEU	2.7
1	O	201	GLU	2.7
4	R	54	ASP	2.7
8	H	219	ASN	2.7
2	B	61	SER	2.7
7	U	230	GLU	2.7
13	a	35[A]	ARG	2.7
7	U	188	GLU	2.6
1	A	54	PRO	2.6
3	C	203	THR	2.6
4	D	1	ASP	2.6
3	Q	235	GLU	2.6
3	Q	204	GLY	2.6
10	X	174	MET	2.6
6	T	58	GLN	2.5
4	R	224	ASP	2.5
4	R	242	GLU	2.5
6	T	178	HIS	2.5
12	Z	173	LYS	2.5
1	A	250	LEU	2.5
13	M	47	ASP	2.5
1	O	4	ARG	2.5
3	C	47	ARG	2.5
1	A	229	THR	2.5
13	M	35[A]	ARG	2.5
5	S	203	GLU	2.5
5	E	201	ARG	2.4
6	F	243	ILE	2.4
6	F	228	LYS	2.4
2	B	220	ASN	2.4
10	J	95	ARG	2.4
6	T	2	THR	2.4
9	W	192	ASP	2.4
11	K	144	LYS	2.4
11	Y	182	ASP	2.4
5	E	173	ARG	2.4
7	U	206	GLY	2.4
7	G	181	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
4	R	230	GLU	2.3
2	P	217	LYS	2.3
10	X	24	GLY	2.3
4	R	1	ASP	2.3
8	V	145	ASP	2.3
3	C	181	GLU	2.3
2	P	230	LYS	2.3
2	B	52	THR	2.3
13	M	1	THR	2.3
3	C	139	ARG	2.3
2	P	50	LYS	2.3
10	X	195	PHE	2.3
12	Z	106	TYR	2.3
6	T	181	GLU	2.3
11	K	30	ARG	2.3
5	S	233	ILE	2.3
7	G	240	ALA	2.3
9	I	192	ASP	2.3
11	K	146	ASP	2.3
6	F	201	GLU	2.3
3	C	216	ASP	2.2
11	Y	146	ASP	2.2
1	O	231	LYS	2.2
2	B	50	LYS	2.2
3	Q	46	ARG	2.2
6	T	166	GLN	2.2
3	Q	139	ARG	2.2
11	Y	30	ARG	2.2
11	Y	67	TYR	2.2
7	U	183	ASP	2.2
9	I	133	LYS	2.2
1	O	250	LEU	2.2
4	R	201	GLU	2.2
5	S	227	GLU	2.2
1	A	51	SER	2.2
2	B	93	HIS	2.2
5	S	165	GLN	2.2
7	G	188	GLU	2.2
5	S	207	VAL	2.2
3	C	185	THR	2.2
5	E	3	ASN	2.2
3	C	204	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
3	Q	60	SER	2.2
9	W	133	LYS	2.2
3	Q	216	ASP	2.2
5	E	210	LEU	2.2
3	Q	237	GLU	2.2
3	Q	51	LYS	2.1
10	X	95	ARG	2.1
6	T	180	PRO	2.1
11	K	147	LEU	2.1
11	Y	179	VAL	2.1
1	O	203	GLU	2.1
8	H	196	ARG	2.1
4	D	202	GLU	2.1
2	B	240	LYS	2.1
3	C	1	GLY	2.1
3	Q	171	GLU	2.1
3	C	141	ASP	2.1
4	R	177	ASN	2.1
6	F	51	THR	2.1
14	b	107	LYS	2.1
1	O	229	THR	2.1
4	R	47	THR	2.1
5	S	218	ASP	2.1
8	V	91	GLN	2.1
1	A	248	GLU	2.1
3	Q	167	LYS	2.1
5	E	218	ASP	2.0
2	B	222	GLY	2.0
3	C	234	ILE	2.0
10	J	24	GLY	2.0
3	Q	201	VAL	2.0
8	H	198	GLU	2.0
4	R	203	LYS	2.0
4	R	238	LYS	2.0
12	L	173	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

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
15	MG	I	301	1/1	0.93	0.15	1.40	51,51,51,51	0
15	MG	Z	301	1/1	0.94	0.15	0.65	60,60,60,60	0
15	MG	G	301	1/1	0.99	0.11	-0.07	39,39,39,39	0
15	MG	J	201	1/1	0.98	0.10	-0.47	52,52,52,52	0
15	MG	L	301	1/1	0.97	0.07	-1.82	43,43,43,43	0
15	MG	N	201	1/1	0.99	0.05	-2.10	38,38,38,38	0
15	MG	K	301	1/1	0.93	0.06	-2.28	46,46,46,46	0
15	MG	I	302	1/1	0.97	0.05	-3.25	41,41,41,41	0
15	MG	K	302	1/1	0.92	0.39	-	64,64,64,64	0
16	CL	U	301	1/1	0.99	0.14	-	30,30,30,30	0
15	MG	H	301	1/1	0.93	0.09	-	57,57,57,57	0
16	CL	G	302	1/1	0.99	0.07	-	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.