Full wwPDB X-ray Structure Validation Report (i)

Jan 19, 2017 – 02:08 PM EST

PDB ID	:	5M2B
Title	:	Yeast 20S proteasome with human beta5i (1-138) and human beta6 (97-111; 118-133) in complex with thiazole based inhibitor Ro19
Authors	:	Groll, M.
Deposited on	:	2016-10-12
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

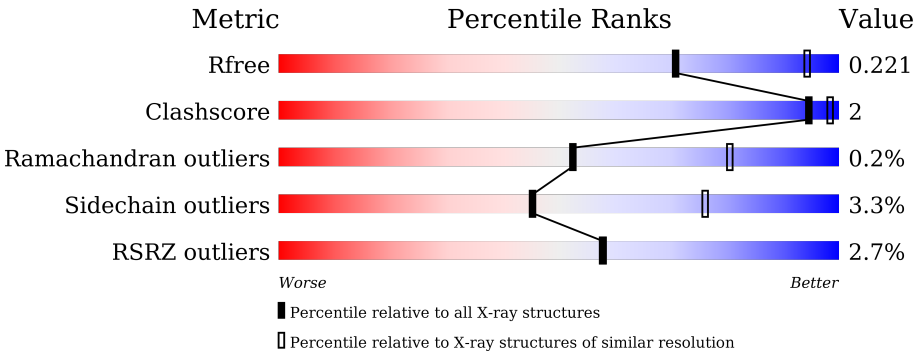
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	3% 98% ·
1	O	250	2% 97% ·
2	B	258	3% 88% 6% · 5%
2	P	258	4% 87% 7% 5%
3	C	254	8% 87% 6% · 6%
3	Q	254	7% 87% 6% · 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	260	2% 85% 5% 10%
4	R	260	4% 85% 5% 10%
5	E	234	3% 94%
5	S	234	3% 94% 5%
6	F	288	% 81% 16%
6	T	288	2% 80% 16%
7	G	252	2% 90% 5%
7	U	252	3% 90% 5%
8	H	232	3% 90% 6%
8	V	232	3% 90% 6%
9	I	205	% 92% 8%
9	W	205	2% 92% 8%
10	J	198	3% 91% 6%
10	X	198	3% 91% 6%
11	K	211	88% 10%
11	Y	211	2% 90% 9%
12	L	222	94% 5%
12	Z	222	% 94% 5%
13	M	246	% 89% 5% 5%
13	a	246	92% 5%
14	N	196	% 94% 5%
14	b	196	% 97%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	MG	J	201	-	-	-	X
15	MG	Z	301	-	-	-	X
17	7DX	K	301	-	-	-	X
17	7DX	Y	301	-	-	-	X

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 49899 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	0	0
			1719	1082	298	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			

Continued on next page...

Continued from previous page...

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
			1640	1035	282	311	12			
11	Y	211	Total	C	N	O	S	0	0	0
			1640	1035	282	311	12			

- Molecule 12 is a protein called Proteasome subunit beta type-6,Proteasome subunit beta type,Proteasome subunit beta type-6,Proteasome subunit beta type,Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1764	1119	305	336	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1764	1119	305	336	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			

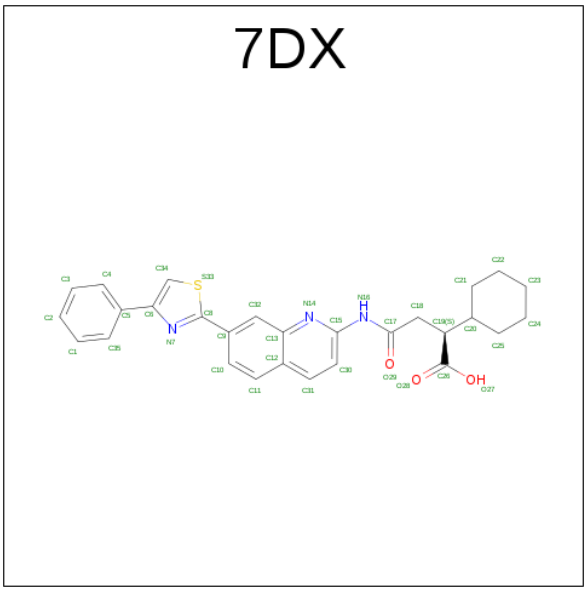
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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	1	Total Mg 1 1	0	0
15	I	1	Total Mg 1 1	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	b	1	Total Cl 1 1	0	0
16	N	1	Total Cl 1 1	0	0
16	U	1	Total Cl 1 1	0	0

- Molecule 17 is (2 {S})-2-cyclohexyl-4-oxidanylidene-4-[[7-(4-phenyl-1,3-thiazol-2-yl)quinolin-2-yl]amino]butanoic acid (three-letter code: 7DX) (formula: $C_{28}H_{27}N_3O_3S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	K	1	Total C N O S 35 28 3 3 1	0	0
17	Y	1	Total C N O S 35 28 3 3 1	0	0

- Molecule 18 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	20	Total O 20 20	0	0
18	B	13	Total O 13 13	0	0
18	C	12	Total O 12 12	0	0
18	D	12	Total O 12 12	0	0
18	E	8	Total O 8 8	0	0
18	F	14	Total O 14 14	0	0
18	G	18	Total O 18 18	0	0
18	H	22	Total O 22 22	0	0
18	I	17	Total O 17 17	0	0
18	J	18	Total O 18 18	0	0

Continued on next page...

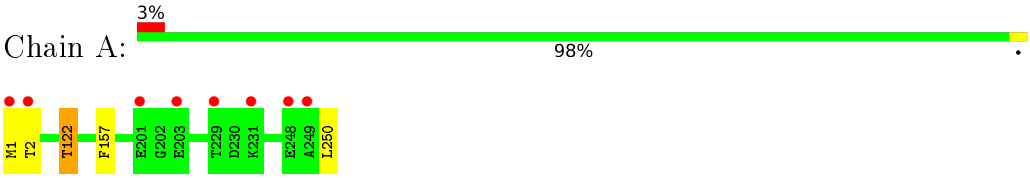
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	K	15	Total O 15 15	0	0
18	L	15	Total O 15 15	0	0
18	M	25	Total O 25 25	0	0
18	N	19	Total O 19 19	0	0
18	O	18	Total O 18 18	0	0
18	P	16	Total O 16 16	0	0
18	Q	4	Total O 4 4	0	0
18	R	15	Total O 15 15	0	0
18	S	7	Total O 7 7	0	0
18	T	11	Total O 11 11	0	0
18	U	25	Total O 25 25	0	0
18	V	17	Total O 17 17	0	0
18	W	20	Total O 20 20	0	0
18	X	20	Total O 20 20	0	0
18	Y	11	Total O 11 11	0	0
18	Z	13	Total O 13 13	0	0
18	a	22	Total O 22 22	0	0
18	b	19	Total O 19 19	0	0

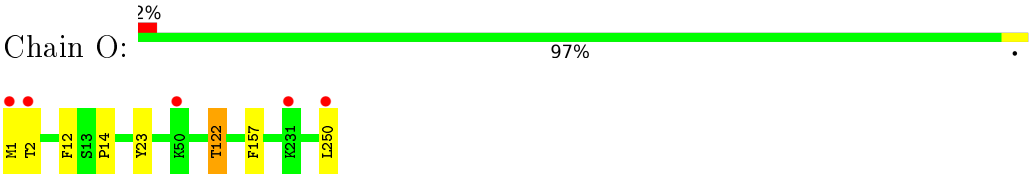
3 Residue-property plots (i)

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.

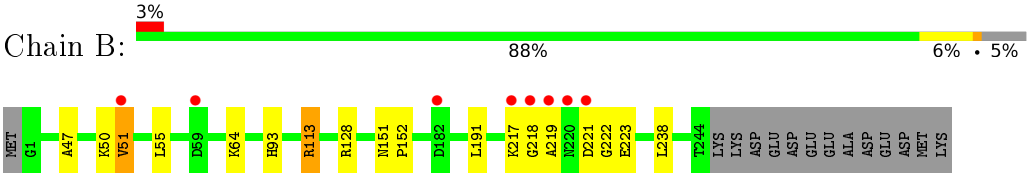
- Molecule 1: Proteasome subunit alpha type-2



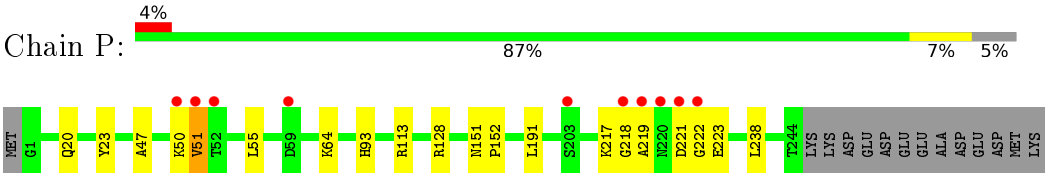
- Molecule 1: Proteasome subunit alpha type-2



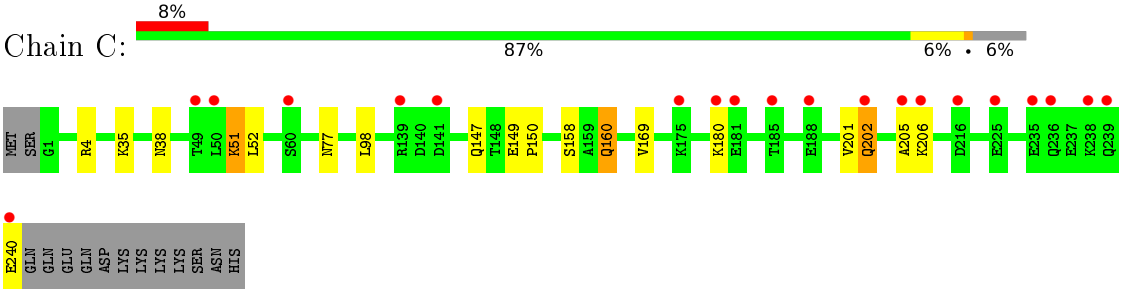
- Molecule 2: Proteasome subunit alpha type-3



- Molecule 2: Proteasome subunit alpha type-3

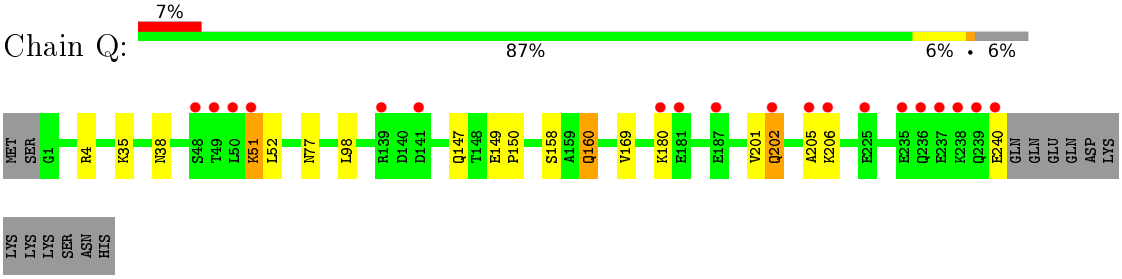


- Molecule 3: Proteasome subunit alpha type-4



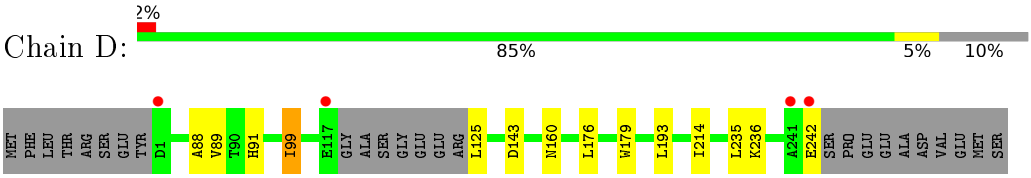
• Molecule 3: Proteasome subunit alpha type-4

Chain Q:



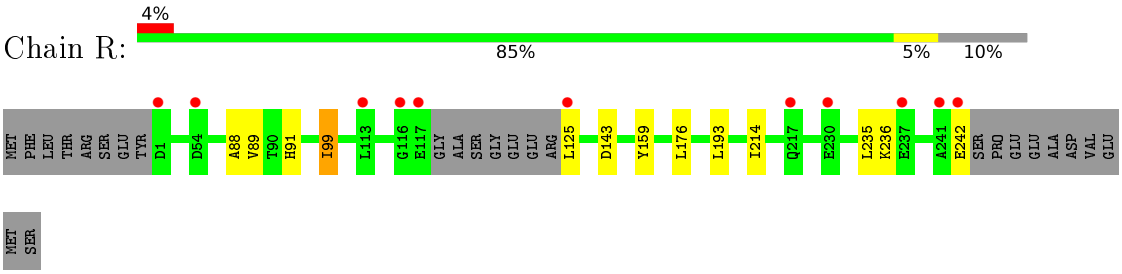
• Molecule 4: Proteasome subunit alpha type-5

Chain D:



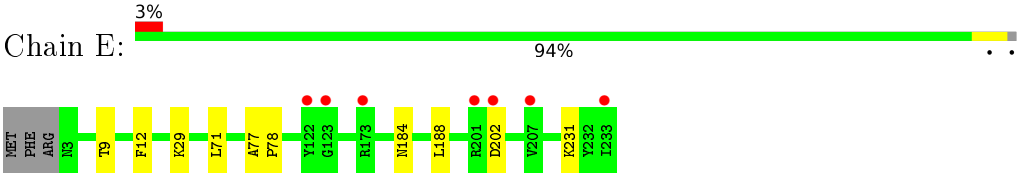
• Molecule 4: Proteasome subunit alpha type-5

Chain R:



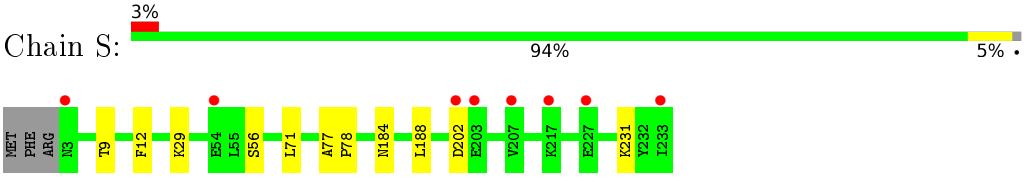
• Molecule 5: Proteasome subunit alpha type-6

Chain E:



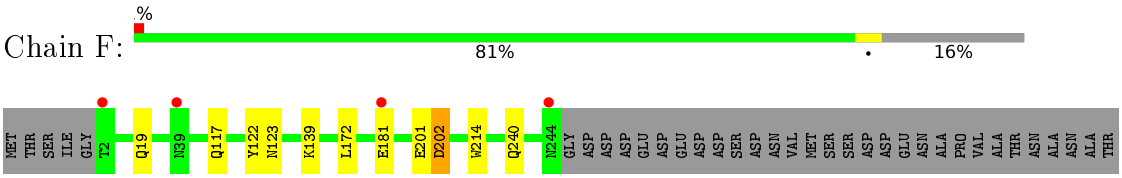
• Molecule 5: Proteasome subunit alpha type-6

Chain S:

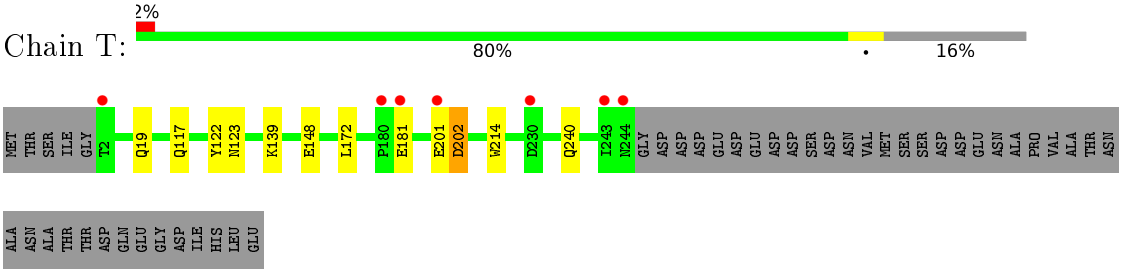


• Molecule 6: Probable proteasome subunit alpha type-7

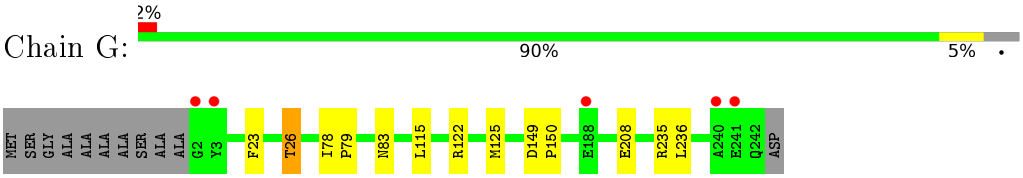
Chain F:



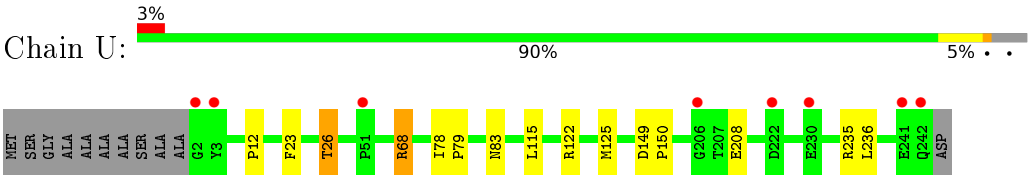
• Molecule 6: Probable proteasome subunit alpha type-7



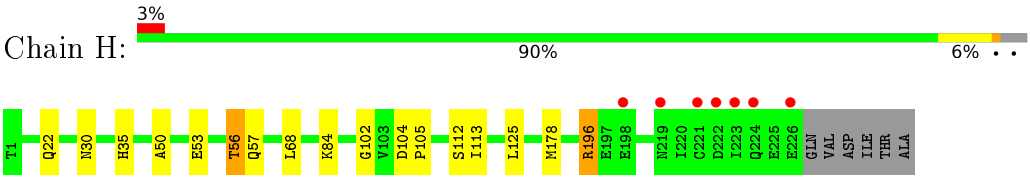
• Molecule 7: Proteasome subunit alpha type-1



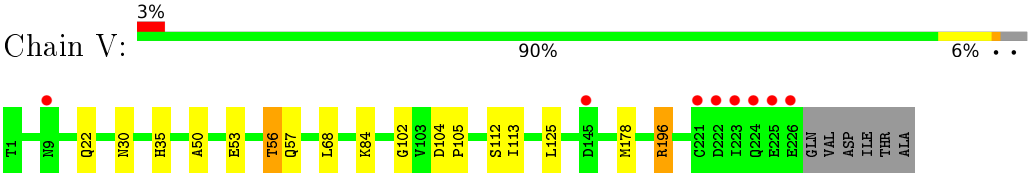
• Molecule 7: Proteasome subunit alpha type-1



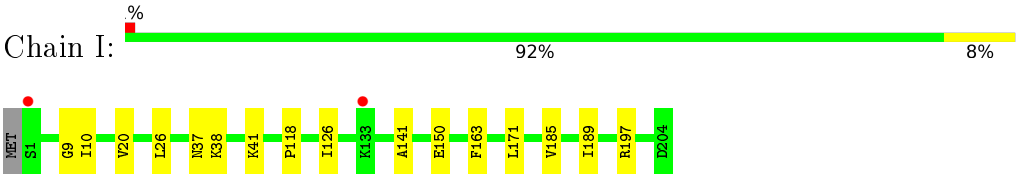
• Molecule 8: Proteasome subunit beta type-2



• Molecule 8: Proteasome subunit beta type-2

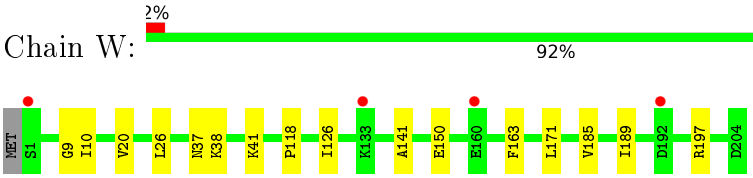


• Molecule 9: Proteasome subunit beta type-3



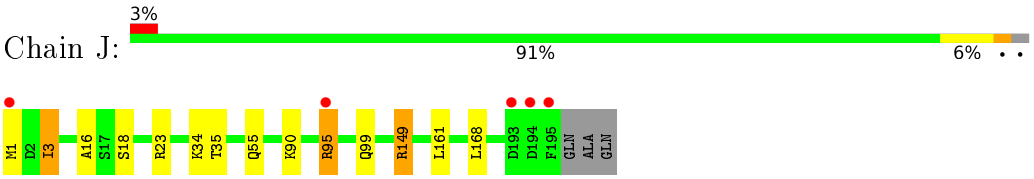
• Molecule 9: Proteasome subunit beta type-3

Chain W:



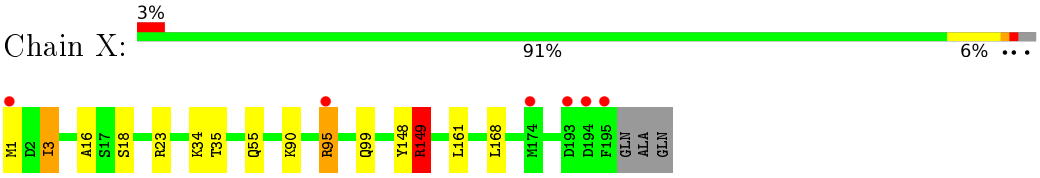
• Molecule 10: Proteasome subunit beta type-4

Chain J:



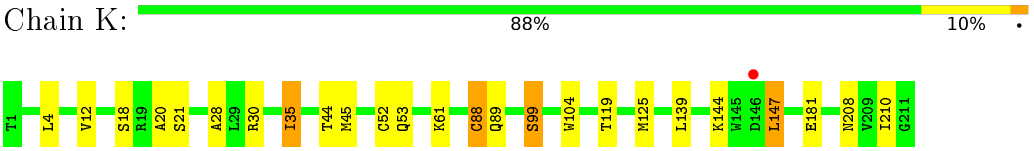
• Molecule 10: Proteasome subunit beta type-4

Chain X:



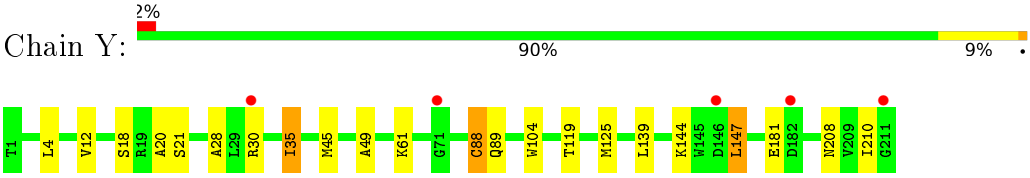
• Molecule 11: Proteasome subunit beta type-8,Proteasome subunit beta type-5

Chain K:



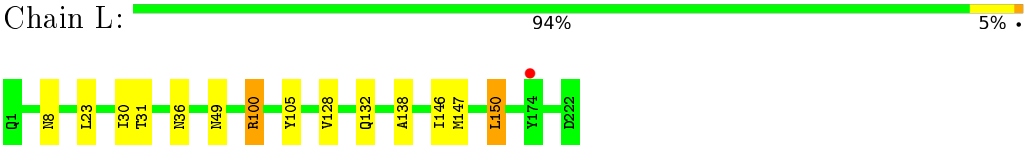
• Molecule 11: Proteasome subunit beta type-8,Proteasome subunit beta type-5

Chain Y:



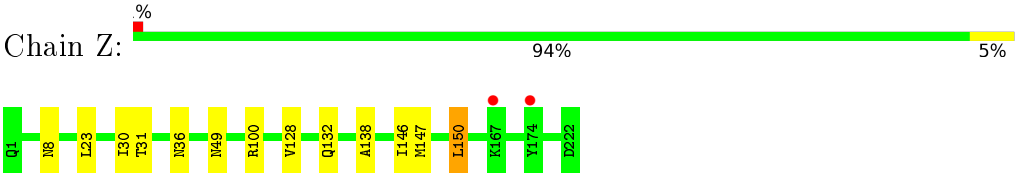
• Molecule 12: Proteasome subunit beta type-6,Proteasome subunit beta type,Proteasome subunit beta type-6,Proteasome subunit beta type,Proteasome subunit beta type-6

Chain L:



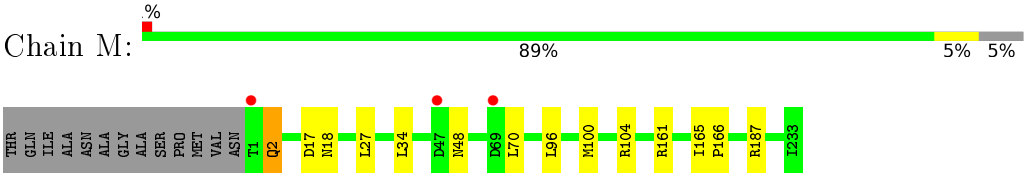
• Molecule 12: Proteasome subunit beta type-6,Proteasome subunit beta type,Proteasome subunit beta type-6,Proteasome subunit beta type,Proteasome subunit beta type-6

Chain Z:



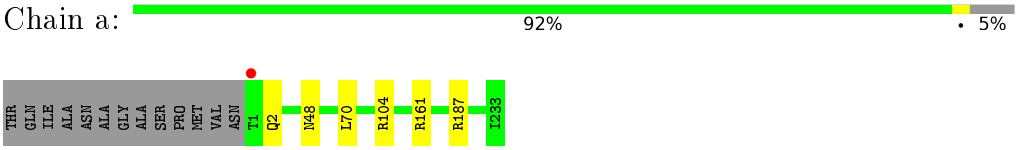
• Molecule 13: Proteasome subunit beta type-7

Chain M:



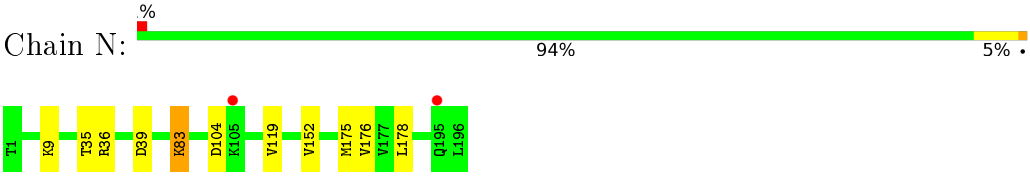
• Molecule 13: Proteasome subunit beta type-7

Chain a:



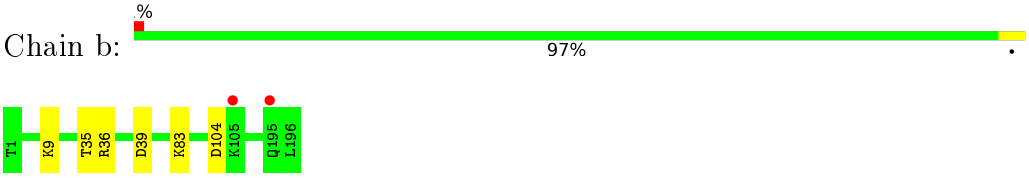
• Molecule 14: Proteasome subunit beta type-1

Chain N:



• Molecule 14: Proteasome subunit beta type-1

Chain b:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	135.16Å 301.15Å 145.98Å 90.00° 112.81° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.7 (15.00-2.70) 96.7 (15.00-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.22 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.200 , 0.218 0.204 , 0.221	Depositor DCC
R_{free} test set	14094 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	53.9	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 35.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	49899	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% 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: 7DX, 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	0.26	0/1952	0.47	0/2642
1	O	0.26	0/1952	0.47	0/2642
2	B	0.29	0/1934	0.50	0/2618
2	P	0.27	0/1934	0.49	0/2618
3	C	0.28	0/1910	0.50	0/2586
3	Q	0.28	0/1910	0.50	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	0.44	0/2609
6	T	0.27	0/1932	0.45	0/2609
7	G	0.29	0/1945	0.47	0/2634
7	U	0.28	0/1945	0.77	4/2634 (0.2%)
8	H	0.25	0/1750	0.51	0/2373
8	V	0.25	0/1750	0.51	0/2373
9	I	0.27	0/1611	0.53	0/2174
9	W	0.27	0/1611	0.53	0/2174
10	J	0.27	0/1589	0.97	6/2142 (0.3%)
10	X	0.30	0/1589	0.94	6/2142 (0.3%)
11	K	0.30	0/1677	0.54	0/2263
11	Y	0.28	0/1677	0.54	0/2263
12	L	0.29	0/1802	0.77	3/2430 (0.1%)
12	Z	0.29	0/1802	0.74	3/2430 (0.1%)
13	M	0.26	0/1855	0.54	0/2514
13	a	0.28	0/1855	0.55	0/2514
14	N	0.25	0/1541	0.49	0/2087
14	b	0.25	0/1541	0.49	0/2087
All	All	0.27	0/50270	0.57	22/67960 (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
7	U	0	1
10	J	0	2
10	X	0	2
All	All	0	5

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	U	68	ARG	NE-CZ-NH2	-22.67	108.97	120.30
10	J	95	ARG	NE-CZ-NH2	-20.64	109.98	120.30
12	L	100	ARG	NE-CZ-NH1	-20.41	110.10	120.30
10	J	149	ARG	NE-CZ-NH1	-20.40	110.10	120.30
10	X	149	ARG	NE-CZ-NH2	-19.92	110.34	120.30
12	Z	100	ARG	NE-CZ-NH2	-19.51	110.55	120.30
10	X	95	ARG	NE-CZ-NH1	-18.86	110.87	120.30
12	L	100	ARG	NE-CZ-NH2	17.68	129.14	120.30
7	U	68	ARG	NE-CZ-NH1	17.06	128.83	120.30
12	Z	100	ARG	NE-CZ-NH1	16.57	128.58	120.30
10	J	149	ARG	NE-CZ-NH2	16.23	128.41	120.30
10	X	95	ARG	NE-CZ-NH2	15.81	128.21	120.30
10	X	149	ARG	NE-CZ-NH1	14.97	127.78	120.30
10	J	95	ARG	NE-CZ-NH1	13.77	127.19	120.30
7	U	68	ARG	CD-NE-CZ	10.87	138.82	123.60
10	J	95	ARG	CD-NE-CZ	10.45	138.23	123.60
10	J	149	ARG	CD-NE-CZ	10.29	138.00	123.60
10	X	149	ARG	CD-NE-CZ	9.65	137.11	123.60
10	X	95	ARG	CD-NE-CZ	9.05	136.27	123.60
12	L	100	ARG	CD-NE-CZ	8.71	135.80	123.60
12	Z	100	ARG	CD-NE-CZ	8.59	135.62	123.60
7	U	68	ARG	CG-CD-NE	-7.27	96.53	111.80

There are no chirality outliers.

All (5) planarity outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
7	U	68	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	15	0
2	P	1904	0	1904	9	0
3	C	1881	0	1895	6	0
3	Q	1881	0	1895	6	0
4	D	1813	0	1797	5	0
4	R	1813	0	1797	5	0
5	E	1773	0	1775	2	0
5	S	1773	0	1775	3	0
6	F	1892	0	1883	3	0
6	T	1892	0	1883	4	0
7	G	1907	0	1901	3	0
7	U	1907	0	1901	4	0
8	H	1719	0	1719	11	0
8	V	1719	0	1719	9	0
9	I	1581	0	1574	12	0
9	W	1581	0	1574	10	0
10	J	1561	0	1569	9	0
10	X	1561	0	1569	10	0
11	K	1640	0	1581	18	0
11	Y	1640	0	1581	14	0
12	L	1764	0	1716	5	0
12	Z	1764	0	1716	4	0
13	M	1824	0	1832	5	0
13	a	1824	0	1832	0	0
14	N	1512	0	1481	3	0
14	b	1512	0	1481	0	0
15	G	1	0	0	0	0
15	I	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	J	1	0	0	0	0
15	K	1	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
16	N	1	0	0	0	0
16	U	1	0	0	0	0
16	b	1	0	0	0	0
17	K	35	0	0	0	0
17	Y	35	0	0	1	0
18	A	20	0	0	0	0
18	B	13	0	0	0	0
18	C	12	0	0	0	0
18	D	12	0	0	0	0
18	E	8	0	0	0	0
18	F	14	0	0	0	0
18	G	18	0	0	0	0
18	H	22	0	0	0	0
18	I	17	0	0	0	0
18	J	18	0	0	0	0
18	K	15	0	0	0	0
18	L	15	0	0	0	0
18	M	25	0	0	1	0
18	N	19	0	0	0	0
18	O	18	0	0	0	0
18	P	16	0	0	1	0
18	Q	4	0	0	0	0
18	R	15	0	0	0	0
18	S	7	0	0	0	0
18	T	11	0	0	1	0
18	U	25	0	0	0	0
18	V	17	0	0	0	0
18	W	20	0	0	0	0
18	X	20	0	0	0	0
18	Y	11	0	0	0	0
18	Z	13	0	0	0	0
18	a	22	0	0	0	0
18	b	19	0	0	0	0
All	All	49899	0	49112	154	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 (154) 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)
2:B:93:HIS:NE2	2:B:113:ARG:HD3	1.60	1.15
2:B:113:ARG:HH11	2:B:113:ARG:HG3	1.21	1.00
11:Y:35:ILE:HG22	11:Y:45:MET:HE3	1.45	0.97
11:K:35:ILE:HG22	11:K:45:MET:HE3	1.58	0.85
11:K:44:THR:O	11:K:99:SER:OG	1.96	0.82
11:Y:35:ILE:HG22	11:Y:45:MET:CE	2.17	0.74
11:K:35:ILE:HG22	11:K:45:MET:CE	2.19	0.73
10:J:3:ILE:HD11	10:J:168:LEU:HD13	1.75	0.68
10:X:3:ILE:HD11	10:X:168:LEU:HD13	1.75	0.68
2:B:93:HIS:CE1	2:B:113:ARG:HD3	2.28	0.67
10:J:23:ARG:NH2	11:K:119:THR:OG1	2.26	0.67
10:X:23:ARG:NH2	11:Y:119:THR:OG1	2.29	0.66
2:B:113:ARG:NH1	2:B:113:ARG:HG3	2.01	0.65
10:J:55:GLN:CD	11:K:88:CYS:SG	2.76	0.64
10:X:55:GLN:CD	11:Y:88:CYS:SG	2.80	0.60
2:B:113:ARG:CG	2:B:113:ARG:HH11	2.05	0.59
10:J:3:ILE:CD1	10:J:168:LEU:HD13	2.33	0.59
2:B:93:HIS:NE2	2:B:113:ARG:CD	2.53	0.58
10:J:55:GLN:NE2	11:K:88:CYS:SG	2.76	0.58
14:N:152:VAL:HA	14:N:175:MET:HE1	1.86	0.57
10:X:3:ILE:CD1	10:X:168:LEU:HD13	2.33	0.57
11:K:20:ALA:HB3	11:K:28:ALA:HB3	1.86	0.56
11:K:208:ASN:O	9:W:38:LYS:NZ	2.38	0.56
4:R:89:VAL:HG12	11:Y:61:LYS:HG3	1.87	0.56
11:Y:20:ALA:HB3	11:Y:28:ALA:HB3	1.87	0.56
8:H:50:ALA:CB	9:I:126:ILE:HG23	2.36	0.55
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.42	0.54
10:X:55:GLN:NE2	11:Y:88:CYS:SG	2.81	0.54
2:P:93:HIS:HB3	18:P:301:HOH:O	2.07	0.54
11:K:144:LYS:HB2	11:K:147:LEU:HD13	1.90	0.54
4:D:89:VAL:HG12	11:K:61:LYS:HG3	1.89	0.53
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.74	0.53
11:Y:144:LYS:HB2	11:Y:147:LEU:HD13	1.90	0.53
11:K:35:ILE:CG2	11:K:45:MET:CE	2.86	0.52
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.91	0.52
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.91	0.52
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.74	0.52
9:I:38:LYS:NZ	11:Y:208:ASN:O	2.42	0.52
7:U:23:PHE:O	7:U:26:THR:HB	2.10	0.51
12:L:100:ARG:HD2	12:L:105:TYR:CE2	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:ARG:NH1	2:B:113:ARG:CG	2.71	0.51
3:C:201:VAL:O	3:C:202:GLN:CB	2.58	0.51
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.59	0.51
7:G:23:PHE:O	7:G:26:THR:HB	2.11	0.50
11:Y:35:ILE:CG2	11:Y:45:MET:CE	2.88	0.50
8:H:50:ALA:CB	9:I:126:ILE:CG2	2.90	0.50
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.42	0.49
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.12	0.49
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.77	0.49
8:H:196:ARG:NH2	9:I:150:GLU:HG3	2.27	0.49
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.95	0.49
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.95	0.49
3:C:51:LYS:O	3:C:52:LEU:HB2	2.12	0.48
8:V:50:ALA:CB	9:W:126:ILE:HG23	2.43	0.48
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.94	0.48
1:O:1:MET:HG3	6:T:122:TYR:CZ	2.48	0.48
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.95	0.48
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.95	0.48
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.94	0.48
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.96	0.47
9:I:20:VAL:HG23	9:I:189:ILE:HB	1.95	0.47
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.78	0.47
9:W:20:VAL:HG23	9:W:189:ILE:HB	1.95	0.47
11:Y:49:ALA:HB2	17:Y:301:7DX:C32	2.44	0.47
10:J:3:ILE:HG22	10:J:18:SER:CB	2.45	0.47
8:V:196:ARG:NH2	9:W:150:GLU:HG3	2.30	0.47
10:X:3:ILE:HG22	10:X:18:SER:CB	2.45	0.47
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.96	0.47
2:B:93:HIS:CD2	2:B:113:ARG:HG2	2.49	0.47
10:J:3:ILE:HG22	10:J:18:SER:HB3	1.95	0.47
13:M:96:LEU:O	13:M:100:MET:HG2	2.15	0.47
10:X:3:ILE:HG22	10:X:18:SER:HB3	1.96	0.47
11:K:18:SER:OG	11:K:30:ARG:HA	2.14	0.46
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.97	0.46
5:E:12:PHE:H	6:F:19:GLN:HE22	1.64	0.46
8:V:53:GLU:O	8:V:57:GLN:HG2	2.16	0.46
6:T:148:GLU:HG2	18:T:304:HOH:O	2.15	0.46
10:X:148:TYR:O	10:X:149:ARG:HD3	2.15	0.46
11:Y:18:SER:OG	11:Y:30:ARG:HA	2.15	0.46
12:Z:138:ALA:HB3	12:Z:147:MET:HG2	1.98	0.46
2:B:217:LYS:C	2:B:219:ALA:H	2.19	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:196:ARG:NH2	9:I:150:GLU:O	2.49	0.45
8:V:50:ALA:CB	9:W:126:ILE:CG2	2.94	0.45
11:Y:104:TRP:CE2	11:Y:181:GLU:HB3	2.52	0.45
2:P:50:LYS:O	2:P:51:VAL:C	2.55	0.44
9:W:26:LEU:HD21	9:W:185:VAL:HG23	1.98	0.44
11:K:35:ILE:CG2	11:K:45:MET:HE2	2.46	0.44
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.17	0.44
12:Z:146:ILE:HG22	12:Z:150:LEU:HD22	2.00	0.44
9:I:26:LEU:HD21	9:I:185:VAL:HG23	1.98	0.44
2:P:217:LYS:C	2:P:219:ALA:H	2.20	0.44
8:H:53:GLU:O	8:H:57:GLN:HG2	2.16	0.44
2:B:50:LYS:O	2:B:51:VAL:C	2.56	0.44
12:L:138:ALA:HB3	12:L:147:MET:HG2	1.98	0.44
1:A:1:MET:HG3	6:F:122:TYR:CZ	2.53	0.44
3:C:35:LYS:HG2	3:C:158:SER:O	2.17	0.44
9:I:163:PHE:CE1	9:I:197:ARG:HD2	2.53	0.44
12:L:146:ILE:HG22	12:L:150:LEU:HD22	2.00	0.44
9:W:9:GLY:HA3	9:W:41:LYS:HE2	2.00	0.43
8:H:84:LYS:HA	8:H:113:ILE:HD11	2.01	0.43
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.53	0.43
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.00	0.43
11:K:104:TRP:CE2	11:K:181:GLU:HB3	2.52	0.43
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.99	0.43
2:B:93:HIS:CD2	2:B:113:ARG:HD3	2.44	0.43
1:O:14:PRO:HA	2:P:23:TYR:CD1	2.54	0.43
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.00	0.43
3:C:201:VAL:O	3:C:202:GLN:HB3	2.18	0.43
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.99	0.43
3:Q:201:VAL:O	3:Q:202:GLN:HB3	2.18	0.43
2:B:221:ASP:O	2:B:223:GLU:N	2.52	0.43
8:V:84:LYS:HA	8:V:113:ILE:HD11	2.01	0.43
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.84	0.42
2:P:221:ASP:O	2:P:223:GLU:N	2.52	0.42
9:W:163:PHE:CE1	9:W:197:ARG:HD2	2.54	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.42
9:I:9:GLY:HA3	9:I:41:LYS:HE2	2.01	0.42
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.50	0.42
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.50	0.42
9:I:10:ILE:HG21	9:I:141:ALA:HB3	2.02	0.42
11:K:45:MET:HE1	11:K:53:GLN:HG2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:45:MET:HG2	11:K:52:CYS:HB3	2.02	0.42
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.02	0.42
4:R:91:HIS:CD2	4:R:99:ILE:HG22	2.55	0.42
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.50	0.41
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.50	0.41
5:S:12:PHE:H	6:T:19:GLN:HE22	1.68	0.41
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.51	0.41
4:D:91:HIS:CD2	4:D:99:ILE:HG22	2.56	0.41
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.50	0.41
2:P:47:ALA:HB1	2:P:64:LYS:HD2	2.03	0.41
2:B:47:ALA:HB1	2:B:64:LYS:HD2	2.03	0.41
8:H:102:GLY:HA2	8:H:178:MET:SD	2.61	0.41
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.86	0.41
13:M:27:LEU:HD21	13:M:34:LEU:HD22	2.03	0.41
8:H:50:ALA:HB3	9:I:126:ILE:CG2	2.51	0.41
11:Y:125:MET:SD	11:Y:139:LEU:HB3	2.61	0.41
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.21	0.41
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.56	0.40
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.03	0.40
11:K:35:ILE:HG21	11:K:45:MET:HE2	2.03	0.40
8:V:102:GLY:HA2	8:V:178:MET:SD	2.60	0.40
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.03	0.40
5:S:77:ALA:N	5:S:78:PRO:CD	2.85	0.40
9:W:10:ILE:HG21	9:W:141:ALA:HB3	2.02	0.40
6:F:202:ASP:OD1	6:F:202:ASP:N	2.55	0.40
5:E:77:ALA:N	5:E:78:PRO:CD	2.85	0.40
11:K:125:MET:SD	11:K:139:LEU:HB3	2.62	0.40
13:M:2:GLN:NE2	18:M:302:HOH:O	2.55	0.40
6:T:202:ASP:OD1	6:T:202:ASP:N	2.55	0.40
12:L:8:ASN:HA	12:L:30:ILE:O	2.22	0.40
13:M:17:ASP:OD1	13:M:18:ASN:N	2.55	0.40
1:O:12:PHE:H	2:P:20:GLN:HE22	1.70	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	69
1	O	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	39	69
2	B	242/258 (94%)	235 (97%)	4 (2%)	3 (1%)	16	39
2	P	242/258 (94%)	235 (97%)	4 (2%)	3 (1%)	16	39
3	C	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	24	51
3	Q	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	24	51
4	D	231/260 (89%)	228 (99%)	3 (1%)	0	100	100
4	R	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
5	E	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
5	S	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
6	F	241/288 (84%)	239 (99%)	2 (1%)	0	100	100
6	T	241/288 (84%)	239 (99%)	2 (1%)	0	100	100
7	G	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
7	U	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
8	H	224/232 (97%)	218 (97%)	6 (3%)	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%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	190 (98%)	3 (2%)	0	100	100
10	X	193/198 (98%)	190 (98%)	3 (2%)	0	100	100
11	K	209/211 (99%)	204 (98%)	5 (2%)	0	100	100
11	Y	209/211 (99%)	203 (97%)	6 (3%)	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%)	221 (96%)	10 (4%)	0	100	100
13	a	231/246 (94%)	221 (96%)	10 (4%)	0	100	100
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	b	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
All	All	6282/6612 (95%)	6132 (98%)	138 (2%)	12 (0%)	52	80

All (12) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	206 (99%)	3 (1%)	74	92
1	O	209/209 (100%)	206 (99%)	3 (1%)	74	92
2	B	203/216 (94%)	199 (98%)	4 (2%)	63	87
2	P	203/216 (94%)	199 (98%)	4 (2%)	63	87
3	C	212/226 (94%)	201 (95%)	11 (5%)	29	58
3	Q	212/226 (94%)	201 (95%)	11 (5%)	29	58
4	D	194/215 (90%)	185 (95%)	9 (5%)	33	64
4	R	194/215 (90%)	185 (95%)	9 (5%)	33	64
5	E	190/193 (98%)	183 (96%)	7 (4%)	41	72
5	S	190/193 (98%)	183 (96%)	7 (4%)	41	72
6	F	201/239 (84%)	192 (96%)	9 (4%)	34	65
6	T	201/239 (84%)	192 (96%)	9 (4%)	34	65
7	G	206/210 (98%)	198 (96%)	8 (4%)	39	70
7	U	206/210 (98%)	198 (96%)	8 (4%)	39	70

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	H	185/190 (97%)	180 (97%)	5 (3%)	52 82
8	V	185/190 (97%)	180 (97%)	5 (3%)	52 82
9	I	172/173 (99%)	170 (99%)	2 (1%)	78 93
9	W	172/173 (99%)	170 (99%)	2 (1%)	78 93
10	J	173/175 (99%)	169 (98%)	4 (2%)	58 85
10	X	173/175 (99%)	169 (98%)	4 (2%)	58 85
11	K	170/170 (100%)	161 (95%)	9 (5%)	28 57
11	Y	170/170 (100%)	162 (95%)	8 (5%)	32 63
12	L	186/186 (100%)	181 (97%)	5 (3%)	52 82
12	Z	186/186 (100%)	181 (97%)	5 (3%)	52 82
13	M	199/208 (96%)	193 (97%)	6 (3%)	48 79
13	a	199/208 (96%)	193 (97%)	6 (3%)	48 79
14	N	162/162 (100%)	156 (96%)	6 (4%)	41 72
14	b	162/162 (100%)	156 (96%)	6 (4%)	41 72
All	All	5324/5544 (96%)	5149 (97%)	175 (3%)	45 76

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	55	LEU
2	B	113	ARG
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	51	LYS
3	C	77	ASN
3	C	98	LEU
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	206	LYS
3	C	240	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	71	LEU
5	E	184	ASN
5	E	188	LEU
5	E	202	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	214	TRP
6	F	240	GLN
7	G	26	THR
7	G	83	ASN
7	G	115	LEU
7	G	122	ARG
7	G	125	MET
7	G	208	GLU
7	G	235	ARG
7	G	236	LEU
8	H	22	GLN
8	H	30	ASN
8	H	56	THR
8	H	68	LEU
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
10	J	3	ILE
10	J	35	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	J	90	LYS
10	J	99	GLN
11	K	4	LEU
11	K	12	VAL
11	K	21	SER
11	K	35	ILE
11	K	88	CYS
11	K	89	GLN
11	K	99	SER
11	K	147	LEU
11	K	210	ILE
12	L	23	LEU
12	L	49	ASN
12	L	128	VAL
12	L	132	GLN
12	L	150	LEU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
14	N	9	LYS
14	N	35	THR
14	N	36	ARG
14	N	39	ASP
14	N	83	LYS
14	N	104	ASP
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	55	LEU
2	P	113	ARG
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	51	LYS
3	Q	77	ASN
3	Q	98	LEU
3	Q	147	GLN
3	Q	160	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	71	LEU
5	S	184	ASN
5	S	188	LEU
5	S	202	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	214	TRP
6	T	240	GLN
7	U	26	THR
7	U	83	ASN
7	U	115	LEU
7	U	122	ARG
7	U	125	MET
7	U	208	GLU
7	U	235	ARG
7	U	236	LEU
8	V	22	GLN
8	V	30	ASN
8	V	56	THR
8	V	68	LEU
8	V	196	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	W	37	ASN
9	W	171	LEU
10	X	3	ILE
10	X	35	THR
10	X	90	LYS
10	X	99	GLN
11	Y	4	LEU
11	Y	12	VAL
11	Y	21	SER
11	Y	35	ILE
11	Y	88	CYS
11	Y	89	GLN
11	Y	147	LEU
11	Y	210	ILE
12	Z	23	LEU
12	Z	49	ASN
12	Z	128	VAL
12	Z	132	GLN
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	35	THR
14	b	36	ARG
14	b	39	ASP
14	b	83	LYS
14	b	104	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (99) 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
2	B	155	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	91	HIS
4	D	146	GLN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	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
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
8	H	86	HIS
8	H	165	ASN
9	I	37	ASN
10	J	55	GLN
11	K	32	ASN
11	K	85	ASN
11	K	175	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
12	L	158	ASN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS
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
6	T	117	GLN
6	T	191	GLN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
8	V	86	HIS
8	V	165	ASN
9	W	37	ASN
10	X	55	GLN
11	Y	32	ASN
11	Y	85	ASN
11	Y	175	ASN
12	Z	3	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	Z	49	ASN
12	Z	158	ASN
13	a	48	ASN
13	a	102	GLN
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN
14	b	161	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 11 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	$\#\|Z\| > 2$
17	7DX	K	301	-	34,39,39	4.01	7 (20%)	41,54,54	2.03	9 (21%)
17	7DX	Y	301	-	34,39,39	4.54	6 (17%)	41,54,54	2.21	10 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	7DX	K	301	-	-	0/20/32/32	0/5/5/5
17	7DX	Y	301	-	-	0/20/32/32	0/5/5/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Y	301	7DX	C8-S33	-20.57	1.45	1.73
17	K	301	7DX	C8-S33	-16.25	1.51	1.73
17	K	301	7DX	C5-C6	-11.11	1.31	1.48
17	Y	301	7DX	C5-C6	-10.66	1.32	1.48
17	Y	301	7DX	C34-S33	-10.22	1.54	1.70
17	K	301	7DX	C34-S33	-9.83	1.55	1.70
17	K	301	7DX	C15-N16	-4.20	1.32	1.40
17	Y	301	7DX	C15-N16	-3.79	1.32	1.40
17	Y	301	7DX	C12-C13	-3.19	1.37	1.42
17	K	301	7DX	C13-N14	-3.12	1.32	1.37
17	K	301	7DX	C12-C13	-3.10	1.37	1.42
17	Y	301	7DX	C13-N14	-3.00	1.32	1.37
17	K	301	7DX	C32-C13	-2.11	1.38	1.41

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	Y	301	7DX	C6-C34-S33	-5.71	104.78	111.79
17	K	301	7DX	C6-C34-S33	-5.17	105.44	111.79
17	Y	301	7DX	C22-C21-C20	-4.59	104.75	111.91
17	Y	301	7DX	C24-C25-C20	-4.09	105.53	111.91
17	K	301	7DX	C18-C19-C20	-3.78	106.42	111.93
17	K	301	7DX	C34-C6-C5	-3.73	124.22	129.45
17	Y	301	7DX	C18-C19-C20	-3.47	106.87	111.93
17	Y	301	7DX	C25-C20-C21	-2.77	104.82	109.45
17	Y	301	7DX	C34-C6-C5	-2.70	125.66	129.45
17	K	301	7DX	C15-N16-C17	-2.61	123.70	128.07
17	Y	301	7DX	C15-N16-C17	-2.61	123.71	128.07
17	Y	301	7DX	C30-C15-N14	-2.58	119.67	123.55
17	K	301	7DX	C24-C25-C20	-2.52	107.98	111.91
17	K	301	7DX	C30-C15-N14	-2.37	119.98	123.55
17	K	301	7DX	C22-C21-C20	-2.37	108.21	111.91
17	K	301	7DX	C23-C22-C21	-2.03	107.24	111.44
17	Y	301	7DX	C21-C20-C19	2.25	115.93	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	Y	301	7DX	C15-N14-C13	7.82	123.21	117.05
17	K	301	7DX	C15-N14-C13	8.14	123.46	117.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	Y	301	7DX	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%)	-0.35	8 (3%)	51	51	33, 48, 84, 123	0
1	O	250/250 (100%)	-0.29	5 (2%)	68	69	36, 53, 99, 132	0
2	B	244/258 (94%)	-0.15	8 (3%)	50	50	35, 55, 104, 155	0
2	P	244/258 (94%)	-0.15	10 (4%)	41	41	37, 57, 102, 151	0
3	C	240/254 (94%)	0.13	20 (8%)	14	11	33, 60, 132, 169	0
3	Q	240/254 (94%)	0.18	19 (7%)	15	13	26, 69, 147, 188	0
4	D	235/260 (90%)	-0.18	4 (1%)	73	74	41, 59, 92, 130	0
4	R	235/260 (90%)	0.03	11 (4%)	35	34	51, 71, 113, 144	0
5	E	231/234 (98%)	-0.15	7 (3%)	54	54	40, 61, 101, 149	0
5	S	231/234 (98%)	-0.04	8 (3%)	48	48	44, 67, 109, 146	0
6	F	243/288 (84%)	-0.33	4 (1%)	74	75	33, 53, 105, 130	0
6	T	243/288 (84%)	-0.20	7 (2%)	55	55	39, 62, 119, 149	0
7	G	241/252 (95%)	-0.34	5 (2%)	67	68	32, 49, 88, 141	0
7	U	241/252 (95%)	-0.30	8 (3%)	50	50	34, 50, 86, 128	0
8	H	226/232 (97%)	-0.20	7 (3%)	52	52	33, 50, 86, 151	0
8	V	226/232 (97%)	-0.18	8 (3%)	48	48	35, 51, 85, 157	0
9	I	204/205 (99%)	-0.58	2 (0%)	84	85	32, 46, 77, 96	0
9	W	204/205 (99%)	-0.54	4 (1%)	68	69	31, 46, 77, 99	0
10	J	195/198 (98%)	-0.30	5 (2%)	59	59	31, 49, 74, 122	0
10	X	195/198 (98%)	-0.31	6 (3%)	52	52	33, 50, 77, 135	0
11	K	211/211 (100%)	-0.20	1 (0%)	91	93	38, 57, 88, 106	0
11	Y	211/211 (100%)	-0.19	5 (2%)	62	62	39, 58, 90, 115	0
12	L	222/222 (100%)	-0.33	1 (0%)	91	93	37, 54, 99, 126	0
12	Z	222/222 (100%)	-0.29	2 (0%)	85	86	34, 55, 98, 132	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	233/246 (94%)	-0.49	3 (1%) 79 79	31, 49, 73, 93	0
13	a	233/246 (94%)	-0.45	1 (0%) 93 94	32, 50, 75, 93	0
14	N	196/196 (100%)	-0.44	2 (1%) 84 85	32, 44, 72, 102	0
14	b	196/196 (100%)	-0.47	2 (1%) 84 85	32, 45, 74, 104	0
All	All	6342/6612 (95%)	-0.25	173 (2%) 58 58	26, 54, 100, 188	0

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	206	LYS	6.8
3	C	206	LYS	6.8
2	B	221	ASP	6.7
10	X	1	MET	6.2
2	P	219	ALA	6.0
2	B	218	GLY	5.6
2	P	218	GLY	5.3
2	B	51	VAL	5.1
2	P	51	VAL	5.1
5	E	202	ASP	5.0
10	J	1	MET	4.9
10	X	194	ASP	4.9
8	H	221	CYS	4.8
9	I	1	SER	4.8
1	A	1	MET	4.7
3	Q	237	GLU	4.7
12	L	174	TYR	4.7
3	Q	239	GLN	4.7
8	V	226	GLU	4.6
2	B	219	ALA	4.5
5	S	202	ASP	4.4
3	Q	236	GLN	4.3
3	Q	49	THR	4.2
3	C	49	THR	4.2
8	H	226	GLU	4.2
4	R	217	GLN	4.2
8	V	224	GLN	4.1
2	P	220	ASN	4.1
3	C	238	LYS	4.1
3	C	202	GLN	4.0
8	V	222	ASP	4.0
9	W	1	SER	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	Q	240	GLU	3.9
3	Q	50	LEU	3.8
1	O	1	MET	3.8
3	C	50	LEU	3.7
9	W	133	LYS	3.7
2	P	221	ASP	3.7
6	F	181	GLU	3.7
6	T	243	ILE	3.6
14	N	195	GLN	3.5
1	O	2	THR	3.5
3	Q	141	ASP	3.5
7	U	2	GLY	3.5
10	J	194	ASP	3.5
6	F	244	ASN	3.4
3	Q	202	GLN	3.4
3	C	205	ALA	3.4
3	Q	48	SER	3.4
7	U	242	GLN	3.4
2	B	217	LYS	3.4
3	Q	238	LYS	3.3
4	R	125	LEU	3.3
2	B	220	ASN	3.3
10	X	195	PHE	3.3
3	Q	205	ALA	3.3
3	C	236	GLN	3.3
1	A	249	ALA	3.2
2	P	59	ASP	3.2
12	Z	174	TYR	3.2
3	C	239	GLN	3.2
3	C	216	ASP	3.1
4	R	117	GLU	3.1
4	R	241	ALA	3.1
10	J	195	PHE	3.0
4	R	113	LEU	3.0
10	X	95	ARG	3.0
14	b	195	GLN	3.0
11	Y	146	ASP	3.0
6	T	181	GLU	3.0
4	R	230	GLU	2.9
8	H	222	ASP	2.9
3	C	225	GLU	2.9
2	B	59	ASP	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	117	GLU	2.9
10	X	193	ASP	2.9
7	U	206	GLY	2.9
7	G	241	GLU	2.9
3	C	175	LYS	2.8
13	a	1	THR	2.8
13	M	47	ASP	2.8
8	H	224	GLN	2.8
3	C	139	ARG	2.8
8	V	221	CYS	2.7
4	R	1	ASP	2.7
3	C	240	GLU	2.7
5	S	217	LYS	2.7
2	P	203	SER	2.7
5	E	233	ILE	2.7
7	G	3	TYR	2.7
6	T	230	ASP	2.7
7	U	241	GLU	2.7
8	V	223	ILE	2.7
12	Z	167	LYS	2.6
1	A	2	THR	2.6
3	Q	139	ARG	2.6
5	S	227	GLU	2.6
3	C	235	GLU	2.6
3	Q	181	GLU	2.6
6	T	244	ASN	2.5
8	H	219	ASN	2.5
5	E	122	TYR	2.5
3	C	141	ASP	2.5
1	O	250	LEU	2.5
1	A	231	LYS	2.5
2	P	52	THR	2.5
11	K	146	ASP	2.5
2	P	222	GLY	2.5
1	O	231	LYS	2.5
5	S	233	ILE	2.5
5	S	3	ASN	2.5
6	T	180	PRO	2.5
13	M	69	ASP	2.5
1	O	50	LYS	2.5
7	U	222	ASP	2.5
4	R	116	GLY	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	V	9	ASN	2.4
4	R	242	GLU	2.4
5	S	54	GLU	2.4
14	N	105	LYS	2.4
3	Q	225	GLU	2.4
5	E	173	ARG	2.4
3	Q	187	GLU	2.4
4	R	54	ASP	2.4
2	P	50	LYS	2.4
5	E	123	GLY	2.4
5	E	207	VAL	2.4
7	U	230	GLU	2.4
6	T	2	THR	2.4
8	V	225	GLU	2.4
8	V	145	ASP	2.3
11	Y	182	ASP	2.3
5	S	203	GLU	2.3
6	T	201	GLU	2.3
3	Q	51	LYS	2.3
7	U	51	PRO	2.3
10	X	174	MET	2.3
6	F	2	THR	2.3
10	J	95	ARG	2.3
9	I	133	LYS	2.3
9	W	160	GLU	2.3
1	A	229	THR	2.3
13	M	1	THR	2.3
7	G	240	ALA	2.3
5	S	207	VAL	2.3
2	B	182	ASP	2.3
1	A	203	GLU	2.2
14	b	105	LYS	2.2
11	Y	211	GLY	2.2
3	Q	235	GLU	2.2
4	D	241	ALA	2.2
4	R	237	GLU	2.2
10	J	193	ASP	2.2
3	C	181	GLU	2.2
7	G	2	GLY	2.1
9	W	192	ASP	2.1
4	D	1	ASP	2.1
8	H	223	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	60	SER	2.1
1	A	248	GLU	2.1
3	Q	180	LYS	2.1
7	G	188	GLU	2.1
11	Y	71	GLY	2.1
1	A	201	GLU	2.1
5	E	201	ARG	2.1
4	D	242	GLU	2.1
7	U	3	TYR	2.1
6	F	39	ASN	2.1
8	H	198	GLU	2.0
3	C	188	GLU	2.0
3	C	180	LYS	2.0
3	C	185	THR	2.0
11	Y	30	ARG	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
17	7DX	K	301	35/35	0.86	0.29	5.63	42,44,47,52	0
17	7DX	Y	301	35/35	0.88	0.31	5.07	42,44,47,53	0
15	MG	Z	301	1/1	0.94	0.27	4.74	49,49,49,49	0
15	MG	J	201	1/1	0.94	0.15	2.03	47,47,47,47	0
16	CL	N	202	1/1	0.97	0.22	1.78	53,53,53,53	0
15	MG	I	301	1/1	0.96	0.15	0.94	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
16	CL	b	201	1/1	0.85	0.14	0.30	61,61,61,61	0
15	MG	K	302	1/1	0.90	0.13	0.19	52,52,52,52	0
15	MG	G	301	1/1	0.91	0.13	0.16	48,48,48,48	0
15	MG	N	201	1/1	0.97	0.07	-2.59	42,42,42,42	0
15	MG	L	301	1/1	0.98	0.04	-4.59	52,52,52,52	0
16	CL	G	302	1/1	0.97	0.18	-	30,30,30,30	0
16	CL	U	301	1/1	0.99	0.21	-	30,30,30,30	0

6.5 Other polymers

There are no such residues in this entry.