



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:29 PM GMT

PDB ID : 4RUR
Title : Yeast 20S proteasome in complex with the alkaloid indolo-phakellin (4)
Authors : Beck, P.; Lansdell, T.A.; Hewlett, N.M.; Tepe, J.J.; Groll, M.
Deposited on : 2014-11-21
Resolution : 2.50 Å(reported)

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

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

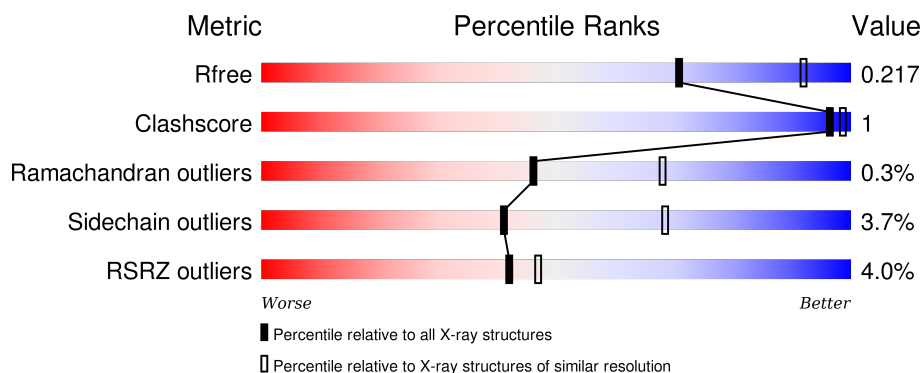
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div> <div>4%</div> <div>98%</div> <div>•</div> </div>
1	O	250	<div> <div>6%</div> <div>96%</div> <div>•</div> </div>
2	B	258	<div> <div>5%</div> <div>86%</div> <div>8% • 5%</div> </div>
2	P	258	<div> <div>5%</div> <div>85%</div> <div>9% • 5%</div> </div>
3	C	254	<div> <div>8%</div> <div>85%</div> <div>8% • 6%</div> </div>

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Mol	Chain	Length	Quality of chain
3	Q	254	
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	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	

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	N	201	-	-	-	X
15	MG	Z	302	-	-	-	X
16	3WE	L	301	-	-	-	X
16	3WE	Z	301	-	-	-	X

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 50389 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			

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	G	1	Total	Mg	0	0
			1	1		
15	K	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	I	1	Total 1	Mg 1	0	0
15	V	1	Total 1	Mg 1	0	0
15	W	1	Total 1	Mg 1	0	0
15	Z	1	Total 1	Mg 1	0	0
15	N	2	Total 2	Mg 2	0	0
15	Y	1	Total 1	Mg 1	0	0

-

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	L	1	Total 22	Br 1	C 15	N 5	O 1	0	0
16	Z	1	Total 22	Br 1	C 15	N 5	O 1	0	0

- 
- WORLD WIDE
PDB
PROTEIN DATA BANK

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	44	Total O 44 44	0	0
17	B	30	Total O 30 30	0	0
17	C	30	Total O 30 30	0	0
17	D	20	Total O 20 20	0	0
17	E	13	Total O 13 13	0	0
17	F	38	Total O 38 38	0	0
17	G	45	Total O 45 45	0	0
17	H	35	Total O 35 35	0	0
17	I	49	Total O 49 49	0	0
17	J	46	Total O 46 46	0	0
17	K	35	Total O 35 35	0	0
17	L	43	Total O 43 43	0	0
17	M	51	Total O 51 51	0	0
17	N	38	Total O 38 38	0	0
17	O	26	Total O 26 26	0	0
17	P	21	Total O 21 21	0	0
17	Q	25	Total O 25 25	0	0
17	R	20	Total O 20 20	0	0
17	S	11	Total O 11 11	0	0
17	T	28	Total O 28 28	0	0
17	U	43	Total O 43 43	0	0
17	V	31	Total O 31 31	0	0

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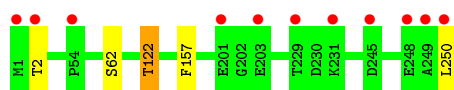
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	W	44	Total 44	O 44	0	0
17	X	34	Total 34	O 34	0	0
17	Y	39	Total 39	O 39	0	0
17	Z	36	Total 36	O 36	0	0
17	a	53	Total 53	O 53	0	0
17	b	42	Total 42	O 42	0	0

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.

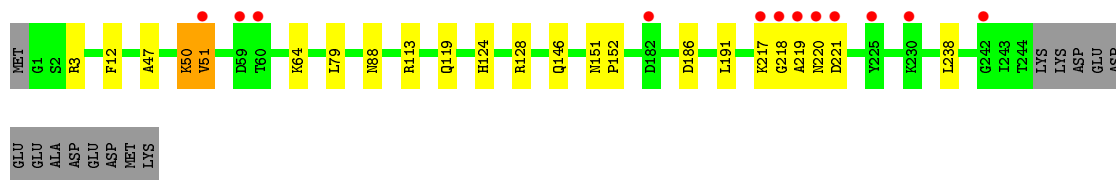
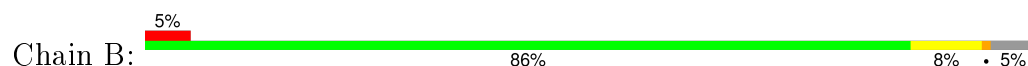
- Molecule 1: Proteasome subunit alpha type-2



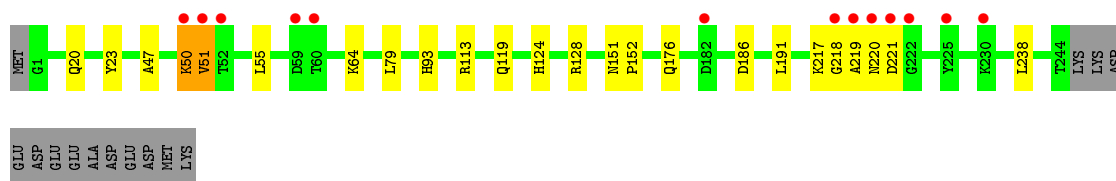
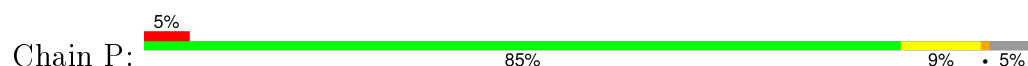
- Molecule 1: Proteasome subunit alpha type-2



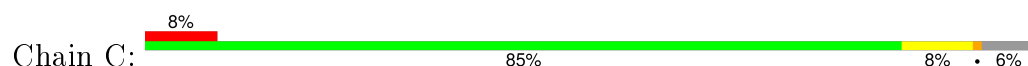
- Molecule 2: Proteasome subunit alpha type-3

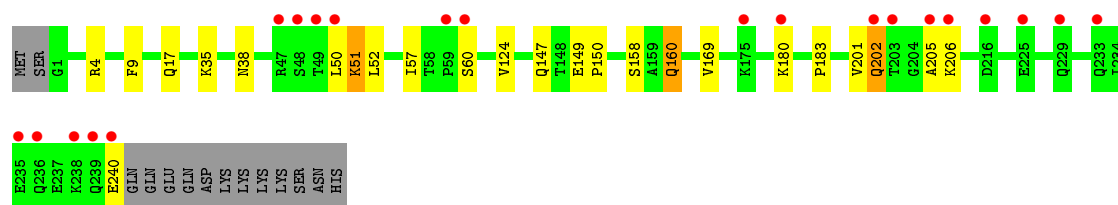


- Molecule 2: Proteasome subunit alpha type-3

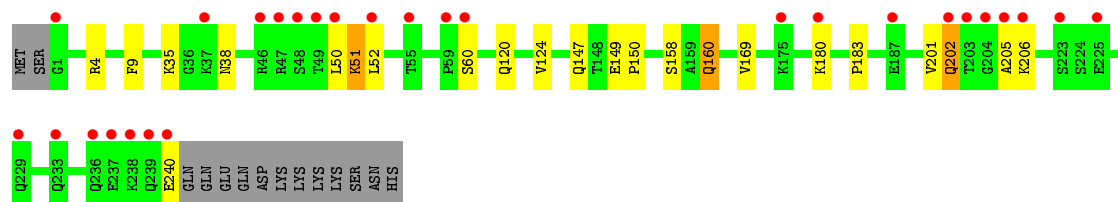
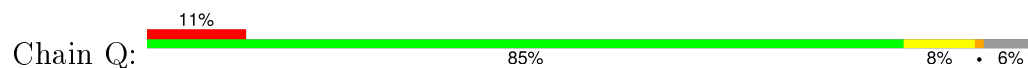


- Molecule 3: Proteasome subunit alpha type-4

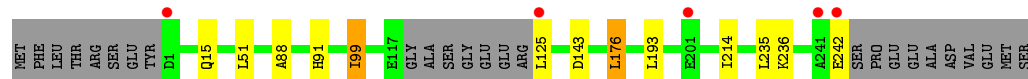
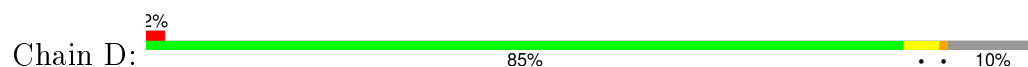




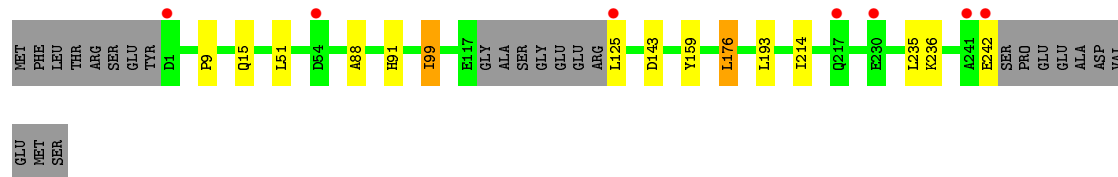
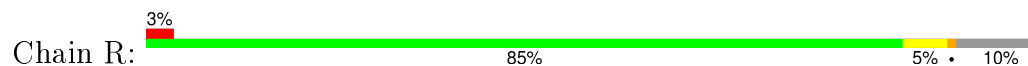
- Molecule 3: Proteasome subunit alpha type-4



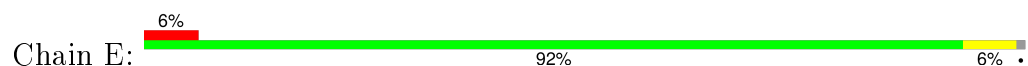
- Molecule 4: Proteasome subunit alpha type-5



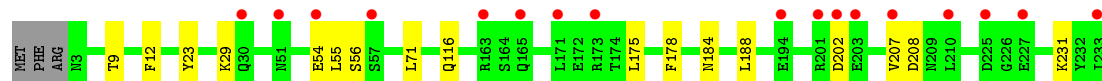
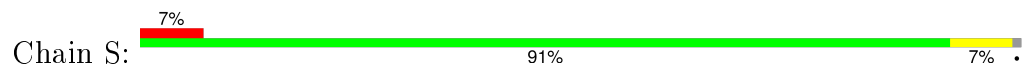
- Molecule 4: Proteasome subunit alpha type-5



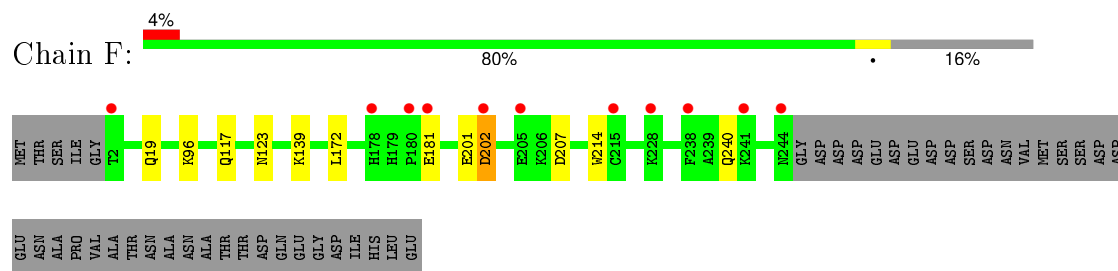
- Molecule 5: Proteasome subunit alpha type-6



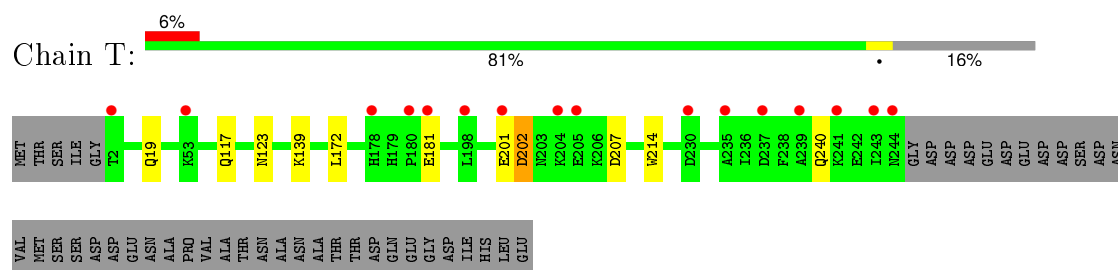
- Molecule 5: Proteasome subunit alpha type-6



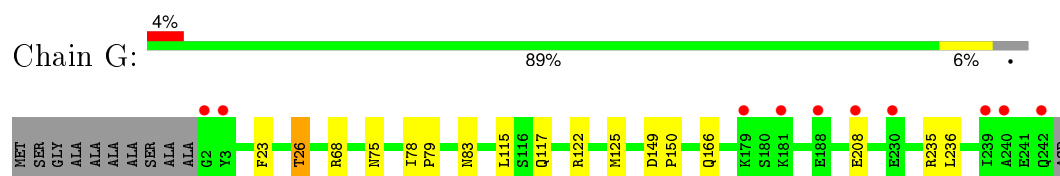
- Molecule 6: Probable proteasome subunit alpha type-7



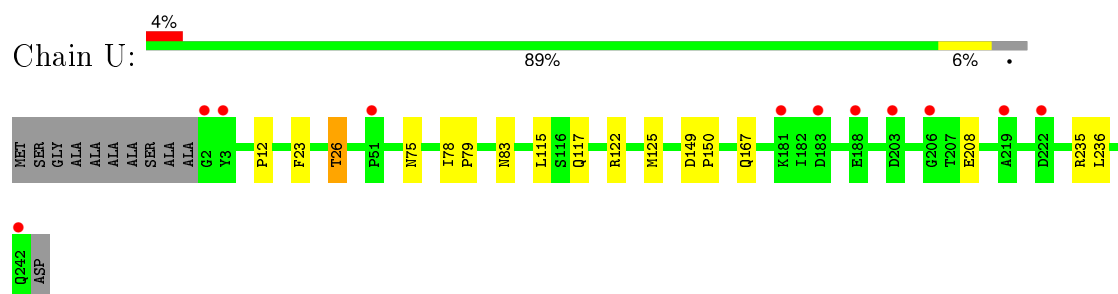
- Molecule 6: Probable proteasome subunit alpha type-7



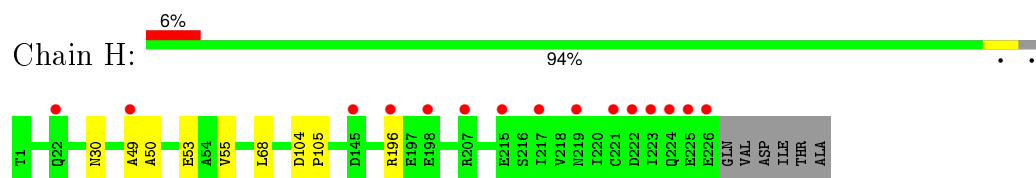
- Molecule 7: Proteasome subunit alpha type-1



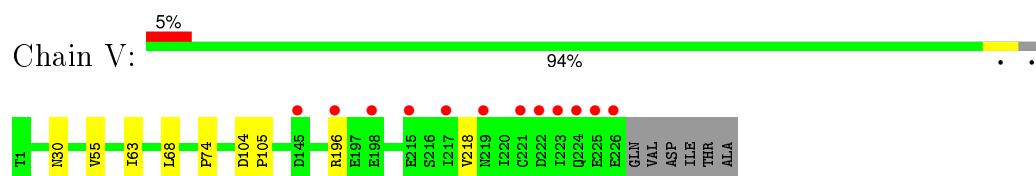
- Molecule 7: Proteasome subunit alpha type-1



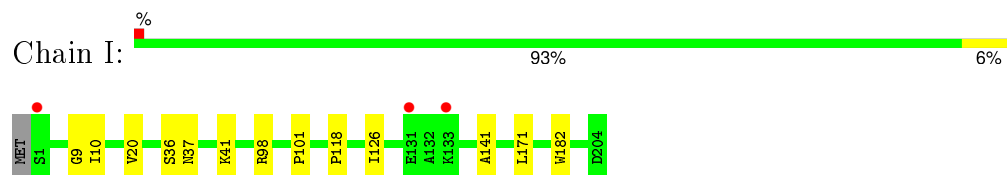
- Molecule 8: Proteasome subunit beta type-2



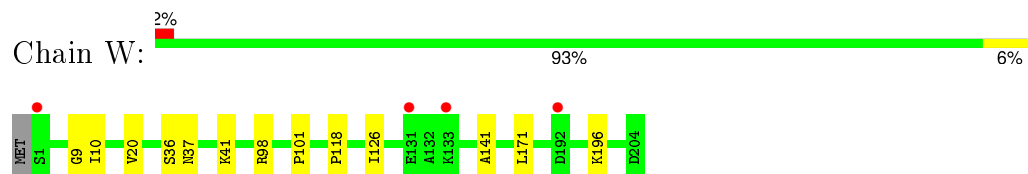
- Molecule 8: Proteasome subunit beta type-2



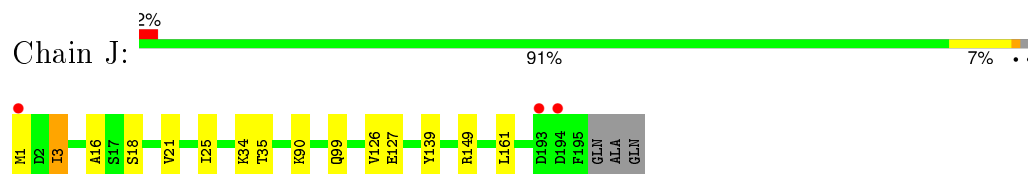
- Molecule 9: Proteasome subunit beta type-3



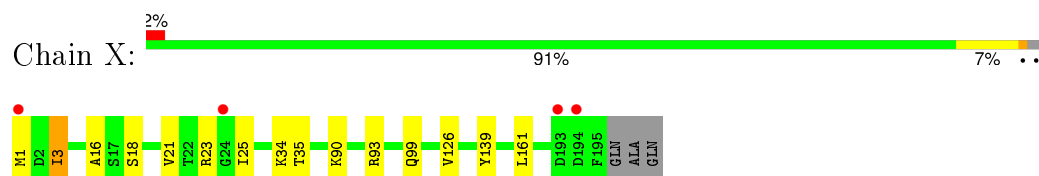
- Molecule 9: Proteasome subunit beta type-3



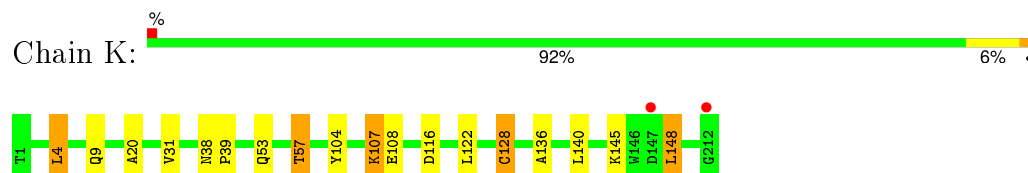
- Molecule 10: Proteasome subunit beta type-4



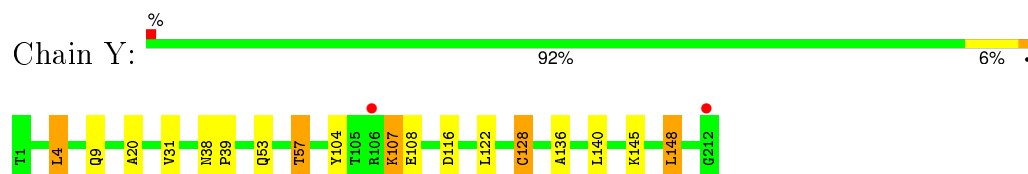
- Molecule 10: Proteasome subunit beta type-4



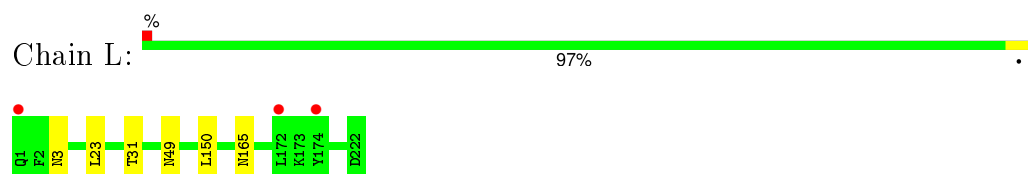
- Molecule 11: Proteasome subunit beta type-5



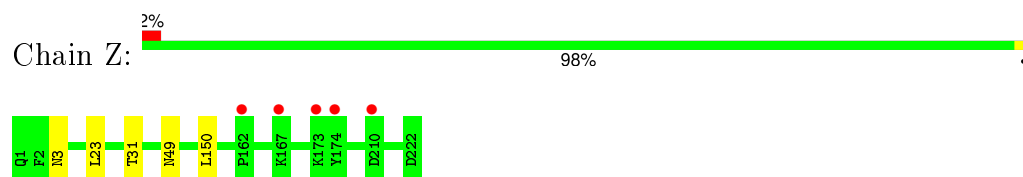
- Molecule 11: Proteasome subunit beta type-5



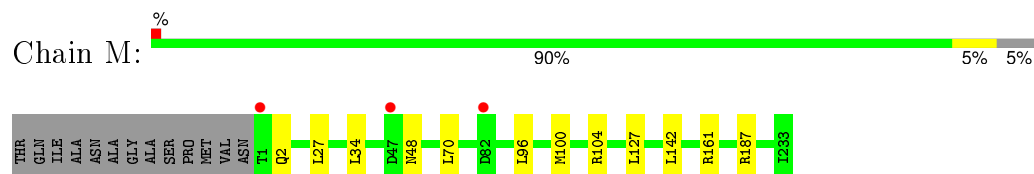
- Molecule 12: Proteasome subunit beta type-6



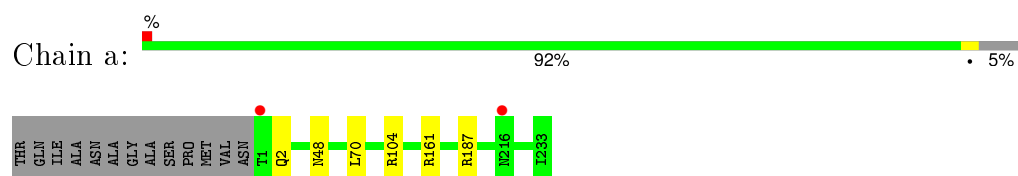
- Molecule 12: Proteasome subunit beta type-6



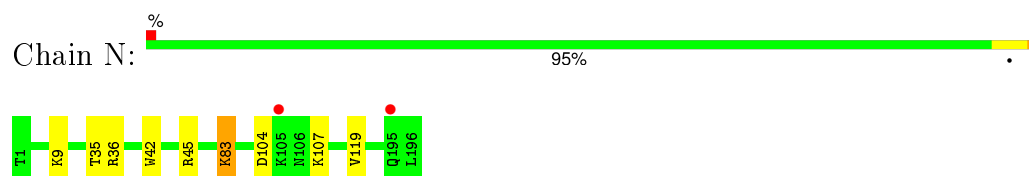
- Molecule 13: Proteasome subunit beta type-7



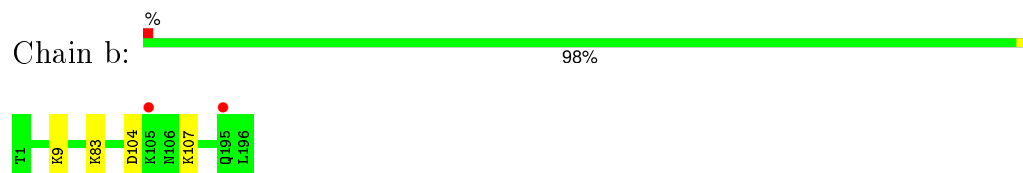
- Molecule 13: Proteasome subunit beta type-7



- Molecule 14: Proteasome subunit beta type-1



- Molecule 14: Proteasome subunit beta type-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.08Å 300.88Å 145.99Å 90.00° 113.11° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 15.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.8 (15.00-2.50) 98.8 (15.00-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.190 , 0.213 0.196 , 0.217	Depositor DCC
R_{free} test set	18230 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	50.4	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	4 of 364602 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	50389	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 3WE

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	0.47	0/2642
1	O	0.27	0/1952	0.47	0/2642
2	B	0.28	0/1934	0.50	0/2618
2	P	0.28	0/1934	0.50	0/2618
3	C	0.28	0/1910	0.51	0/2586
3	Q	0.28	0/1910	0.51	0/2586
4	D	0.27	0/1837	0.48	0/2475
4	R	0.27	0/1837	0.48	0/2475
5	E	0.27	0/1800	0.47	0/2433
5	S	0.27	0/1800	0.48	0/2433
6	F	0.27	0/1932	0.45	0/2609
6	T	0.27	0/1932	0.45	0/2609
7	G	0.27	0/1945	0.47	0/2634
7	U	0.27	0/1945	0.47	0/2634
8	H	0.31	0/1750	0.47	0/2373
8	V	0.28	0/1750	0.47	0/2373
9	I	0.28	0/1611	0.48	0/2174
9	W	0.28	0/1611	0.48	0/2174
10	J	0.27	0/1589	0.48	0/2142
10	X	0.27	0/1589	0.48	0/2142
11	K	0.27	0/1681	0.49	1/2274 (0.0%)
11	Y	0.26	0/1681	0.49	1/2274 (0.0%)
12	L	0.27	0/1795	0.48	0/2420
12	Z	0.27	0/1795	0.48	0/2420
13	M	0.28	0/1855	0.51	0/2514
13	a	0.28	0/1855	0.51	0/2514
14	N	0.26	0/1541	0.48	0/2087
14	b	0.26	0/1541	0.47	0/2087
All	All	0.27	0/50264	0.48	2/67962 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	4	LEU	CA-CB-CG	5.03	126.87	115.30
11	Y	4	LEU	CA-CB-CG	5.03	126.87	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1	0
1	O	1915	0	1929	5	0
2	B	1904	0	1904	12	0
2	P	1904	0	1904	11	0
3	C	1881	0	1895	9	0
3	Q	1881	0	1895	9	0
4	D	1813	0	1797	6	0
4	R	1813	0	1797	9	0
5	E	1773	0	1775	5	0
5	S	1773	0	1775	5	0
6	F	1892	0	1883	3	0
6	T	1892	0	1883	2	0
7	G	1907	0	1901	5	0
7	U	1907	0	1901	5	0
8	H	1719	0	1719	4	0
8	V	1719	0	1719	4	0
9	I	1581	0	1574	7	0
9	W	1581	0	1574	7	0
10	J	1561	0	1569	9	0
10	X	1561	0	1569	9	0
11	K	1644	0	1595	7	0
11	Y	1644	0	1595	7	0
12	L	1757	0	1711	2	0
12	Z	1757	0	1711	0	0
13	M	1824	0	1832	3	0
13	a	1824	0	1832	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	N	1512	0	1481	6	0
14	b	1512	0	1481	0	0
15	G	1	0	0	0	0
15	I	1	0	0	0	0
15	K	1	0	0	0	0
15	N	2	0	0	0	0
15	V	1	0	0	0	0
15	W	1	0	0	0	0
15	Y	1	0	0	0	0
15	Z	1	0	0	0	0
16	L	22	0	13	0	0
16	Z	22	0	13	0	0
17	A	44	0	0	0	0
17	B	30	0	0	1	0
17	C	30	0	0	0	0
17	D	20	0	0	0	0
17	E	13	0	0	1	0
17	F	38	0	0	1	0
17	G	45	0	0	1	0
17	H	35	0	0	0	0
17	I	49	0	0	0	0
17	J	46	0	0	2	0
17	K	35	0	0	0	0
17	L	43	0	0	2	0
17	M	51	0	0	0	0
17	N	38	0	0	1	0
17	O	26	0	0	0	0
17	P	21	0	0	1	0
17	Q	25	0	0	1	0
17	R	20	0	0	1	0
17	S	11	0	0	0	0
17	T	28	0	0	0	0
17	U	43	0	0	2	0
17	V	31	0	0	0	0
17	W	44	0	0	0	0
17	X	34	0	0	2	0
17	Y	39	0	0	0	0
17	Z	36	0	0	0	0
17	a	53	0	0	0	0
17	b	42	0	0	0	0
All	All	50389	0	49156	124	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 1.

All (124) 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)
7:G:166:GLN:NE2	17:G:427:HOH:O	2.26	0.67
12:L:165:ASN:ND2	17:L:435:HOH:O	2.30	0.64
7:G:68:ARG:HH12	14:N:36:ARG:HH22	1.47	0.62
10:X:23:ARG:NE	17:X:214:HOH:O	2.36	0.59
14:N:35:THR:HG21	14:N:45:ARG:HE	1.69	0.57
12:L:165:ASN:CG	17:L:435:HOH:O	2.43	0.56
14:N:35:THR:HG22	17:N:324:HOH:O	2.06	0.54
2:P:217:LYS:C	2:P:219:ALA:H	2.12	0.54
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.43	0.53
2:B:12:PHE:H	3:C:17:GLN:HE22	1.54	0.53
5:E:147:GLN:NE2	17:E:310:HOH:O	2.41	0.52
2:B:217:LYS:C	2:B:219:ALA:H	2.12	0.52
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	1.92	0.52
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.58	0.51
3:C:201:VAL:O	3:C:202:GLN:CB	2.58	0.51
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.10	0.51
5:E:12:PHE:H	6:F:19:GLN:HE22	1.57	0.51
2:B:3:ARG:HB3	5:E:122:TYR:OH	2.10	0.51
3:C:51:LYS:O	3:C:52:LEU:HB2	2.10	0.51
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.93	0.50
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.93	0.50
10:J:25:ILE:O	10:X:139:TYR:OH	2.30	0.50
8:H:49:ALA:O	8:H:53:GLU:HG3	2.12	0.50
4:R:99:ILE:HG23	17:R:302:HOH:O	2.11	0.50
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.93	0.50
5:S:12:PHE:H	6:T:19:GLN:HE22	1.59	0.50
2:B:88:ASN:OD1	17:B:325:HOH:O	2.20	0.50
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.42	0.49
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.93	0.49
6:F:96:LYS:NZ	17:F:337:HOH:O	2.44	0.49
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.78	0.49
7:G:23:PHE:O	7:G:26:THR:HB	2.13	0.48
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.78	0.48
7:U:23:PHE:O	7:U:26:THR:HB	2.14	0.48
7:U:167:GLN:NE2	17:U:335:HOH:O	2.40	0.48
10:J:149:ARG:NH2	17:J:222:HOH:O	2.46	0.48
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.96	0.48
10:J:127:GLU:OE2	17:J:211:HOH:O	2.20	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.78	0.47
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.96	0.47
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.50	0.47
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.97	0.47
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.97	0.46
1:O:57:MET:HE1	17:U:315:HOH:O	2.15	0.46
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.96	0.46
11:Y:53:GLN:O	11:Y:57:THR:OG1	2.33	0.46
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.97	0.46
4:R:91:HIS:HB3	4:R:99:ILE:HG22	1.98	0.46
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.81	0.45
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.97	0.45
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.16	0.45
4:D:176:LEU:HD22	5:E:55:LEU:CD2	2.46	0.45
11:K:107:LYS:HG3	11:K:108:GLU:HG3	1.98	0.45
3:C:35:LYS:HG2	3:C:158:SER:O	2.16	0.45
2:B:50:LYS:HD3	2:B:50:LYS:HA	1.86	0.45
4:D:91:HIS:HB3	4:D:99:ILE:HG22	1.98	0.45
11:K:128:CYS:SG	11:K:136:ALA:HB3	2.57	0.45
11:Y:128:CYS:SG	11:Y:136:ALA:HB3	2.56	0.45
11:K:53:GLN:O	11:K:57:THR:OG1	2.33	0.45
11:Y:107:LYS:HG3	11:Y:108:GLU:HG3	1.98	0.45
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.99	0.45
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.47	0.44
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.00	0.44
14:N:35:THR:CG2	14:N:45:ARG:HE	2.31	0.44
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.97	0.44
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.99	0.44
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.47	0.44
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	1.99	0.44
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.52	0.44
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.48	0.44
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.48	0.43
2:B:146:GLN:HG2	3:C:57:ILE:HG21	1.99	0.43
11:K:145:LYS:HB2	11:K:148:LEU:HD13	2.00	0.43
2:P:93:HIS:CD2	17:P:304:HOH:O	2.71	0.43
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.01	0.43
8:H:50:ALA:CB	9:I:126:ILE:HG23	2.49	0.43
4:R:176:LEU:HD11	5:S:54:GLU:HB2	2.00	0.43
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.01	0.43
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:96:LEU:O	13:M:100:MET:HG2	2.19	0.42
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.01	0.42
11:K:38:ASN:HB2	11:K:39:PRO:CD	2.49	0.42
10:J:139:TYR:OH	10:X:25:ILE:O	2.38	0.42
8:V:218:VAL:CG2	9:W:196:LYS:HB2	2.49	0.42
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.49	0.42
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.49	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.83	0.42
9:I:101:PRO:HB3	9:I:126:ILE:HD12	2.02	0.42
1:O:14:PRO:HA	2:P:23:TYR:CD1	2.55	0.42
6:F:202:ASP:OD1	6:F:202:ASP:N	2.53	0.42
10:X:3:ILE:HG23	10:X:18:SER:HB3	2.01	0.42
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.49	0.42
1:O:12:PHE:H	2:P:20:GLN:HE22	1.67	0.42
9:W:101:PRO:HB3	9:W:126:ILE:HD12	2.02	0.42
2:B:124:HIS:HB3	3:C:124:VAL:HG12	2.02	0.42
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.02	0.42
9:W:98:ARG:O	9:W:126:ILE:HD11	2.20	0.42
10:J:3:ILE:HG23	10:J:18:SER:HB3	2.01	0.41
7:G:78:ILE:N	7:G:79:PRO:CD	2.83	0.41
9:I:98:ARG:O	9:I:126:ILE:HD11	2.20	0.41
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.56	0.41
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.03	0.41
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	2.03	0.41
13:M:27:LEU:HD21	13:M:34:LEU:HD22	2.02	0.41
2:P:176:GLN:HG3	3:Q:52:LEU:HD13	2.03	0.41
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.03	0.41
4:R:91:HIS:CD2	4:R:99:ILE:HG22	2.56	0.41
2:B:151:ASN:HB2	2:B:152:PRO:HD2	2.02	0.41
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.55	0.41
6:T:202:ASP:N	6:T:202:ASP:OD1	2.54	0.41
11:K:20:ALA:HB2	11:K:31:VAL:HG21	2.03	0.41
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.69	0.41
4:R:9:PRO:HA	5:S:23:TYR:CD1	2.56	0.41
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	2.03	0.41
3:Q:120:GLN:NE2	17:Q:317:HOH:O	2.54	0.41
2:P:50:LYS:O	2:P:51:VAL:C	2.59	0.40
8:V:63:ILE:HG23	8:V:74:PRO:HB3	2.04	0.40
4:D:91:HIS:CD2	4:D:99:ILE:HG22	2.57	0.40
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.52	0.40
2:B:50:LYS:O	2:B:51:VAL:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.52	0.40
9:W:36:SER:HB2	10:X:126:VAL:HG11	2.03	0.40
3:C:9:PHE:H	4:D:15:GLN:HE22	1.69	0.40
10:X:93:ARG:NH1	17:X:207:HOH:O	2.53	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	61
1	O	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	39	61
2	B	242/258 (94%)	236 (98%)	2 (1%)	4 (2%)	11	19
2	P	242/258 (94%)	235 (97%)	3 (1%)	4 (2%)	11	19
3	C	238/254 (94%)	232 (98%)	3 (1%)	3 (1%)	15	26
3	Q	238/254 (94%)	232 (98%)	3 (1%)	3 (1%)	15	26
4	D	231/260 (89%)	229 (99%)	2 (1%)	0	100	100
4	R	231/260 (89%)	229 (99%)	2 (1%)	0	100	100
5	E	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
5	S	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
6	F	241/288 (84%)	238 (99%)	3 (1%)	0	100	100
6	T	241/288 (84%)	238 (99%)	3 (1%)	0	100	100
7	G	239/252 (95%)	238 (100%)	1 (0%)	0	100	100
7	U	239/252 (95%)	239 (100%)	0	0	100	100
8	H	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
8	V	224/232 (97%)	218 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	188 (97%)	5 (3%)	0	100	100
10	X	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
11	K	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
11	Y	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
12	L	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
12	Z	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
13	M	231/246 (94%)	223 (96%)	8 (4%)	0	100	100
13	a	231/246 (94%)	223 (96%)	8 (4%)	0	100	100
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
14	b	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
All	All	6284/6614 (95%)	6140 (98%)	128 (2%)	16 (0%)	46	68

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
2	B	221	ASP
3	C	202	GLN
2	P	51	VAL
2	P	221	ASP
3	Q	202	GLN
1	A	2	THR
2	B	220	ASN
1	O	2	THR
2	P	220	ASN
2	B	218	GLY
2	P	218	GLY
3	C	205	ALA
3	Q	205	ALA
3	C	183	PRO
3	Q	183	PRO

5.3.2 Protein sidechains ⓘ

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	87
1	O	209/209 (100%)	205 (98%)	4 (2%)	65	87
2	B	203/216 (94%)	196 (97%)	7 (3%)	44	72
2	P	203/216 (94%)	195 (96%)	8 (4%)	39	66
3	C	212/226 (94%)	201 (95%)	11 (5%)	29	51
3	Q	212/226 (94%)	201 (95%)	11 (5%)	29	51
4	D	194/215 (90%)	184 (95%)	10 (5%)	29	51
4	R	194/215 (90%)	184 (95%)	10 (5%)	29	51
5	E	190/193 (98%)	179 (94%)	11 (6%)	25	45
5	S	190/193 (98%)	179 (94%)	11 (6%)	25	45
6	F	201/239 (84%)	191 (95%)	10 (5%)	30	53
6	T	201/239 (84%)	191 (95%)	10 (5%)	30	53
7	G	206/210 (98%)	196 (95%)	10 (5%)	31	55
7	U	206/210 (98%)	196 (95%)	10 (5%)	31	55
8	H	185/190 (97%)	181 (98%)	4 (2%)	60	84
8	V	185/190 (97%)	181 (98%)	4 (2%)	60	84
9	I	172/173 (99%)	169 (98%)	3 (2%)	68	89
9	W	172/173 (99%)	170 (99%)	2 (1%)	78	93
10	J	173/175 (99%)	169 (98%)	4 (2%)	58	83
10	X	173/175 (99%)	169 (98%)	4 (2%)	58	83
11	K	169/169 (100%)	160 (95%)	9 (5%)	28	50
11	Y	169/169 (100%)	160 (95%)	9 (5%)	28	50
12	L	185/185 (100%)	180 (97%)	5 (3%)	52	79
12	Z	185/185 (100%)	180 (97%)	5 (3%)	52	79
13	M	199/208 (96%)	193 (97%)	6 (3%)	48	76
13	a	199/208 (96%)	193 (97%)	6 (3%)	48	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	162/162 (100%)	158 (98%)	4 (2%)	55	82
14	b	162/162 (100%)	158 (98%)	4 (2%)	55	82
All	All	5320/5540 (96%)	5124 (96%)	196 (4%)	41	68

All (196) 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	79	LEU
2	B	113	ARG
2	B	119	GLN
2	B	186	ASP
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	50	LEU
3	C	51	LYS
3	C	60	SER
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	206	LYS
3	C	240	GLU
4	D	51	LEU
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

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Mol	Chain	Res	Type
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	207	VAL
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	75	ASN
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	122	ARG
7	G	125	MET
7	G	208	GLU
7	G	235	ARG
7	G	236	LEU
8	H	30	ASN
8	H	55	VAL
8	H	68	LEU
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
9	I	182	TRP
10	J	3	ILE
10	J	35	THR
10	J	90	LYS
10	J	99	GLN
11	K	4	LEU
11	K	9	GLN

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Mol	Chain	Res	Type
11	K	57	THR
11	K	104	TYR
11	K	107	LYS
11	K	116	ASP
11	K	128	CYS
11	K	140	LEU
11	K	148	LEU
12	L	3	ASN
12	L	23	LEU
12	L	31	THR
12	L	49	ASN
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	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
2	P	79	LEU
2	P	113	ARG
2	P	119	GLN
2	P	186	ASP
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	50	LEU
3	Q	51	LYS
3	Q	60	SER
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL

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Mol	Chain	Res	Type
3	Q	180	LYS
3	Q	206	LYS
3	Q	240	GLU
4	R	51	LEU
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	207	VAL
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
6	T	214	TRP
6	T	240	GLN
7	U	26	THR
7	U	75	ASN
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	122	ARG
7	U	125	MET
7	U	208	GLU

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Mol	Chain	Res	Type
7	U	235	ARG
7	U	236	LEU
8	V	30	ASN
8	V	55	VAL
8	V	68	LEU
8	V	196	ARG
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	9	GLN
11	Y	57	THR
11	Y	104	TYR
11	Y	107	LYS
11	Y	116	ASP
11	Y	128	CYS
11	Y	140	LEU
11	Y	148	LEU
12	Z	3	ASN
12	Z	23	LEU
12	Z	31	THR
12	Z	49	ASN
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	83	LYS
14	b	104	ASP
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

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Mol	Chain	Res	Type
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
3	C	17	GLN
3	C	77	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	100	ASN
4	D	146	GLN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	120	GLN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
6	F	240	GLN
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
8	H	66	HIS
8	H	165	ASN
9	I	37	ASN
10	J	55	GLN
10	J	146	HIS
11	K	85	ASN
11	K	176	ASN

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Mol	Chain	Res	Type
11	K	190	ASN
11	K	208	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
13	M	18	ASN
13	M	48	ASN
13	M	102	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
2	P	176	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	92	ASN
5	S	99	ASN
5	S	116	GLN
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	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN

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Mol	Chain	Res	Type
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	167	GLN
8	V	165	ASN
9	W	37	ASN
10	X	55	GLN
10	X	86	GLN
11	Y	85	ASN
11	Y	176	ASN
11	Y	190	ASN
11	Y	208	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
13	a	18	ASN
13	a	48	ASN
13	a	102	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 11 ligands modelled in this entry, 9 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	$\# Z > 2$
16	3WE	L	301	-	21,26,26	2.16	4 (19%)	15,42,42	2.27	5 (33%)
16	3WE	Z	301	-	21,26,26	2.15	4 (19%)	15,42,42	2.35	5 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	3WE	L	301	-	-	0/0/40/40	0/4/5/5
16	3WE	Z	301	-	-	0/0/40/40	0/4/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	L	301	3WE	C18-N19	-5.00	1.26	1.35
16	Z	301	3WE	C18-N19	-4.99	1.26	1.35
16	Z	301	3WE	C5-N14	-2.33	1.36	1.39
16	L	301	3WE	C5-N14	-2.30	1.36	1.39
16	Z	301	3WE	C18-N22	2.16	1.34	1.29
16	L	301	3WE	C18-N22	2.21	1.34	1.29
16	Z	301	3WE	C7-C4	6.75	1.50	1.41
16	L	301	3WE	C7-C4	6.85	1.50	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Z	301	3WE	C2-C3-C4	-2.95	116.71	120.88
16	L	301	3WE	C2-C3-C4	-2.88	116.81	120.88
16	Z	301	3WE	C20-N14-C5	-2.64	125.16	128.35
16	Z	301	3WE	C23-C13-N12	-2.63	100.05	103.34
16	L	301	3WE	C20-N14-C5	-2.43	125.41	128.35
16	L	301	3WE	C23-C13-N12	-2.32	100.44	103.34
16	L	301	3WE	C3-C4-C5	3.54	123.46	119.56
16	Z	301	3WE	C3-C4-C5	3.68	123.61	119.56
16	L	301	3WE	N19-C18-N17	6.26	115.95	109.27
16	Z	301	3WE	N19-C18-N17	6.33	116.02	109.27

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 [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, 95th 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%)	-0.13	11 (4%)	38	43	40, 53, 86, 124	0
1	O	250/250 (100%)	-0.03	15 (6%)	25	28	43, 60, 102, 131	0
2	B	244/258 (94%)	0.04	12 (4%)	33	38	39, 58, 99, 147	0
2	P	244/258 (94%)	0.13	13 (5%)	30	34	45, 61, 105, 149	0
3	C	240/254 (94%)	0.22	21 (8%)	12	13	39, 62, 124, 149	0
3	Q	240/254 (94%)	0.44	28 (11%)	6	6	41, 71, 150, 176	0
4	D	235/260 (90%)	-0.13	5 (2%)	67	71	43, 63, 96, 136	0
4	R	235/260 (90%)	-0.05	7 (2%)	54	59	45, 66, 102, 137	0
5	E	231/234 (98%)	0.05	14 (6%)	25	27	46, 66, 104, 150	0
5	S	231/234 (98%)	0.23	17 (7%)	17	19	49, 73, 112, 160	0
6	F	243/288 (84%)	-0.09	11 (4%)	37	42	42, 59, 110, 140	0
6	T	243/288 (84%)	0.05	16 (6%)	22	24	41, 68, 124, 152	0
7	G	241/252 (95%)	-0.15	10 (4%)	41	46	35, 54, 88, 137	0
7	U	241/252 (95%)	-0.03	11 (4%)	36	41	43, 58, 89, 135	0
8	H	226/232 (97%)	0.13	15 (6%)	22	24	35, 52, 86, 152	0
8	V	226/232 (97%)	0.10	12 (5%)	30	34	41, 54, 86, 157	0
9	I	204/205 (99%)	-0.28	3 (1%)	76	79	36, 48, 77, 98	0
9	W	204/205 (99%)	-0.31	4 (1%)	68	72	39, 51, 80, 104	0
10	J	195/198 (98%)	-0.23	3 (1%)	76	79	37, 51, 76, 129	0
10	X	195/198 (98%)	-0.17	4 (2%)	67	71	37, 52, 76, 140	0
11	K	212/212 (100%)	-0.28	2 (0%)	85	88	34, 50, 71, 90	0
11	Y	212/212 (100%)	-0.26	2 (0%)	85	88	39, 50, 73, 92	0
12	L	222/222 (100%)	-0.23	3 (1%)	78	80	37, 52, 83, 118	0
12	Z	222/222 (100%)	-0.27	5 (2%)	64	67	37, 52, 84, 120	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.37	3 (1%)	79	82	36, 52, 73, 91	0
13	a	233/246 (94%)	-0.31	2 (0%)	85	88	36, 50, 72, 90	0
14	N	196/196 (100%)	-0.33	2 (1%)	84	86	38, 48, 75, 104	0
14	b	196/196 (100%)	-0.31	2 (1%)	84	86	38, 49, 75, 109	0
All	All	6344/6614 (95%)	-0.08	253 (3%)	42	47	34, 56, 100, 176	0

All (253) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	X	1	MET	10.8
3	Q	49	THR	10.5
3	Q	50	LEU	8.8
8	V	221	CYS	8.4
2	B	221	ASP	8.4
3	Q	206	LYS	8.4
8	V	224	GLN	7.5
8	H	221	CYS	7.4
3	C	49	THR	7.4
2	P	219	ALA	6.9
10	J	1	MET	6.9
8	H	223	ILE	6.8
2	P	51	VAL	6.7
8	V	226	GLU	6.7
2	B	51	VAL	6.4
5	S	202	ASP	6.4
10	X	194	ASP	6.2
3	C	50	LEU	6.2
2	B	219	ALA	6.1
12	L	174	TYR	6.1
3	Q	239	GLN	5.9
2	P	220	ASN	5.9
2	B	218	GLY	5.8
2	P	221	ASP	5.7
3	C	206	LYS	5.7
2	P	218	GLY	5.6
2	P	59	ASP	5.5
8	V	223	ILE	5.5
4	R	241	ALA	5.5
3	C	236	GLN	5.4
3	Q	236	GLN	5.4
9	W	1	SER	5.4

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Mol	Chain	Res	Type	RSRZ
5	E	202	ASP	5.3
7	U	242	GLN	5.3
1	O	1	MET	5.2
12	Z	174	TYR	5.2
1	A	249	ALA	5.0
6	T	178	HIS	5.0
8	V	222	ASP	4.9
9	I	1	SER	4.9
8	H	226	GLU	4.8
1	A	1	MET	4.8
2	B	220	ASN	4.8
6	F	244	ASN	4.8
8	H	222	ASP	4.8
3	Q	205	ALA	4.7
1	O	249	ALA	4.7
9	I	131	GLU	4.7
8	H	224	GLN	4.4
14	b	195	GLN	4.4
2	P	52	THR	4.2
3	C	202	GLN	4.2
3	Q	202	GLN	4.2
10	J	194	ASP	4.2
6	F	205	GLU	4.1
6	T	243	ILE	4.1
5	S	54	GLU	4.1
1	O	250	LEU	4.1
1	O	2	THR	4.1
6	F	178	HIS	4.0
3	C	205	ALA	4.0
4	R	125	LEU	3.9
1	A	2	THR	3.9
8	V	225	GLU	3.9
14	b	105	LYS	3.9
3	Q	238	LYS	3.8
3	Q	204	GLY	3.8
9	W	133	LYS	3.8
3	Q	55	THR	3.7
3	C	238	LYS	3.7
5	E	122	TYR	3.7
3	C	240	GLU	3.7
8	H	217	ILE	3.6
2	P	225	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
9	I	133	LYS	3.6
2	B	217	LYS	3.5
4	R	217	GLN	3.5
7	G	3	TYR	3.5
6	T	244	ASN	3.5
5	E	233	ILE	3.5
5	S	233	ILE	3.5
13	M	47	ASP	3.4
6	F	181	GLU	3.4
9	W	192	ASP	3.4
8	H	215	GLU	3.4
3	Q	240	GLU	3.3
2	B	60	THR	3.3
1	O	201	GLU	3.3
2	B	59	ASP	3.3
1	A	231	LYS	3.3
3	C	225	GLU	3.3
3	Q	52	LEU	3.2
8	H	198	GLU	3.2
6	T	181	GLU	3.2
12	Z	167	LYS	3.1
3	Q	187	GLU	3.1
5	S	227	GLU	3.1
7	U	2	GLY	3.1
10	X	193	ASP	3.1
13	a	1	THR	3.1
1	O	50	LYS	3.1
8	V	145	ASP	3.1
3	Q	59	PRO	3.1
6	T	180	PRO	3.1
7	U	206	GLY	3.1
5	S	194	GLU	3.1
3	C	180	LYS	3.0
10	J	193	ASP	3.0
7	G	242	GLN	3.0
3	Q	237	GLU	3.0
4	D	242	GLU	3.0
8	V	215	GLU	3.0
14	N	195	GLN	3.0
2	P	50	LYS	3.0
3	C	239	GLN	2.9
6	T	230	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
3	C	235	GLU	2.9
3	Q	223	SER	2.9
3	Q	225	GLU	2.9
4	R	1	ASP	2.9
6	T	204	LYS	2.9
7	U	181	LYS	2.9
3	C	47	ARG	2.9
6	F	202	ASP	2.9
7	U	188	GLU	2.9
7	U	51	PRO	2.9
1	A	201	GLU	2.9
3	Q	203	THR	2.9
3	Q	37	LYS	2.9
3	C	203	THR	2.8
5	S	201	ARG	2.8
5	S	57	SER	2.8
1	A	229	THR	2.8
6	T	201	GLU	2.8
2	P	222	GLY	2.8
3	C	216	ASP	2.8
2	B	242	GLY	2.8
1	O	248	GLU	2.8
5	E	54	GLU	2.8
4	D	125	LEU	2.8
5	S	173	ARG	2.8
4	D	1	ASP	2.7
4	D	241	ALA	2.7
5	E	227	GLU	2.7
5	E	173	ARG	2.7
6	T	205	GLU	2.7
11	Y	212	GLY	2.7
8	H	219	ASN	2.7
1	A	248	GLU	2.7
5	E	217	LYS	2.7
2	P	230	LYS	2.7
6	T	241	LYS	2.7
3	Q	48	SER	2.6
7	G	230	GLU	2.6
8	V	219	ASN	2.6
6	F	180	PRO	2.6
7	U	3	TYR	2.6
3	C	175	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
4	R	230	GLU	2.6
4	R	242	GLU	2.6
3	C	48	SER	2.6
8	H	196	ARG	2.6
3	Q	180	LYS	2.5
5	E	201	ARG	2.5
4	D	201	GLU	2.5
9	W	131	GLU	2.5
3	Q	175	LYS	2.5
1	A	250	LEU	2.5
5	E	210	LEU	2.5
3	Q	60	SER	2.5
5	S	30	GLN	2.5
1	A	54	PRO	2.5
7	G	208	GLU	2.5
12	Z	162	PRO	2.5
3	Q	229	GLN	2.5
8	V	217	ILE	2.5
13	M	82	ASP	2.4
5	E	123	GLY	2.4
6	T	198	LEU	2.4
5	E	203	GLU	2.4
6	F	228	LYS	2.4
2	P	182	ASP	2.4
3	Q	1	GLY	2.4
5	E	3	ASN	2.4
10	X	24	GLY	2.4
14	N	105	LYS	2.4
13	a	216	ASN	2.4
6	F	2	THR	2.4
8	H	22	GLN	2.3
1	O	52	SER	2.3
8	H	207	ARG	2.3
8	H	145	ASP	2.3
5	S	210	LEU	2.3
5	S	165	GLN	2.3
5	S	163	ARG	2.3
5	S	51	ASN	2.3
5	S	203	GLU	2.3
7	G	179	LYS	2.3
7	U	203	ASP	2.3
3	C	59	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
11	Y	106	ARG	2.3
6	T	239	ALA	2.2
2	B	230	LYS	2.2
5	S	207	VAL	2.2
7	G	240	ALA	2.2
3	C	60	SER	2.2
1	O	203	GLU	2.2
6	T	2	THR	2.2
8	H	225	GLU	2.2
7	G	2	GLY	2.2
3	Q	233	GLN	2.2
1	A	203	GLU	2.2
7	U	219	ALA	2.2
3	Q	46	ARG	2.2
1	O	229	THR	2.2
2	P	60	THR	2.2
13	M	1	THR	2.2
3	Q	47	ARG	2.2
3	C	233	GLN	2.2
5	S	171	LEU	2.2
6	T	237	ASP	2.2
12	Z	210	ASP	2.2
12	L	1	GLN	2.2
11	K	212	GLY	2.1
1	O	184	GLU	2.1
3	C	229	GLN	2.1
5	S	225	ASP	2.1
8	H	49	ALA	2.1
6	F	215	CYS	2.1
5	E	117	LYS	2.1
12	Z	173	LYS	2.1
2	B	182	ASP	2.1
7	G	181	LYS	2.1
12	L	172	LEU	2.1
6	F	241	LYS	2.1
1	O	178	ARG	2.1
7	G	188	GLU	2.1
1	O	177	LYS	2.1
7	U	222	ASP	2.1
7	G	239	ILE	2.1
8	V	198	GLU	2.1
1	A	245	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
4	R	54	ASP	2.1
8	V	196	ARG	2.1
1	O	182	GLU	2.1
2	B	225	TYR	2.1
6	T	235	ALA	2.0
11	K	147	ASP	2.0
5	E	180	LYS	2.0
6	T	53	LYS	2.0
6	F	238	PHE	2.0
1	O	231	LYS	2.0
7	U	183	ASP	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, 95th 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	Z	302	1/1	0.73	0.45	11.20	101,101,101,101	0
15	MG	N	201	1/1	0.47	0.36	7.57	65,65,65,65	0
16	3WE	L	301	22/22	0.83	0.24	2.85	73,89,98,115	0
16	3WE	Z	301	22/22	0.85	0.22	2.27	73,84,97,120	0
15	MG	G	301	1/1	0.70	0.13	0.39	66,66,66,66	0
15	MG	Y	301	1/1	0.99	0.11	-0.02	49,49,49,49	0
15	MG	K	301	1/1	0.94	0.09	-0.93	53,53,53,53	0
15	MG	I	301	1/1	0.97	0.08	-1.20	70,70,70,70	0
15	MG	W	301	1/1	0.91	0.07	-1.67	64,64,64,64	0
15	MG	V	301	1/1	0.99	0.05	-2.27	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
15	MG	N	202	1/1	0.78	0.20	-	73,73,73,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.