



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 07:57 am GMT

PDB ID : 4Y8H
Title : Yeast 20S proteasome in complex with N3-APAL-ep
Authors : Huber, E.M.; Groll, M.
Deposited on : 2015-02-16
Resolution : 2.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

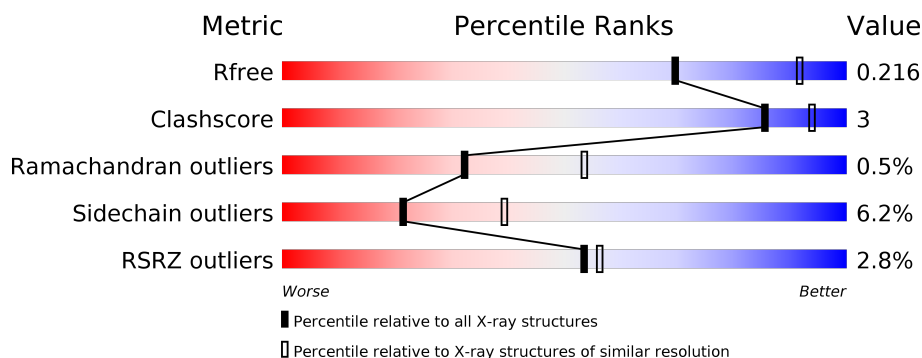
1 Overall quality at a glance

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}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (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>2%</div> <div> <div></div> <div>92%</div> <div>6%</div> </div> <div>•</div> </div>
1	O	250	<div> <div>3%</div> <div> <div></div> <div>92%</div> <div>6%</div> </div> <div>•</div> </div>
2	B	258	<div> <div>6%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>5%</div> </div> <div>•</div> </div>
2	P	258	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>5%</div> </div> <div>•</div> </div>
3	C	254	<div> <div>7%</div> <div> <div></div> <div>82%</div> <div>10%</div> <div>6%</div> </div> <div>•</div> </div>
3	Q	254	<div> <div>10%</div> <div> <div></div> <div>82%</div> <div>10%</div> <div>6%</div> </div> <div>•</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	
15	c	6	
15	d	6	
15	e	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	f	6	
15	g	6	
15	h	6	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	MG	I	301	-	-	-	X
16	MG	Z	301	-	-	-	X
18	MES	K	302	-	-	-	X
18	MES	g	101	-	-	-	X

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 50485 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

- Molecule 2 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			
2	P	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	240	Total	C	N	O	S	0	0	0
			1881	1176	329	372	4			
3	Q	240	Total	C	N	O	S	0	0	0
			1881	1176	329	372	4			

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	7			
4	R	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	7			

- Molecule 5 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			
5	S	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			

- Molecule 6 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	243	Total	C	N	O	S	0	0	0
			1892	1203	329	356	4			
6	T	243	Total	C	N	O	S	0	0	0
			1892	1203	329	356	4			

- Molecule 7 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	241	Total	C	N	O	S	0	0	0
			1907	1214	320	365	8			
7	U	241	Total	C	N	O	S	0	0	0
			1907	1214	320	365	8			

- Molecule 8 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			
8	V	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			

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

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

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

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

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-5.

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

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

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

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

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

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

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

- Molecule 15 is a protein called N3-APAL-ep.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	c	6	Total	C	N	O	0	0	0
			35	22	7	6			
15	d	6	Total	C	N	O	0	0	0
			35	22	7	6			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	e	6	Total	C	N	O	0	0	0
			35	22	7	6			
15	f	6	Total	C	N	O	0	0	0
			35	22	7	6			
15	g	6	Total	C	N	O	0	0	0
			35	22	7	6			
15	h	6	Total	C	N	O	0	0	0
			35	22	7	6			

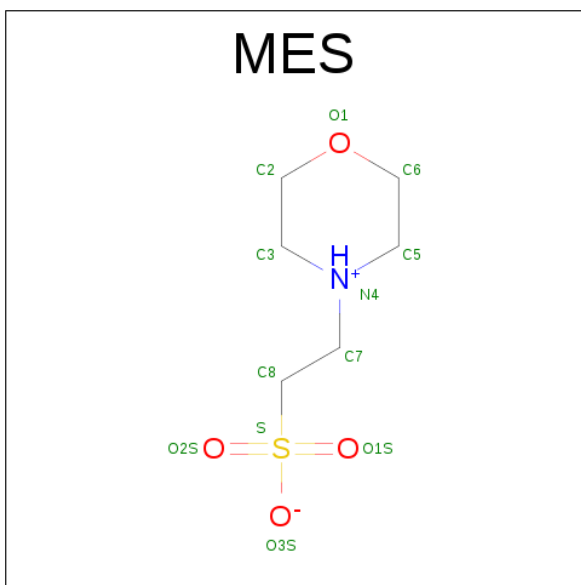
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

- Molecule 18 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	44	Total	O	0	0
			44	44		
19	B	37	Total	O	0	0
			37	37		
19	C	22	Total	O	0	0
			22	22		
19	D	19	Total	O	0	0
			19	19		
19	E	19	Total	O	0	0
			19	19		
19	F	29	Total	O	0	0
			29	29		
19	G	46	Total	O	0	0
			46	46		
19	H	55	Total	O	0	0
			55	55		
19	I	42	Total	O	0	0
			42	42		
19	J	34	Total	O	0	0
			34	34		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	K	43	Total O 43 43	0	0
19	L	48	Total O 48 48	0	0
19	M	43	Total O 43 43	0	0
19	N	37	Total O 37 37	0	0
19	O	21	Total O 21 21	0	0
19	P	21	Total O 21 21	0	0
19	Q	20	Total O 20 20	0	0
19	R	16	Total O 16 16	0	0
19	S	13	Total O 13 13	0	0
19	T	23	Total O 23 23	0	0
19	U	30	Total O 30 30	0	0
19	V	38	Total O 38 38	0	0
19	W	34	Total O 34 34	0	0
19	X	31	Total O 31 31	0	0
19	Y	34	Total O 34 34	0	0
19	Z	41	Total O 41 41	0	0
19	a	55	Total O 55 55	0	0
19	b	35	Total O 35 35	0	0
19	c	3	Total O 3 3	0	0
19	d	2	Total O 2 2	0	0
19	e	2	Total O 2 2	0	0

Continued on next page...

Continued from previous page...

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

3 Residue-property plots [i](#)

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

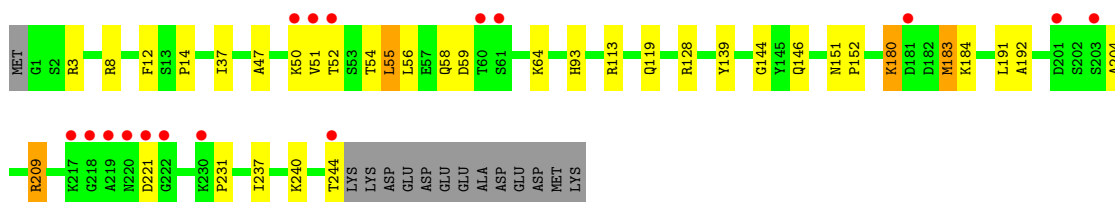
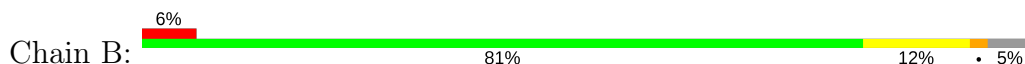
- Molecule 1: Proteasome subunit alpha type-2



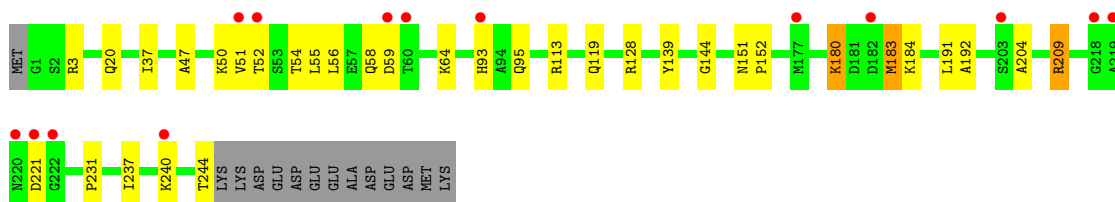
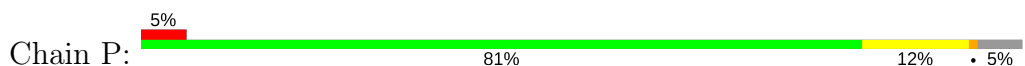
- Molecule 1: Proteasome subunit alpha type-2



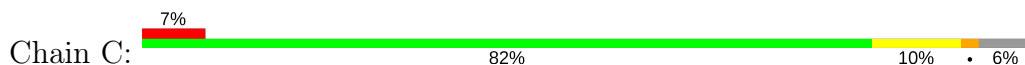
- Molecule 2: Proteasome subunit alpha type-3

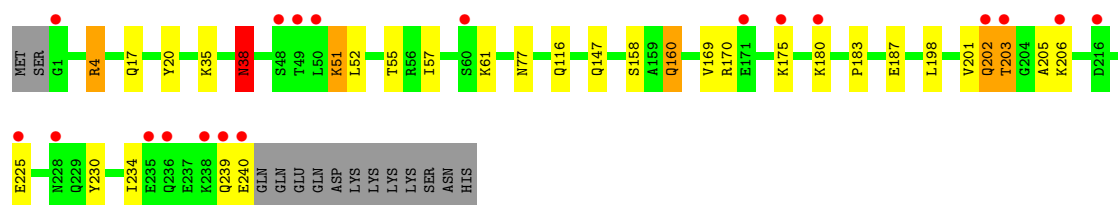


- Molecule 2: Proteasome subunit alpha type-3

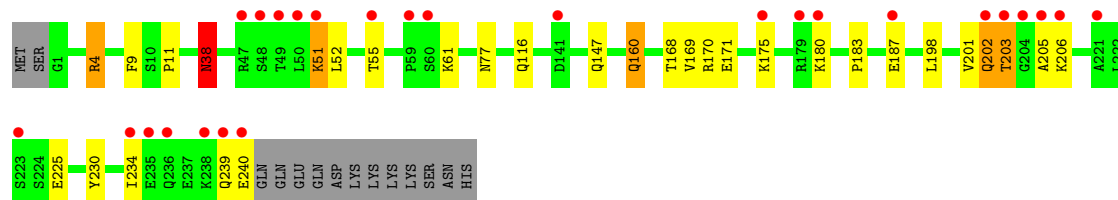
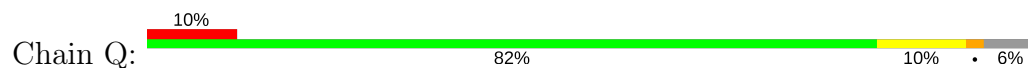


- Molecule 3: Proteasome subunit alpha type-4

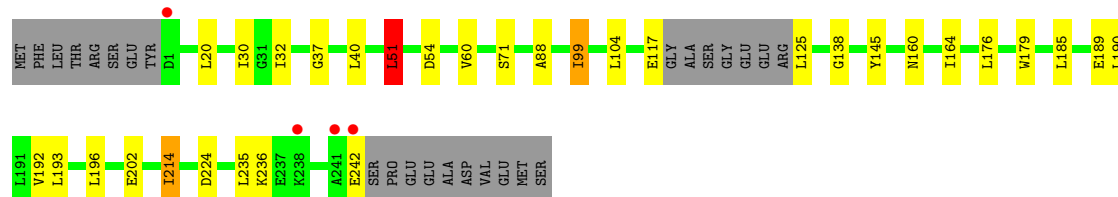
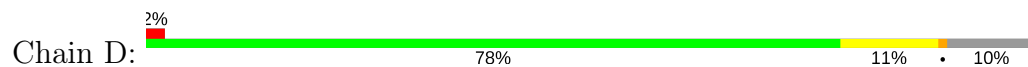




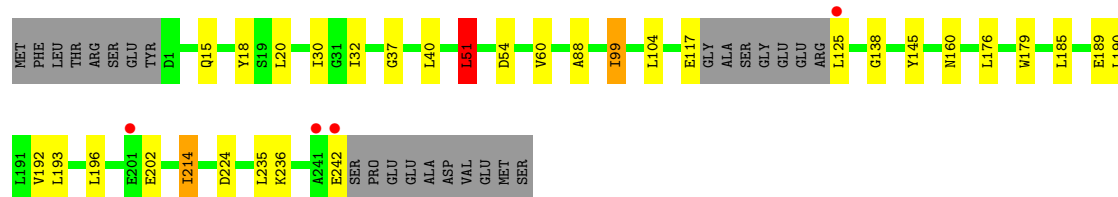
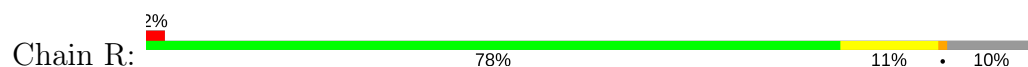
• Molecule 3: Proteasome subunit alpha type-4



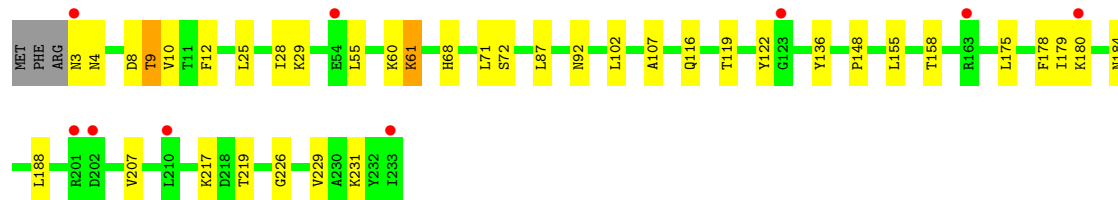
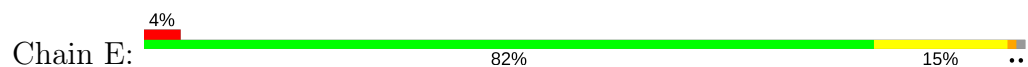
• Molecule 4: Proteasome subunit alpha type-5



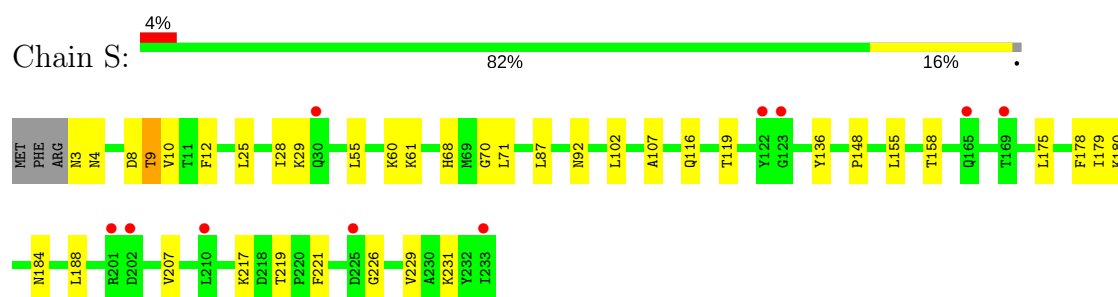
• Molecule 4: Proteasome subunit alpha type-5



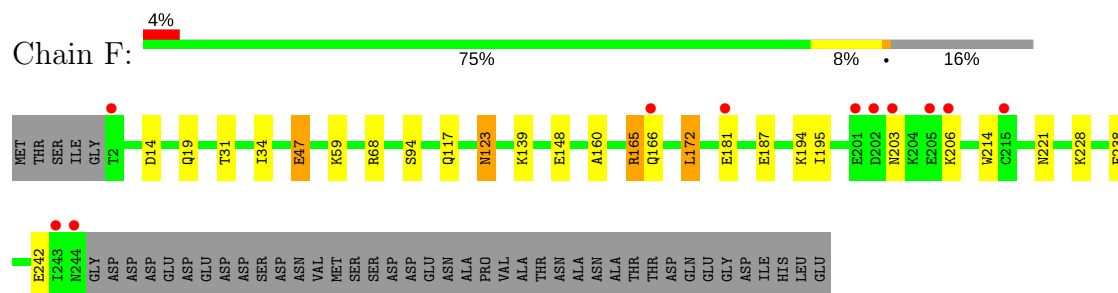
• Molecule 5: Proteasome subunit alpha type-6



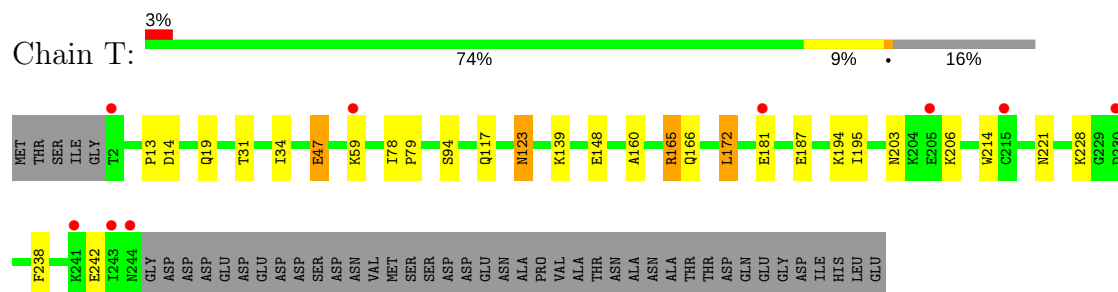
• Molecule 5: Proteasome subunit alpha type-6



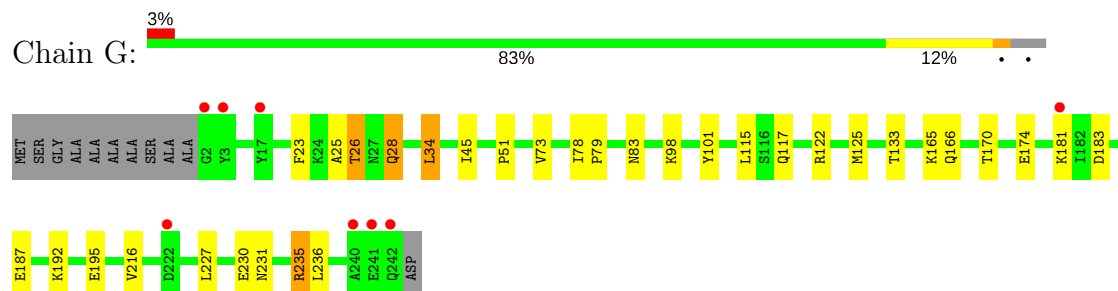
- Molecule 6: Probable proteasome subunit alpha type-7



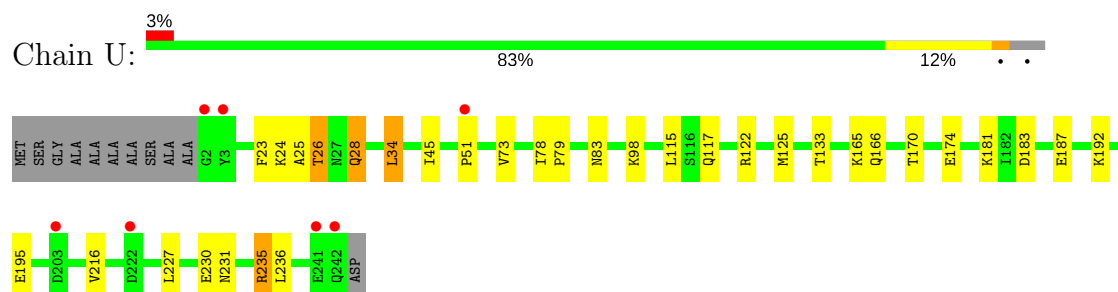
- Molecule 6: Probable proteasome subunit alpha type-7



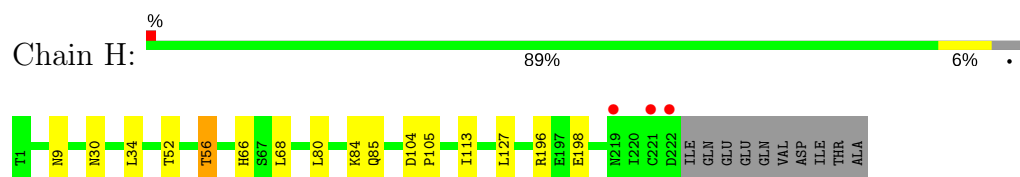
- Molecule 7: Proteasome subunit alpha type-1



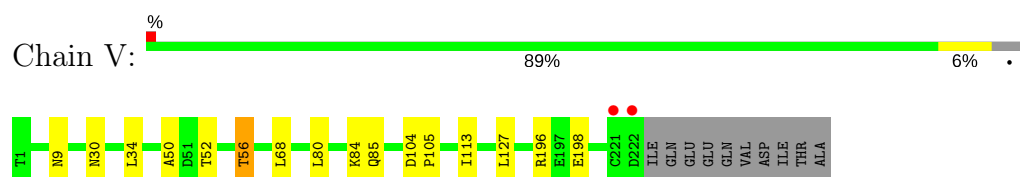
- Molecule 7: Proteasome subunit alpha type-1



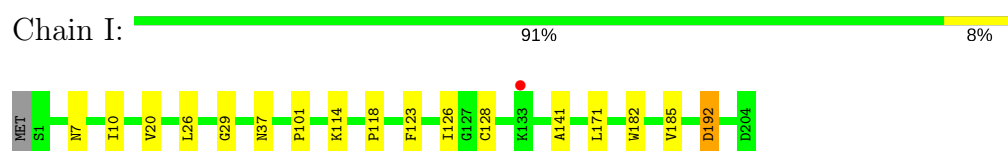
- Molecule 8: Proteasome subunit beta type-2



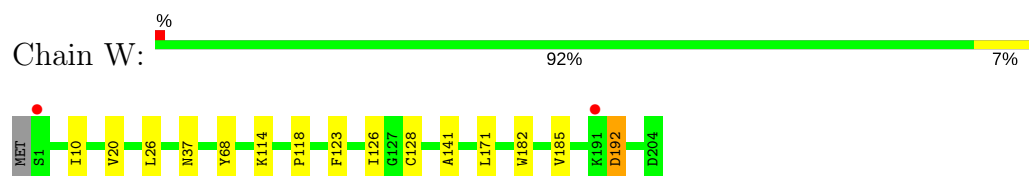
- Molecule 8: Proteasome subunit beta type-2



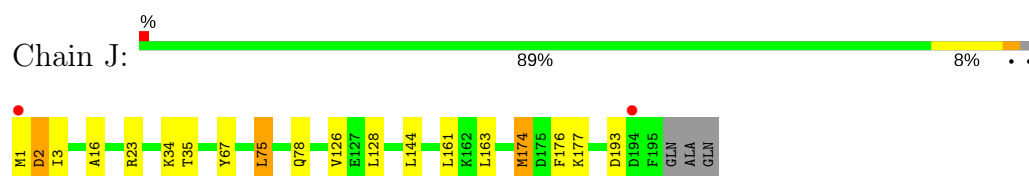
- Molecule 9: Proteasome subunit beta type-3



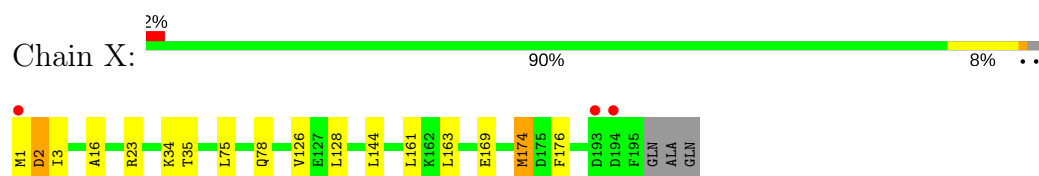
- Molecule 9: Proteasome subunit beta type-3



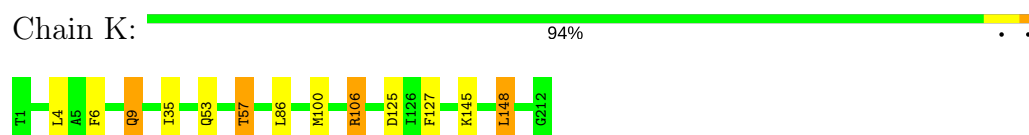
- Molecule 10: Proteasome subunit beta type-4



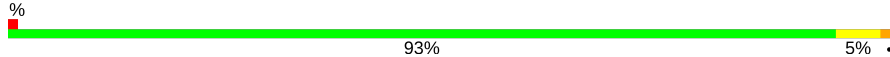
- Molecule 10: Proteasome subunit beta type-4

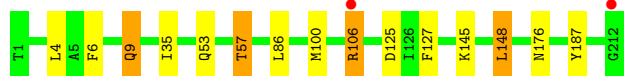


- Molecule 11: PROTEASOME SUBUNIT BETA TYPE-5




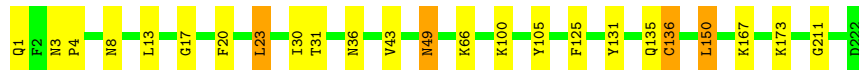
- Molecule 11: PROTEASOME SUBUNIT BETA TYPE-5

Chain Y:  93% 5%




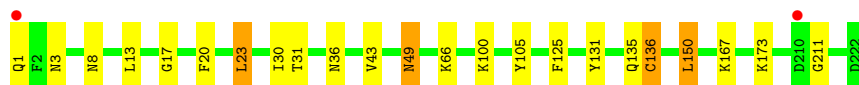
- Molecule 12: Proteasome subunit beta type-6

Chain L:  89% 9%




- Molecule 12: Proteasome subunit beta type-6

Chain Z:  90% 9%




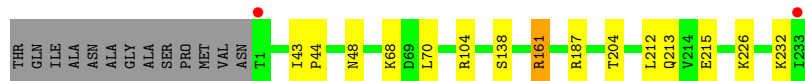
- Molecule 13: Proteasome subunit beta type-7

Chain M:  83% 10% 5%



- Molecule 13: Proteasome subunit beta type-7

Chain a:  89% 6% 5%



- Molecule 14: Proteasome subunit beta type-1

Chain N:  95% 5%

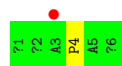
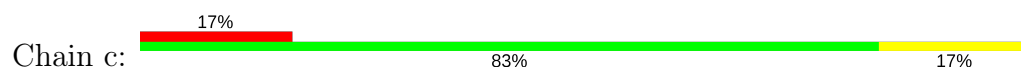


- Molecule 14: Proteasome subunit beta type-1

Chain b:  97%



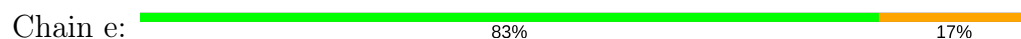
- Molecule 15: N3-APAL-ep



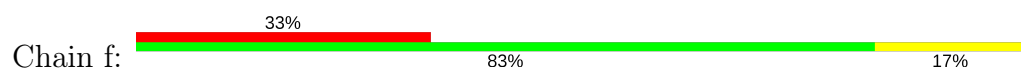
- Molecule 15: N3-APAL-ep



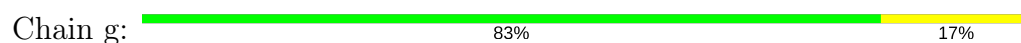
- Molecule 15: N3-APAL-ep



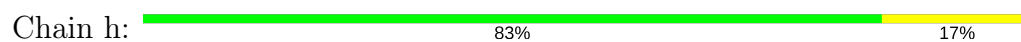
- Molecule 15: N3-APAL-ep



- Molecule 15: N3-APAL-ep



- Molecule 15: N3-APAL-ep



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.32Å 300.79Å 145.46Å 90.00° 113.64° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 15.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (15.00-2.50) 99.2 (15.00-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.201 , 0.214 0.203 , 0.216	Depositor DCC
R_{free} test set	18194 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	49.3	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	50485	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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, 0.333 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: AZI, MG, ACE, CL, MES, 05W

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	0.53	0/2642
1	O	0.27	0/1952	0.53	0/2642
2	B	0.27	0/1934	0.56	0/2618
2	P	0.27	0/1934	0.56	0/2618
3	C	0.28	0/1910	0.57	0/2586
3	Q	0.28	0/1910	0.57	0/2586
4	D	0.27	0/1837	0.55	1/2475 (0.0%)
4	R	0.27	0/1837	0.55	1/2475 (0.0%)
5	E	0.27	0/1800	0.55	0/2433
5	S	0.27	0/1800	0.55	0/2433
6	F	0.28	0/1932	0.50	0/2609
6	T	0.28	0/1932	0.50	0/2609
7	G	0.28	0/1945	0.53	0/2634
7	U	0.28	0/1945	0.53	0/2634
8	H	0.26	0/1715	0.52	0/2326
8	V	0.30	0/1715	0.52	0/2326
9	I	0.27	0/1611	0.53	0/2174
9	W	0.28	0/1611	0.54	0/2174
10	J	0.27	0/1589	0.53	0/2142
10	X	0.27	0/1589	0.53	0/2142
11	K	0.29	0/1681	0.54	0/2274
11	Y	0.31	0/1681	0.55	0/2274
12	L	0.28	0/1795	0.51	0/2420
12	Z	0.27	0/1795	0.51	0/2420
13	M	0.27	0/1855	0.57	1/2514 (0.0%)
13	a	0.28	0/1855	0.58	1/2514 (0.0%)
14	N	0.35	0/1541	0.53	0/2087
14	b	0.32	0/1541	0.52	0/2087
15	c	1.64	1/18 (5.6%)	1.03	0/25
15	d	2.34	1/18 (5.6%)	1.64	0/25
15	e	2.57	1/18 (5.6%)	1.38	0/25
15	f	1.86	1/18 (5.6%)	1.40	0/25

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	g	2.20	1/18 (5.6%)	1.66	0/25
15	h	1.46	1/18 (5.6%)	0.89	0/25
All	All	0.30	6/50302 (0.0%)	0.54	4/68018 (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
9	I	0	1
9	W	0	1
12	L	0	1
12	Z	0	1
All	All	0	4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	e	4	PRO	CA-C	-7.66	1.37	1.52
15	g	4	PRO	CA-C	-6.94	1.39	1.52
15	d	4	PRO	CA-C	-6.83	1.39	1.52
15	f	4	PRO	CA-C	-6.43	1.40	1.52
15	c	4	PRO	CA-C	-5.60	1.41	1.52
15	h	4	PRO	CA-C	-5.51	1.41	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	161	ARG	NE-CZ-NH1	5.30	122.95	120.30
13	M	161	ARG	NE-CZ-NH1	5.28	122.94	120.30
4	D	51	LEU	CA-CB-CG	5.08	126.99	115.30
4	R	51	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	I	192	ASP	Peptide
12	L	135	GLN	Peptide
9	W	192	ASP	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
12	Z	135	GLN	Peptide

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	7	0
1	O	1915	0	1929	8	0
2	B	1904	0	1904	18	0
2	P	1904	0	1904	16	0
3	C	1881	0	1895	16	0
3	Q	1881	0	1895	15	0
4	D	1813	0	1797	12	0
4	R	1813	0	1797	12	0
5	E	1773	0	1775	11	0
5	S	1773	0	1775	10	0
6	F	1892	0	1883	9	0
6	T	1892	0	1883	10	0
7	G	1907	0	1901	11	0
7	U	1907	0	1901	11	0
8	H	1684	0	1685	5	0
8	V	1684	0	1685	5	0
9	I	1581	0	1574	7	0
9	W	1581	0	1574	6	0
10	J	1561	0	1569	9	0
10	X	1561	0	1569	8	0
11	K	1644	0	1592	8	0
11	Y	1644	0	1592	9	0
12	L	1757	0	1711	12	0
12	Z	1757	0	1711	11	0
13	M	1824	0	1832	12	0
13	a	1824	0	1832	0	0
14	N	1512	0	1478	2	0
14	b	1512	0	1479	0	0
15	c	35	0	37	0	0
15	d	35	0	36	0	0
15	e	35	0	36	0	0
15	f	35	0	37	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	g	35	0	36	0	0
15	h	35	0	37	0	0
16	G	1	0	0	0	0
16	I	2	0	0	0	0
16	K	1	0	0	0	0
16	L	1	0	0	0	0
16	N	2	0	0	0	0
16	Z	1	0	0	0	0
17	G	1	0	0	0	0
17	N	1	0	0	0	0
17	U	1	0	0	0	0
17	b	1	0	0	0	0
18	K	12	0	13	0	0
18	g	12	0	13	0	0
19	A	44	0	0	0	0
19	B	37	0	0	0	0
19	C	22	0	0	0	0
19	D	19	0	0	1	0
19	E	19	0	0	0	0
19	F	29	0	0	0	0
19	G	46	0	0	0	0
19	H	55	0	0	0	0
19	I	42	0	0	0	0
19	J	34	0	0	0	0
19	K	43	0	0	0	0
19	L	48	0	0	0	0
19	M	43	0	0	0	0
19	N	37	0	0	1	0
19	O	21	0	0	0	0
19	P	21	0	0	0	0
19	Q	20	0	0	0	0
19	R	16	0	0	0	0
19	S	13	0	0	0	0
19	T	23	0	0	0	0
19	U	30	0	0	0	0
19	V	38	0	0	0	0
19	W	34	0	0	0	0
19	X	31	0	0	0	0
19	Y	34	0	0	0	0
19	Z	41	0	0	0	0
19	a	55	0	0	0	0
19	b	35	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	c	3	0	0	0	0
19	d	2	0	0	0	0
19	e	2	0	0	0	0
19	f	2	0	0	0	0
19	g	2	0	0	0	0
19	h	2	0	0	0	0
All	All	50485	0	49296	237	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (237) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:53:GLN:O	11:Y:57:THR:HG23	1.88	0.73
11:K:53:GLN:O	11:K:57:THR:HG23	1.88	0.72
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.73	0.71
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.72	0.70
3:C:201:VAL:O	3:C:202:GLN:HB2	1.92	0.69
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.73	0.69
3:Q:51:LYS:O	3:Q:52:LEU:HB2	1.92	0.69
2:B:93:HIS:HB3	2:B:113:ARG:HH21	1.58	0.69
3:C:51:LYS:O	3:C:52:LEU:HB2	1.92	0.68
3:Q:201:VAL:O	3:Q:202:GLN:HB2	1.92	0.68
2:P:93:HIS:HB3	2:P:113:ARG:HH21	1.59	0.68
3:Q:202:GLN:HG3	3:Q:203:THR:H	1.57	0.68
3:C:202:GLN:HG3	3:C:203:THR:H	1.58	0.67
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.75	0.67
10:J:126:VAL:HG12	10:J:128:LEU:HG	1.77	0.66
11:Y:100:MET:CE	11:Y:127:PHE:HB2	2.26	0.66
11:K:100:MET:CE	11:K:127:PHE:HB2	2.26	0.66
10:X:126:VAL:HG12	10:X:128:LEU:HG	1.77	0.66
7:G:23:PHE:O	7:G:26:THR:HB	1.96	0.66
7:U:23:PHE:O	7:U:26:THR:HB	1.97	0.64
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.81	0.63
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.80	0.62
5:S:12:PHE:H	6:T:19:GLN:HE22	1.51	0.58
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.51	0.58
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.85	0.58
3:C:201:VAL:O	3:C:202:GLN:CB	2.52	0.57
2:B:146:GLN:HG2	3:C:57:ILE:HG21	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.85	0.57
8:H:52:THR:O	8:H:56:THR:HB	2.06	0.56
13:M:161:ARG:HH11	13:M:161:ARG:HG3	1.69	0.56
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.71	0.56
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.71	0.56
1:A:176:GLU:HG3	2:B:55:LEU:HD22	1.88	0.56
8:V:52:THR:O	8:V:56:THR:HB	2.06	0.56
12:Z:23:LEU:HD13	12:Z:43:VAL:HG13	1.88	0.55
2:B:8:ARG:HD2	3:C:4:ARG:NH2	2.21	0.55
12:L:23:LEU:HD13	12:L:43:VAL:HG13	1.88	0.55
3:C:198:LEU:HA	3:C:201:VAL:HG12	1.88	0.55
3:Q:198:LEU:HA	3:Q:201:VAL:HG12	1.88	0.55
6:T:31:THR:HB	6:T:47:GLU:HG2	1.90	0.54
5:E:12:PHE:H	6:F:19:GLN:HE22	1.56	0.54
6:F:31:THR:HB	6:F:47:GLU:HG2	1.90	0.53
14:N:185:ARG:NH1	19:N:321:HOH:O	2.40	0.53
10:X:1:MET:HA	10:X:34:LYS:CE	2.39	0.53
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.09	0.53
4:D:32:ILE:HD12	4:D:192:VAL:HG23	1.92	0.52
12:L:8:ASN:HA	12:L:30:ILE:O	2.09	0.52
11:Y:106:ARG:HH11	11:Y:106:ARG:HB3	1.74	0.52
11:K:106:ARG:HB3	11:K:106:ARG:HH11	1.74	0.52
4:R:32:ILE:HD12	4:R:192:VAL:HG23	1.91	0.52
4:D:30:ILE:HD12	4:D:196:LEU:HG	1.91	0.52
10:J:1:MET:HA	10:J:34:LYS:HE3	1.91	0.52
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.75	0.52
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.58	0.52
10:J:1:MET:HA	10:J:34:LYS:CE	2.39	0.52
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.75	0.52
3:C:230:TYR:O	3:C:234:ILE:HG13	2.09	0.51
3:Q:230:TYR:O	3:Q:234:ILE:HG13	2.09	0.51
4:R:30:ILE:HD12	4:R:196:LEU:HG	1.91	0.51
3:C:160:GLN:HE22	3:C:170:ARG:HE	1.58	0.51
10:X:1:MET:HA	10:X:34:LYS:HE3	1.90	0.51
2:B:204:ALA:O	2:B:209:ARG:NH2	2.44	0.51
6:F:123:ASN:C	6:F:123:ASN:HD22	2.14	0.51
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.46	0.51
9:I:101:PRO:HB3	9:I:126:ILE:CD1	2.41	0.51
3:Q:160:GLN:HE22	3:Q:170:ARG:HE	1.58	0.51
13:M:127:LEU:HG	13:M:142:LEU:HD12	1.93	0.51
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:100:MET:HE3	11:K:127:PHE:CB	2.40	0.50
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.93	0.50
2:P:204:ALA:O	2:P:209:ARG:NH2	2.44	0.50
4:R:138:GLY:HA2	4:R:214:ILE:HG12	1.93	0.50
6:T:123:ASN:HD22	6:T:123:ASN:C	2.14	0.50
13:M:27:LEU:HD21	13:M:34:LEU:HD22	1.94	0.50
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	1.93	0.50
4:D:138:GLY:HA2	4:D:214:ILE:HG12	1.93	0.49
4:D:99:ILE:HG22	19:D:304:HOH:O	2.12	0.49
12:L:17:GLY:HA3	12:L:20:PHE:CE1	2.48	0.49
11:K:145:LYS:HB2	11:K:148:LEU:HD13	1.93	0.49
8:V:84:LYS:HG3	8:V:85:GLN:N	2.27	0.49
7:G:34:LEU:HD23	7:G:34:LEU:C	2.33	0.49
5:E:68:HIS:HE1	5:E:102:LEU:O	1.96	0.49
9:I:101:PRO:HB3	9:I:126:ILE:HD12	1.94	0.48
12:L:49:ASN:HD21	12:L:211:GLY:HA2	1.78	0.48
6:T:172:LEU:HD13	6:T:195:ILE:HD13	1.95	0.48
12:Z:49:ASN:HD21	12:Z:211:GLY:HA2	1.78	0.48
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.94	0.48
12:Z:17:GLY:HA3	12:Z:20:PHE:CE1	2.48	0.48
4:D:99:ILE:HD13	4:D:104:LEU:HB2	1.96	0.48
6:F:194:LYS:HD3	6:F:242:GLU:HG3	1.96	0.48
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.41	0.48
3:Q:202:GLN:CG	3:Q:203:THR:H	2.26	0.48
5:S:68:HIS:HE1	5:S:102:LEU:O	1.96	0.48
6:F:172:LEU:HD13	6:F:195:ILE:HD13	1.95	0.48
6:T:194:LYS:HD3	6:T:242:GLU:HG3	1.96	0.48
8:V:50:ALA:HB3	9:W:126:ILE:HD12	1.94	0.48
5:E:9:THR:HG21	5:E:119:THR:HA	1.96	0.48
7:U:73:VAL:HG12	7:U:133:THR:HB	1.95	0.48
7:G:73:VAL:HG12	7:G:133:THR:HB	1.96	0.47
4:R:99:ILE:HD13	4:R:104:LEU:HB2	1.96	0.47
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.96	0.47
11:Y:100:MET:HE3	11:Y:127:PHE:CB	2.42	0.47
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.41	0.47
3:C:51:LYS:HA	3:C:51:LYS:HD2	1.73	0.47
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.97	0.47
2:P:59:ASP:HB3	2:P:231:PRO:HG2	1.96	0.47
5:S:9:THR:HG21	5:S:119:THR:HA	1.96	0.47
7:U:34:LEU:C	7:U:34:LEU:HD23	2.34	0.47
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:84:LYS:HG3	8:H:85:GLN:N	2.28	0.47
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.96	0.47
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.97	0.47
2:B:3:ARG:NH1	5:E:122:TYR:OH	2.47	0.47
4:R:185:LEU:O	4:R:189:GLU:HG3	2.15	0.47
2:B:237:ILE:HD12	2:B:240:LYS:HE3	1.97	0.47
1:O:149:GLN:O	1:O:156:TYR:HA	2.15	0.47
1:A:149:GLN:O	1:A:156:TYR:HA	2.15	0.46
2:B:59:ASP:HB3	2:B:231:PRO:HG2	1.97	0.46
7:G:187:GLU:HG2	7:G:192:LYS:HB2	1.97	0.46
2:P:180:LYS:O	2:P:183:MET:HB2	2.16	0.46
13:M:43:ILE:HG21	13:M:64:GLU:HG2	1.97	0.46
4:D:185:LEU:O	4:D:189:GLU:HG3	2.16	0.46
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.96	0.46
13:M:182:ARG:NH2	13:M:215:GLU:O	2.49	0.46
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.46	0.46
7:U:45:ILE:HG22	7:U:216:VAL:HG13	1.98	0.46
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.46	0.45
7:G:195:GLU:HG3	7:G:235:ARG:HG3	1.98	0.45
7:G:45:ILE:HG22	7:G:216:VAL:HG13	1.98	0.45
2:P:237:ILE:HD12	2:P:240:LYS:HE3	1.96	0.45
3:C:38:ASN:N	3:C:38:ASN:HD22	2.15	0.45
7:U:187:GLU:HG2	7:U:192:LYS:HB2	1.97	0.45
2:B:180:LYS:O	2:B:183:MET:HB2	2.16	0.45
7:U:195:GLU:HG3	7:U:235:ARG:HG3	1.98	0.45
1:A:50:LYS:O	1:A:50:LYS:HG3	2.17	0.45
2:B:151:ASN:HB2	2:B:152:PRO:HD2	1.98	0.45
3:Q:38:ASN:N	3:Q:38:ASN:HD22	2.15	0.45
2:P:151:ASN:HB2	2:P:152:PRO:HD2	1.99	0.45
4:R:51:LEU:C	4:R:51:LEU:HD12	2.37	0.44
7:U:227:LEU:HB3	7:U:231:ASN:HB2	1.99	0.44
5:S:87:LEU:HD21	5:S:107:ALA:HB1	2.00	0.44
5:E:155:LEU:HD13	5:E:158:THR:HB	2.00	0.44
5:E:226:GLY:O	5:E:229:VAL:HG22	2.18	0.44
5:S:155:LEU:HD13	5:S:158:THR:HB	2.00	0.44
5:S:136:TYR:CE1	5:S:217:LYS:HA	2.52	0.44
1:A:247:LEU:O	1:A:250:LEU:HB2	2.18	0.44
13:M:43:ILE:HA	13:M:44:PRO:HD3	1.91	0.44
10:X:3:ILE:HD12	10:X:176:PHE:CD2	2.53	0.44
5:E:87:LEU:HD21	5:E:107:ALA:HB1	2.00	0.44
5:E:136:TYR:CE1	5:E:217:LYS:HA	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:227:LEU:HB3	7:G:231:ASN:HB2	1.99	0.43
3:Q:51:LYS:HA	3:Q:51:LYS:HD2	1.74	0.43
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.53	0.43
5:S:226:GLY:O	5:S:229:VAL:HG22	2.17	0.43
1:O:12:PHE:H	2:P:20:GLN:HE22	1.66	0.43
10:J:3:ILE:HD12	10:J:176:PHE:CD2	2.53	0.43
1:O:50:LYS:HG3	1:O:50:LYS:O	2.18	0.43
4:D:37:GLY:HA2	4:D:145:TYR:CE1	2.54	0.43
1:O:247:LEU:O	1:O:250:LEU:HB2	2.18	0.43
2:P:37:ILE:HD12	2:P:192:ALA:HB2	2.01	0.43
2:B:37:ILE:HD12	2:B:192:ALA:HB2	2.00	0.43
12:L:136:CYS:SG	12:L:150:LEU:HB3	2.58	0.43
4:R:37:GLY:HA2	4:R:145:TYR:CE1	2.54	0.43
4:D:51:LEU:C	4:D:51:LEU:HD12	2.38	0.43
1:O:122:THR:CG2	2:P:128:ARG:HH21	2.31	0.43
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.54	0.42
11:K:6:PHE:HA	11:K:125:ASP:O	2.19	0.42
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.83	0.42
13:M:27:LEU:HB2	13:M:192:SER:HB3	2.02	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.83	0.42
6:F:68:ARG:NH1	13:M:72:THR:OG1	2.49	0.42
11:Y:6:PHE:HA	11:Y:125:ASP:O	2.19	0.42
3:Q:11:PRO:HA	4:R:18:TYR:CD1	2.54	0.42
2:B:93:HIS:CG	2:B:113:ARG:HE	2.37	0.42
6:T:238:PHE:O	6:T:242:GLU:HG2	2.20	0.42
6:T:34:ILE:HG22	6:T:160:ALA:HB2	2.02	0.42
2:P:95:GLN:HB3	9:W:68:TYR:CD2	2.55	0.42
13:M:25:ASP:HA	13:M:195:PHE:CB	2.49	0.42
2:P:93:HIS:CG	2:P:113:ARG:HE	2.37	0.42
3:C:202:GLN:CG	3:C:203:THR:H	2.26	0.42
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.54	0.42
10:J:193:ASP:OD1	10:J:193:ASP:N	2.52	0.42
1:A:115:ALA:HB1	1:A:154:GLY:O	2.20	0.42
6:F:238:PHE:O	6:F:242:GLU:HG2	2.19	0.42
13:M:93:PHE:CE2	13:M:128:ARG:HD3	2.54	0.42
4:R:99:ILE:CD1	4:R:104:LEU:HB2	2.50	0.42
12:Z:100:LYS:HD3	12:Z:105:TYR:CE2	2.55	0.41
12:Z:136:CYS:SG	12:Z:150:LEU:HB3	2.60	0.41
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.54	0.41
12:L:100:LYS:HD3	12:L:105:TYR:CE2	2.55	0.41
7:U:78:ILE:N	7:U:79:PRO:CD	2.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:177:LYS:NZ	10:X:169:GLU:O	2.53	0.41
12:Z:100:LYS:HD3	12:Z:105:TYR:CZ	2.55	0.41
1:A:110:LEU:O	1:A:114:VAL:HG23	2.20	0.41
7:G:170:THR:O	7:G:174:GLU:HG3	2.20	0.41
1:O:115:ALA:HB1	1:O:154:GLY:O	2.20	0.41
10:J:174:MET:HA	10:X:174:MET:HA	2.02	0.41
9:I:7:ASN:HA	9:I:29:GLY:O	2.21	0.41
6:T:13:PRO:O	7:U:24:LYS:HD2	2.21	0.41
12:L:4:PRO:O	13:M:104:ARG:NH1	2.49	0.41
6:T:165:ARG:HG2	6:T:166:GLN:N	2.36	0.41
6:F:34:ILE:HG22	6:F:160:ALA:HB2	2.02	0.41
12:L:100:LYS:HD3	12:L:105:TYR:CZ	2.56	0.41
8:V:80:LEU:HD12	8:V:113:ILE:HD11	2.03	0.41
2:B:12:PHE:H	3:C:17:GLN:HE22	1.68	0.41
5:E:28:ILE:HD11	5:E:148:PRO:CD	2.50	0.41
9:I:123:PHE:HA	9:I:128:CYS:O	2.20	0.41
7:U:25:ALA:O	7:U:28:GLN:HB2	2.21	0.41
10:X:3:ILE:HD12	10:X:176:PHE:CG	2.55	0.41
11:Y:86:LEU:HD13	11:Y:86:LEU:C	2.42	0.41
2:B:139:TYR:CE2	2:B:144:GLY:HA2	2.56	0.41
4:D:99:ILE:CD1	4:D:104:LEU:HB2	2.50	0.41
4:D:71:SER:HB3	4:D:164:ILE:HD12	2.03	0.41
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.56	0.41
9:W:123:PHE:HA	9:W:128:CYS:O	2.21	0.41
11:Y:176:ASN:ND2	11:Y:187:TYR:OH	2.54	0.41
7:G:25:ALA:O	7:G:28:GLN:HB2	2.21	0.40
7:G:101:TYR:OH	8:H:66:HIS:HE1	2.04	0.40
8:H:80:LEU:HD12	8:H:113:ILE:HD11	2.03	0.40
5:S:28:ILE:HD11	5:S:148:PRO:CD	2.50	0.40
7:U:170:THR:O	7:U:174:GLU:HG3	2.21	0.40
9:W:26:LEU:HD21	9:W:185:VAL:HG23	2.03	0.40
3:C:35:LYS:HG2	3:C:158:SER:O	2.21	0.40
6:F:165:ARG:HG2	6:F:166:GLN:N	2.36	0.40
11:K:86:LEU:HD13	11:K:86:LEU:C	2.42	0.40
2:P:139:TYR:CE2	2:P:144:GLY:HA2	2.57	0.40
9:I:26:LEU:HD21	9:I:185:VAL:HG23	2.03	0.40
13:M:96:LEU:O	13:M:100:MET:HG2	2.22	0.40
3:Q:168:THR:O	3:Q:171:GLU:HB3	2.21	0.40
1:A:122:THR:CG2	2:B:128:ARG:HH21	2.35	0.40
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.57	0.40
5:E:61:LYS:O	5:E:72:SER:HA	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:13:ILE:HG21	14:N:175:MET:CE	2.52	0.40
1:O:110:LEU:O	1:O:114:VAL:HG23	2.22	0.40
2:P:3:ARG:HG3	3:Q:4:ARG:CZ	2.51	0.40
5:S:70:GLY:HA3	5:S:221:PHE:CE2	2.57	0.40
6:T:78:ILE:HB	6:T:79:PRO:HD3	2.04	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%)	7 (3%)	2 (1%)	22	39
1	O	248/250 (99%)	239 (96%)	7 (3%)	2 (1%)	22	39
2	B	242/258 (94%)	230 (95%)	9 (4%)	3 (1%)	15	27
2	P	242/258 (94%)	230 (95%)	9 (4%)	3 (1%)	15	27
3	C	238/254 (94%)	227 (95%)	6 (2%)	5 (2%)	8	13
3	Q	238/254 (94%)	227 (95%)	6 (2%)	5 (2%)	8	13
4	D	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
4	R	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
5	E	229/234 (98%)	217 (95%)	12 (5%)	0	100	100
5	S	229/234 (98%)	217 (95%)	12 (5%)	0	100	100
6	F	241/288 (84%)	233 (97%)	8 (3%)	0	100	100
6	T	241/288 (84%)	233 (97%)	8 (3%)	0	100	100
7	G	239/252 (95%)	236 (99%)	2 (1%)	1 (0%)	38	59
7	U	239/252 (95%)	235 (98%)	3 (1%)	1 (0%)	38	59
8	H	220/232 (95%)	214 (97%)	5 (2%)	1 (0%)	32	53
8	V	220/232 (95%)	214 (97%)	5 (2%)	1 (0%)	32	53

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
9	W	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
10	J	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	32	53
10	X	193/198 (98%)	189 (98%)	3 (2%)	1 (0%)	32	53
11	K	210/212 (99%)	205 (98%)	4 (2%)	1 (0%)	32	53
11	Y	210/212 (99%)	204 (97%)	5 (2%)	1 (0%)	32	53
12	L	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
12	Z	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
13	M	231/246 (94%)	224 (97%)	7 (3%)	0	100	100
13	a	231/246 (94%)	224 (97%)	7 (3%)	0	100	100
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
14	b	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
15	c	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
15	d	2/6 (33%)	1 (50%)	0	1 (50%)	0	0
15	e	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
15	f	2/6 (33%)	2 (100%)	0	0	100	100
15	g	2/6 (33%)	2 (100%)	0	0	100	100
15	h	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
All	All	6288/6650 (95%)	6084 (97%)	175 (3%)	29 (0%)	32	53

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
2	B	52	THR
3	C	202	GLN
3	C	205	ALA
1	O	2	THR
2	P	52	THR
3	Q	202	GLN
3	Q	205	ALA
2	B	51	VAL
3	C	38	ASN
8	H	9	ASN
10	J	2	ASP
2	P	51	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	Q	38	ASN
8	V	9	ASN
10	X	2	ASP
11	K	9	GLN
11	Y	9	GLN
2	B	221	ASP
3	C	183	PRO
2	P	221	ASP
3	Q	183	PRO
15	d	3	ALA
3	C	206	LYS
3	Q	206	LYS
1	A	166	LYS
1	O	166	LYS
7	G	51	PRO
7	U	51	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%)	199 (95%)	10 (5%)	30	53
1	O	209/209 (100%)	199 (95%)	10 (5%)	30	53
2	B	203/216 (94%)	191 (94%)	12 (6%)	23	42
2	P	203/216 (94%)	191 (94%)	12 (6%)	23	42
3	C	212/226 (94%)	195 (92%)	17 (8%)	14	27
3	Q	212/226 (94%)	195 (92%)	17 (8%)	14	27
4	D	194/215 (90%)	177 (91%)	17 (9%)	12	22
4	R	194/215 (90%)	177 (91%)	17 (9%)	12	22
5	E	190/193 (98%)	170 (90%)	20 (10%)	8	15
5	S	190/193 (98%)	170 (90%)	20 (10%)	8	15
6	F	201/239 (84%)	184 (92%)	17 (8%)	12	23

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	T	201/239 (84%)	184 (92%)	17 (8%)	12	23
7	G	206/210 (98%)	190 (92%)	16 (8%)	15	28
7	U	206/210 (98%)	190 (92%)	16 (8%)	15	28
8	H	181/190 (95%)	174 (96%)	7 (4%)	37	63
8	V	181/190 (95%)	174 (96%)	7 (4%)	37	63
9	I	172/173 (99%)	167 (97%)	5 (3%)	48	75
9	W	172/173 (99%)	167 (97%)	5 (3%)	48	75
10	J	173/175 (99%)	165 (95%)	8 (5%)	31	55
10	X	173/175 (99%)	165 (95%)	8 (5%)	31	55
11	K	169/169 (100%)	163 (96%)	6 (4%)	40	67
11	Y	169/169 (100%)	163 (96%)	6 (4%)	40	67
12	L	185/185 (100%)	176 (95%)	9 (5%)	29	52
12	Z	185/185 (100%)	176 (95%)	9 (5%)	29	52
13	M	199/208 (96%)	183 (92%)	16 (8%)	14	27
13	a	199/208 (96%)	184 (92%)	15 (8%)	16	29
14	N	162/162 (100%)	156 (96%)	6 (4%)	39	66
14	b	162/162 (100%)	156 (96%)	6 (4%)	39	66
15	c	1/1 (100%)	1 (100%)	0	100	100
15	d	1/1 (100%)	1 (100%)	0	100	100
15	e	1/1 (100%)	0	1 (100%)	0	0
15	f	1/1 (100%)	1 (100%)	0	100	100
15	g	1/1 (100%)	1 (100%)	0	100	100
15	h	1/1 (100%)	1 (100%)	0	100	100
All	All	5318/5546 (96%)	4986 (94%)	332 (6%)	21	39

All (332) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	17	LYS
1	A	30	GLN
1	A	50	LYS
1	A	59	GLU
1	A	61	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	122	THR
1	A	157	PHE
1	A	231	LYS
1	A	250	LEU
2	B	50	LYS
2	B	54	THR
2	B	55	LEU
2	B	56	LEU
2	B	58	GLN
2	B	119	GLN
2	B	180	LYS
2	B	183	MET
2	B	184	LYS
2	B	191	LEU
2	B	209	ARG
2	B	244	THR
3	C	4	ARG
3	C	38	ASN
3	C	51	LYS
3	C	55	THR
3	C	61	LYS
3	C	77	ASN
3	C	116	GLN
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	175	LYS
3	C	180	LYS
3	C	187	GLU
3	C	203	THR
3	C	225	GLU
3	C	239	GLN
3	C	240	GLU
4	D	20	LEU
4	D	40	LEU
4	D	51	LEU
4	D	54	ASP
4	D	60	VAL
4	D	99	ILE
4	D	117	GLU
4	D	125	LEU
4	D	176	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	190	LEU
4	D	193	LEU
4	D	202	GLU
4	D	214	ILE
4	D	224	ASP
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	3	ASN
5	E	4	ASN
5	E	8	ASP
5	E	9	THR
5	E	10	VAL
5	E	25	LEU
5	E	29	LYS
5	E	55	LEU
5	E	60	LYS
5	E	61	LYS
5	E	71	LEU
5	E	92	ASN
5	E	116	GLN
5	E	179	ILE
5	E	180	LYS
5	E	184	ASN
5	E	188	LEU
5	E	207	VAL
5	E	219	THR
5	E	231	LYS
6	F	14	ASP
6	F	47	GLU
6	F	59	LYS
6	F	94	SER
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	148	GLU
6	F	165	ARG
6	F	172	LEU
6	F	181	GLU
6	F	187	GLU
6	F	203	ASN
6	F	206	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	214	TRP
6	F	221	ASN
6	F	228	LYS
7	G	26	THR
7	G	28	GLN
7	G	34	LEU
7	G	83	ASN
7	G	98	LYS
7	G	115	LEU
7	G	117	GLN
7	G	122	ARG
7	G	125	MET
7	G	165	LYS
7	G	166	GLN
7	G	181	LYS
7	G	183	ASP
7	G	230	GLU
7	G	235	ARG
7	G	236	LEU
8	H	30	ASN
8	H	34	LEU
8	H	56	THR
8	H	68	LEU
8	H	127	LEU
8	H	196	ARG
8	H	198	GLU
9	I	37	ASN
9	I	114	LYS
9	I	171	LEU
9	I	182	TRP
9	I	192	ASP
10	J	2	ASP
10	J	23	ARG
10	J	35	THR
10	J	75	LEU
10	J	78	GLN
10	J	144	LEU
10	J	163	LEU
10	J	174	MET
11	K	4	LEU
11	K	9	GLN
11	K	35	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	K	57	THR
11	K	106	ARG
11	K	148	LEU
12	L	1	GLN
12	L	3	ASN
12	L	23	LEU
12	L	49	ASN
12	L	66	LYS
12	L	136	CYS
12	L	150	LEU
12	L	167	LYS
12	L	173	LYS
13	M	43	ILE
13	M	44	PRO
13	M	48	ASN
13	M	68	LYS
13	M	70	LEU
13	M	79	PRO
13	M	104	ARG
13	M	138	SER
13	M	161	ARG
13	M	187	ARG
13	M	204	THR
13	M	212	LEU
13	M	213	GLN
13	M	215	GLU
13	M	226	LYS
13	M	232	LYS
14	N	21	THR
14	N	22	THR
14	N	36	ARG
14	N	39	ASP
14	N	119	VAL
14	N	178	LEU
1	O	2	THR
1	O	17	LYS
1	O	30	GLN
1	O	50	LYS
1	O	59	GLU
1	O	61	LEU
1	O	122	THR
1	O	157	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	231	LYS
1	O	250	LEU
2	P	50	LYS
2	P	54	THR
2	P	55	LEU
2	P	56	LEU
2	P	58	GLN
2	P	119	GLN
2	P	180	LYS
2	P	183	MET
2	P	184	LYS
2	P	191	LEU
2	P	209	ARG
2	P	244	THR
3	Q	4	ARG
3	Q	38	ASN
3	Q	51	LYS
3	Q	55	THR
3	Q	61	LYS
3	Q	77	ASN
3	Q	116	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	175	LYS
3	Q	180	LYS
3	Q	187	GLU
3	Q	203	THR
3	Q	225	GLU
3	Q	239	GLN
3	Q	240	GLU
4	R	20	LEU
4	R	40	LEU
4	R	51	LEU
4	R	54	ASP
4	R	60	VAL
4	R	99	ILE
4	R	117	GLU
4	R	125	LEU
4	R	176	LEU
4	R	190	LEU
4	R	193	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	R	202	GLU
4	R	214	ILE
4	R	224	ASP
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	3	ASN
5	S	4	ASN
5	S	8	ASP
5	S	9	THR
5	S	10	VAL
5	S	25	LEU
5	S	29	LYS
5	S	55	LEU
5	S	60	LYS
5	S	61	LYS
5	S	71	LEU
5	S	92	ASN
5	S	116	GLN
5	S	179	ILE
5	S	180	LYS
5	S	184	ASN
5	S	188	LEU
5	S	207	VAL
5	S	219	THR
5	S	231	LYS
6	T	14	ASP
6	T	47	GLU
6	T	59	LYS
6	T	94	SER
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	148	GLU
6	T	165	ARG
6	T	172	LEU
6	T	181	GLU
6	T	187	GLU
6	T	203	ASN
6	T	206	LYS
6	T	214	TRP
6	T	221	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	T	228	LYS
7	U	26	THR
7	U	28	GLN
7	U	34	LEU
7	U	83	ASN
7	U	98	LYS
7	U	115	LEU
7	U	117	GLN
7	U	122	ARG
7	U	125	MET
7	U	165	LYS
7	U	166	GLN
7	U	181	LYS
7	U	183	ASP
7	U	230	GLU
7	U	235	ARG
7	U	236	LEU
8	V	30	ASN
8	V	34	LEU
8	V	56	THR
8	V	68	LEU
8	V	127	LEU
8	V	196	ARG
8	V	198	GLU
9	W	37	ASN
9	W	114	LYS
9	W	171	LEU
9	W	182	TRP
9	W	192	ASP
10	X	2	ASP
10	X	23	ARG
10	X	35	THR
10	X	75	LEU
10	X	78	GLN
10	X	144	LEU
10	X	163	LEU
10	X	174	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	35	ILE
11	Y	57	THR
11	Y	106	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	Y	148	LEU
12	Z	1	GLN
12	Z	3	ASN
12	Z	23	LEU
12	Z	49	ASN
12	Z	66	LYS
12	Z	136	CYS
12	Z	150	LEU
12	Z	167	LYS
12	Z	173	LYS
13	a	43	ILE
13	a	44	PRO
13	a	48	ASN
13	a	68	LYS
13	a	70	LEU
13	a	104	ARG
13	a	138	SER
13	a	161	ARG
13	a	187	ARG
13	a	204	THR
13	a	212	LEU
13	a	213	GLN
13	a	215	GLU
13	a	226	LYS
13	a	232	LYS
14	b	21	THR
14	b	22	THR
14	b	36	ARG
14	b	39	ASP
14	b	119	VAL
14	b	178	LEU
15	e	4	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (119) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	155	ASN
2	B	176	GLN
3	C	38	ASN
3	C	77	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	100	ASN
4	D	210	GLN
4	D	225	ASN
5	E	68	HIS
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
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	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	167	GLN
7	G	175	ASN
7	G	186	ASN
8	H	30	ASN
8	H	57	GLN
8	H	66	HIS
8	H	172	ASN
8	H	189	ASN
9	I	37	ASN
10	J	55	GLN
10	J	118	GLN
10	J	191	GLN
11	K	85	ASN
11	K	176	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	L	3	ASN
12	L	36	ASN
12	L	49	ASN
12	L	80	ASN
12	L	158	ASN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	69	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	38	ASN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	100	ASN
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	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	83	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	167	GLN
7	U	175	ASN
7	U	186	ASN
8	V	30	ASN
8	V	57	GLN
8	V	165	ASN
8	V	172	ASN
8	V	189	ASN
10	X	55	GLN
10	X	86	GLN
10	X	191	GLN
11	Y	85	ASN
11	Y	176	ASN
12	Z	3	ASN
12	Z	36	ASN
12	Z	49	ASN
12	Z	80	ASN
12	Z	95	HIS
12	Z	158	ASN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	179	ASN
13	a	194	ASN
14	b	38	HIS
14	b	161	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 12 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
18	MES	K	302	-	12,12,12	2.10	1 (8%)	14,16,16	1.69	3 (21%)
18	MES	g	101	-	12,12,12	2.14	1 (8%)	14,16,16	1.62	3 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	MES	K	302	-	-	0/6/14/14	0/1/1/1
18	MES	g	101	-	-	0/6/14/14	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	g	101	MES	C8-S	-7.14	1.66	1.77
18	K	302	MES	C8-S	-6.95	1.67	1.77

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	g	101	MES	O1S-S-C8	2.20	108.68	106.79
18	K	302	MES	O1S-S-C8	2.81	109.21	106.79
18	g	101	MES	O3S-S-C8	2.96	109.70	106.06
18	K	302	MES	O2S-S-C8	3.05	109.41	106.79
18	K	302	MES	O3S-S-C8	3.69	110.60	106.06
18	g	101	MES	O2S-S-C8	3.81	110.07	106.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.20	6 (2%) 59 61	30, 48, 79, 122	0
1	O	250/250 (100%)	-0.10	8 (3%) 48 51	34, 55, 94, 128	0
2	B	244/258 (94%)	-0.04	16 (6%) 19 19	32, 52, 101, 146	0
2	P	244/258 (94%)	0.06	14 (5%) 24 25	37, 56, 104, 151	0
3	C	240/254 (94%)	0.11	19 (7%) 13 13	32, 55, 119, 144	0
3	Q	240/254 (94%)	0.40	26 (10%) 6 6	36, 68, 144, 165	0
4	D	235/260 (90%)	-0.11	4 (1%) 70 72	34, 57, 90, 141	0
4	R	235/260 (90%)	-0.09	4 (1%) 70 72	37, 59, 98, 144	0
5	E	231/234 (98%)	-0.01	9 (3%) 40 42	38, 60, 92, 132	0
5	S	231/234 (98%)	0.04	10 (4%) 36 38	39, 63, 104, 141	0
6	F	243/288 (84%)	-0.13	11 (4%) 34 36	32, 52, 101, 129	0
6	T	243/288 (84%)	-0.11	9 (3%) 42 44	32, 54, 101, 142	0
7	G	241/252 (95%)	-0.14	8 (3%) 47 50	26, 48, 83, 132	0
7	U	241/252 (95%)	-0.21	7 (2%) 52 55	33, 50, 82, 107	0
8	H	222/232 (95%)	-0.31	3 (1%) 75 76	31, 45, 70, 111	0
8	V	222/232 (95%)	-0.26	2 (0%) 84 85	33, 49, 73, 130	0
9	I	204/205 (99%)	-0.51	1 (0%) 90 91	29, 42, 67, 94	0
9	W	204/205 (99%)	-0.47	2 (0%) 82 83	26, 44, 74, 106	0
10	J	195/198 (98%)	-0.37	2 (1%) 82 83	27, 45, 72, 130	0
10	X	195/198 (98%)	-0.34	3 (1%) 74 75	31, 48, 73, 140	0
11	K	212/212 (100%)	-0.34	0 100 100	30, 44, 72, 96	0
11	Y	212/212 (100%)	-0.42	2 (0%) 84 85	33, 45, 74, 99	0
12	L	222/222 (100%)	-0.41	0 100 100	30, 46, 73, 90	0
12	Z	222/222 (100%)	-0.40	2 (0%) 84 85	30, 45, 73, 97	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%)	-0.43	3 (1%) 77 78	29, 44, 67, 104	0
13	a	233/246 (94%)	-0.41	2 (0%) 84 85	29, 43, 67, 108	0
14	N	196/196 (100%)	-0.48	2 (1%) 82 83	27, 40, 66, 96	0
14	b	196/196 (100%)	-0.41	2 (1%) 82 83	28, 41, 67, 95	0
15	c	3/6 (50%)	0.94	1 (33%) 0 0	53, 53, 55, 65	0
15	d	3/6 (50%)	-0.03	0 100 100	41, 41, 50, 60	0
15	e	3/6 (50%)	-0.60	0 100 100	33, 33, 40, 47	0
15	f	3/6 (50%)	2.56	2 (66%) 0 0	61, 61, 61, 64	0
15	g	3/6 (50%)	-0.62	0 100 100	38, 38, 54, 63	0
15	h	3/6 (50%)	-0.68	0 100 100	41, 41, 44, 49	0
All	All	6354/6650 (95%)	-0.20	180 (2%) 53 56	26, 50, 93, 165	0

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	219	ALA	9.3
3	Q	49	THR	9.2
3	Q	50	LEU	8.4
2	P	51	VAL	7.3
2	B	219	ALA	7.0
3	Q	206	LYS	6.5
3	C	49	THR	6.2
2	B	218	GLY	5.7
3	C	206	LYS	5.6
2	B	51	VAL	5.3
1	O	52	SER	5.2
3	C	238	LYS	5.2
4	D	242	GLU	5.2
5	S	202	ASP	5.1
10	X	194	ASP	5.1
4	R	241	ALA	5.1
1	A	1	MET	5.1
6	F	2	THR	5.0
2	P	218	GLY	4.9
5	E	202	ASP	4.9
3	Q	204	GLY	4.8
2	B	220	ASN	4.7
3	Q	238	LYS	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
10	J	1	MET	4.6
1	O	1	MET	4.6
3	C	202	GLN	4.6
10	J	194	ASP	4.6
3	Q	48	SER	4.5
4	D	241	ALA	4.4
3	Q	51	LYS	4.3
6	T	243	ILE	4.3
8	V	222	ASP	4.3
2	B	222	GLY	4.2
13	a	1	THR	4.2
3	Q	221	ALA	4.1
3	Q	223	SER	4.1
9	W	1	SER	4.1
1	O	201	GLU	4.1
6	T	2	THR	4.1
2	P	221	ASP	4.0
1	A	250	LEU	4.0
2	P	59	ASP	4.0
13	M	1	THR	3.9
15	f	3	ALA	3.9
3	Q	239	GLN	3.9
6	F	205	GLU	3.9
3	Q	240	GLU	3.9
2	P	220	ASN	3.8
2	P	52	THR	3.7
7	G	242	GLN	3.7
1	A	249	ALA	3.7
3	Q	203	THR	3.7
6	F	202	ASP	3.7
3	C	50	LEU	3.6
3	Q	234	ILE	3.5
2	B	221	ASP	3.5
1	A	2	THR	3.5
3	C	239	GLN	3.5
4	R	242	GLU	3.4
5	S	165	GLN	3.4
6	T	241	LYS	3.4
8	H	222	ASP	3.4
6	T	215	CYS	3.4
7	U	242	GLN	3.3
3	Q	236	GLN	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	F	244	ASN	3.3
6	T	244	ASN	3.3
15	c	3	ALA	3.2
1	O	53	SER	3.2
3	C	225	GLU	3.2
10	X	193	ASP	3.2
3	C	240	GLU	3.2
7	U	2	GLY	3.2
7	U	241	GLU	3.2
7	G	181	LYS	3.2
3	Q	47	ARG	3.2
3	C	48	SER	3.1
3	C	236	GLN	3.1
2	B	50	LYS	3.1
2	B	203	SER	3.1
2	B	244	THR	3.1
3	Q	205	ALA	3.1
3	Q	202	GLN	3.0
10	X	1	MET	3.0
7	G	240	ALA	3.0
6	F	215	CYS	3.0
5	S	233	ILE	3.0
7	G	2	GLY	3.0
5	E	233	ILE	2.9
7	G	3	TYR	2.9
6	F	243	ILE	2.9
6	T	181	GLU	2.9
3	Q	55	THR	2.9
13	a	233	ILE	2.9
3	C	235	GLU	2.8
5	S	225	ASP	2.8
3	Q	175	LYS	2.8
5	S	201	ARG	2.8
11	Y	106	ARG	2.7
3	C	171	GLU	2.7
1	O	2	THR	2.7
1	O	250	LEU	2.7
13	M	47	ASP	2.7
6	F	201	GLU	2.7
7	U	222	ASP	2.7
7	G	241	GLU	2.7
2	B	230	LYS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	S	169	THR	2.6
2	B	61	SER	2.6
2	P	222	GLY	2.6
2	B	60	THR	2.5
2	P	60	THR	2.5
6	T	205	GLU	2.5
3	C	180	LYS	2.5
14	N	105	LYS	2.5
2	P	182	ASP	2.5
3	C	1	GLY	2.5
2	P	203	SER	2.5
3	Q	235	GLU	2.5
3	C	203	THR	2.5
14	b	105	LYS	2.5
1	O	249	ALA	2.5
3	Q	179	ARG	2.4
14	b	195	GLN	2.4
5	S	122	TYR	2.4
5	S	210	LEU	2.4
3	Q	180	LYS	2.4
7	U	203	ASP	2.4
6	F	181	GLU	2.4
1	A	52	SER	2.4
12	Z	1	GLN	2.4
6	F	203	ASN	2.4
11	Y	212	GLY	2.4
12	Z	210	ASP	2.4
3	Q	141	ASP	2.3
3	C	216	ASP	2.3
8	H	221	CYS	2.3
15	f	5	ALA	2.3
3	C	60	SER	2.3
5	E	163	ARG	2.3
2	B	217	LYS	2.3
6	T	59	LYS	2.3
4	D	1	ASP	2.3
7	G	222	ASP	2.3
3	C	228	ASN	2.3
5	S	30	GLN	2.2
1	A	248	GLU	2.2
5	E	54	GLU	2.2
1	O	248	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	V	221	CYS	2.2
7	U	51	PRO	2.2
2	B	201	ASP	2.2
5	E	180	LYS	2.2
5	E	210	LEU	2.2
3	Q	60	SER	2.2
5	E	123	GLY	2.2
7	G	17	TYR	2.1
6	T	230	ASP	2.1
2	B	181	ASP	2.1
9	W	191	LYS	2.1
13	M	82	ASP	2.1
4	D	238	LYS	2.1
8	H	219	ASN	2.1
5	S	123	GLY	2.1
3	Q	59	PRO	2.1
4	R	125	LEU	2.1
2	P	93	HIS	2.1
3	C	175	LYS	2.1
2	B	52	THR	2.1
9	I	133	LYS	2.1
2	P	177	MET	2.1
4	R	201	GLU	2.1
6	F	166	GLN	2.1
7	U	3	TYR	2.0
6	F	206	LYS	2.0
5	E	201	ARG	2.0
3	Q	187	GLU	2.0
5	E	3	ASN	2.0
2	P	240	LYS	2.0
14	N	195	GLN	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

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
18	MES	g	101	12/12	0.90	0.22	5.42	59,68,73,76	0
16	MG	Z	301	1/1	0.95	0.29	4.46	56,56,56,56	0
16	MG	I	301	1/1	0.94	0.28	3.64	58,58,58,58	0
18	MES	K	302	12/12	0.92	0.20	3.18	63,72,75,78	0
17	CL	b	201	1/1	0.97	0.13	1.26	30,30,30,30	0
16	MG	N	201	1/1	0.92	0.12	0.50	45,45,45,45	0
16	MG	L	301	1/1	0.95	0.11	-0.99	55,55,55,55	0
16	MG	G	301	1/1	0.96	0.08	-1.34	41,41,41,41	0
16	MG	I	302	1/1	0.99	0.07	-1.46	46,46,46,46	0
16	MG	K	301	1/1	0.96	0.06	-2.03	44,44,44,44	0
17	CL	N	203	1/1	0.99	0.04	-4.46	30,30,30,30	0
17	CL	G	302	1/1	0.98	0.11	-	30,30,30,30	0
16	MG	N	202	1/1	0.83	0.21	-	59,59,59,59	0
17	CL	U	301	1/1	0.99	0.19	-	30,30,30,30	0

6.5 Other polymers

There are no such residues in this entry.