



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 03:16 AM UTC

PDB ID : 6HWF / pdb_00006hwf
Title : Yeast 20S proteasome beta2-G45A mutant in complex with ONX 0914
Authors : Huber, E.M.; Groll, M.
Deposited on : 2018-10-11
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : ?? (??), CSD ??CSD?? (????)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

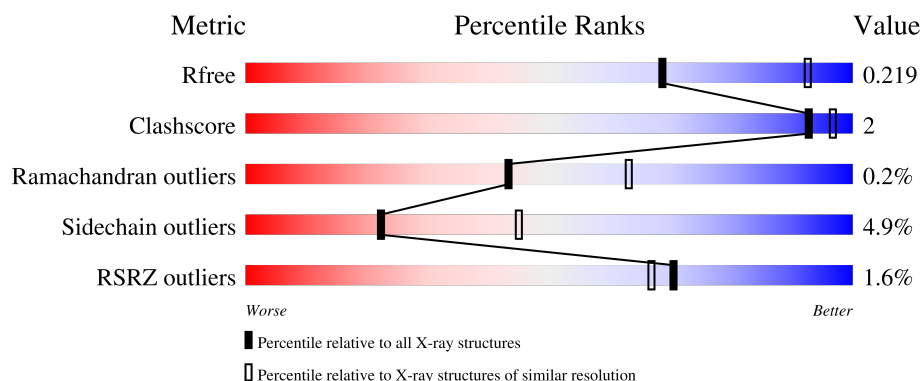
1 Overall quality at a glance

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	 2% 95% 5%
1	O	250	 2% 96% .
2	B	258	 3% 86% 8% 5%
2	P	258	 3% 87% 7% 5%
3	C	254	 2% 87% 6% . 6%

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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	

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 50758 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
			1720	1083	298	332	7			
8	V	226	Total	C	N	O	S	0	0	0
			1720	1083	298	332	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	45	ALA	GLY	engineered mutation	UNP P25043
V	45	ALA	GLY	engineered mutation	UNP P25043

- 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			
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			

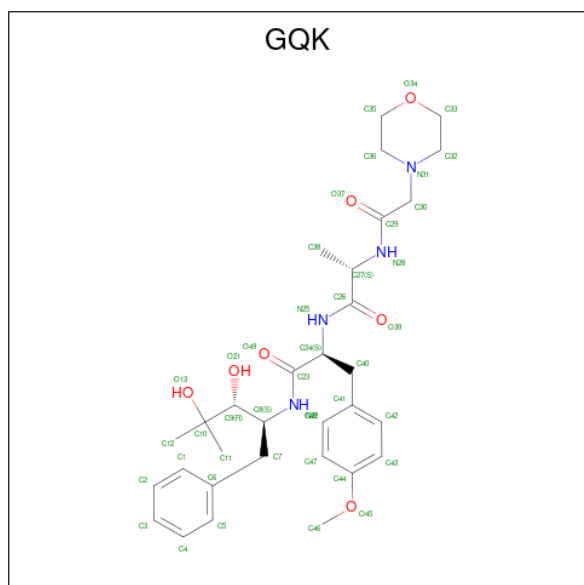
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 16 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

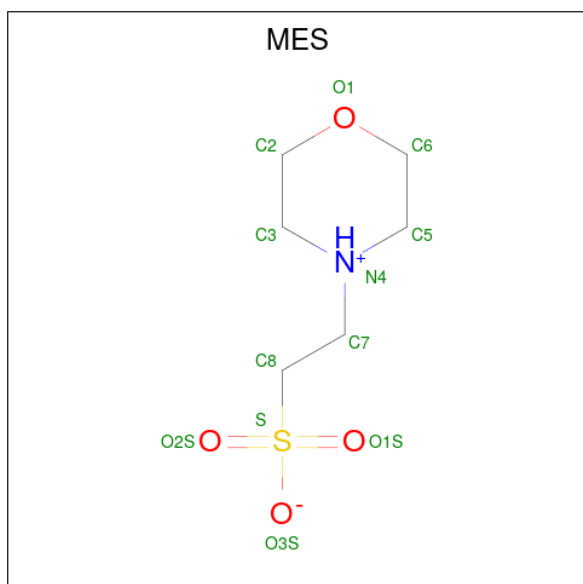
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Cl 1 1	0	0
16	U	1	Total Cl 1 1	0	0

- Molecule 17 is (2 {S})-3-(4-methoxyphenyl)- {N}-[(2 {S},3 {R})-4-methyl-3,4-bis(oxidanyl)-1-phenyl-pentan-2-yl]-2-[[[(2 {S})-2-(2-morpholin-4-ylethanoylamino)propanoyl]amino]prop anamide (CCD ID: GQK) (formula: C₃₁H₄₄N₄O₇).



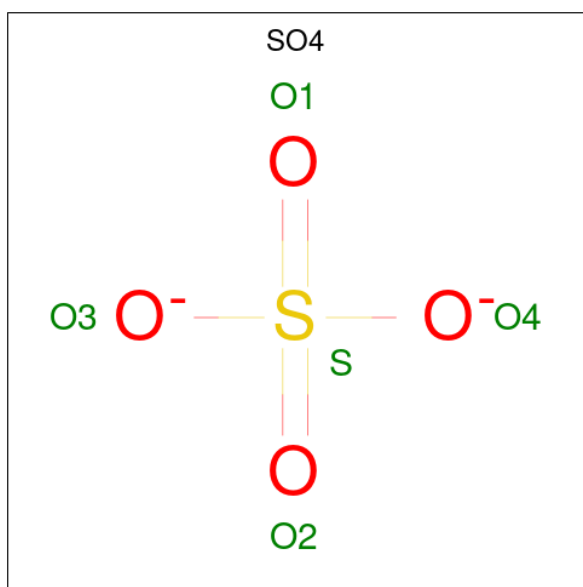
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	H	1	Total	C	N	O	0	0
			42	31	4	7		
17	K	1	Total	C	N	O	0	0
			42	31	4	7		
17	N	1	Total	C	N	O	0	0
			42	31	4	7		
17	V	1	Total	C	N	O	0	0
			42	31	4	7		
17	Y	1	Total	C	N	O	0	0
			42	31	4	7		
17	b	1	Total	C	N	O	0	0
			42	31	4	7		

- Molecule 18 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 19 is SULFATE ION (CCD ID: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	N	1	Total	O	S	0	0
			5	4	1		
19	b	1	Total	O	S	0	0
			5	4	1		

- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	49	Total	O	0	0
			49	49		
20	B	41	Total	O	0	0
			41	41		
20	C	35	Total	O	0	0
			35	35		
20	D	25	Total	O	0	0
			25	25		
20	E	19	Total	O	0	0
			19	19		
20	F	32	Total	O	0	0
			32	32		
20	G	47	Total	O	0	0
			47	47		
20	H	42	Total	O	0	0
			42	42		
20	I	36	Total	O	0	0
			36	36		
20	J	48	Total	O	0	0
			48	48		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	K	64	Total 64	O 64	0	0
20	L	52	Total 52	O 52	0	0
20	M	41	Total 41	O 41	0	0
20	N	35	Total 35	O 35	0	0
20	O	25	Total 25	O 25	0	0
20	P	25	Total 25	O 25	0	0
20	Q	22	Total 22	O 22	0	0
20	R	16	Total 16	O 16	0	0
20	S	21	Total 21	O 21	0	0
20	T	32	Total 32	O 32	0	0
20	U	39	Total 39	O 39	0	0
20	V	43	Total 43	O 43	0	0
20	W	35	Total 35	O 35	0	0
20	X	43	Total 43	O 43	0	0
20	Y	53	Total 53	O 53	0	0
20	Z	47	Total 47	O 47	0	0
20	a	64	Total 64	O 64	0	0
20	b	39	Total 39	O 39	0	0

3 Residue-property plots [i](#)

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

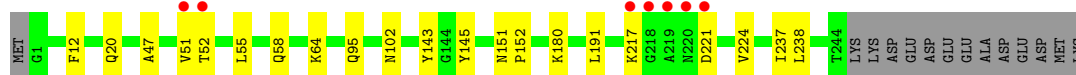
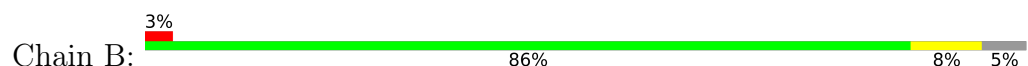
- Molecule 1: Proteasome subunit alpha type-2



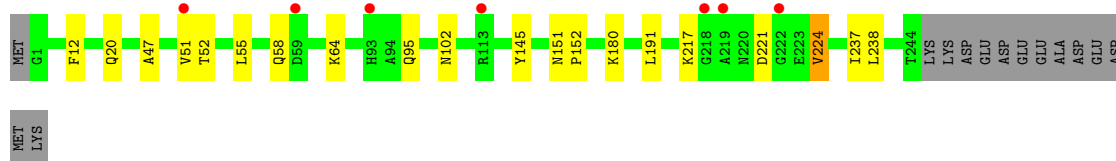
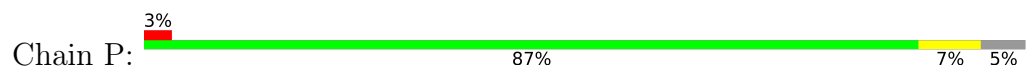
- Molecule 1: Proteasome subunit alpha type-2



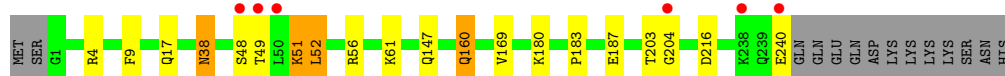
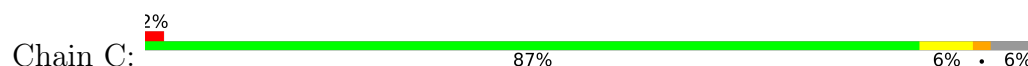
- Molecule 2: Proteasome subunit alpha type-3



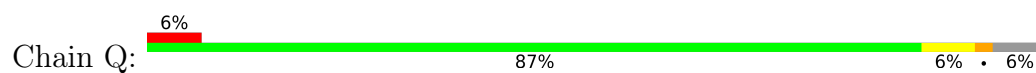
- Molecule 2: Proteasome subunit alpha type-3



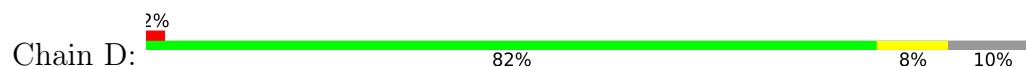
- Molecule 3: Proteasome subunit alpha type-4



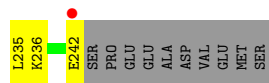
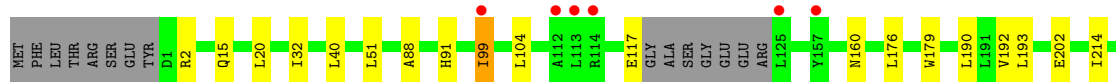
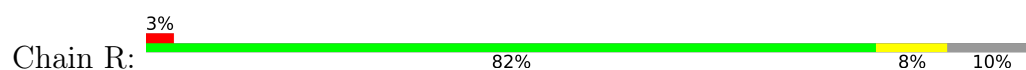
- Molecule 3: Proteasome subunit alpha type-4



- Molecule 4: Proteasome subunit alpha type-5



- Molecule 4: Proteasome subunit alpha type-5



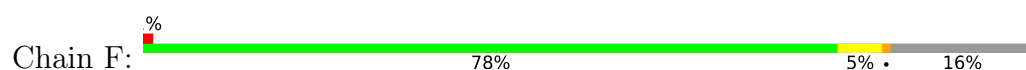
- Molecule 5: Proteasome subunit alpha type-6

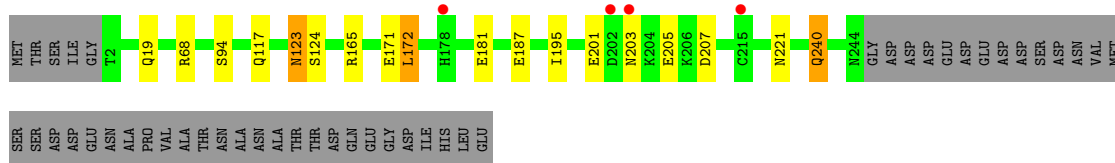


- Molecule 5: Proteasome subunit alpha type-6

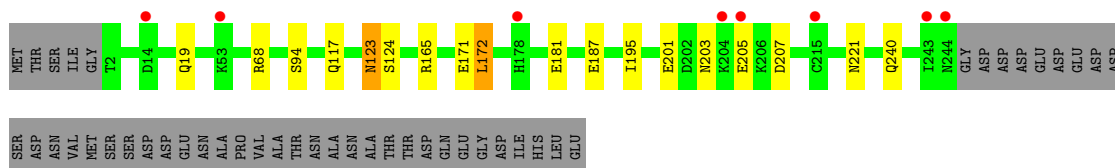
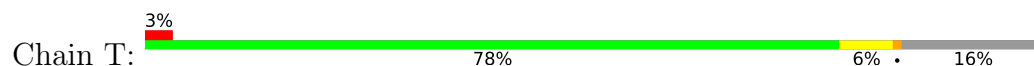


- Molecule 6: Probable proteasome subunit alpha type-7

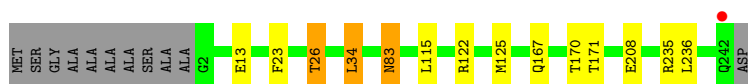




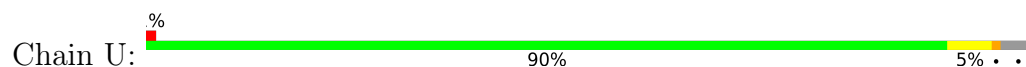
- Molecule 6: Probable proteasome subunit alpha type-7



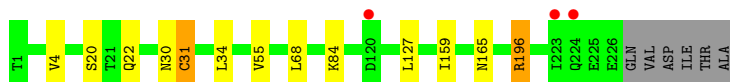
- Molecule 7: Proteasome subunit alpha type-1



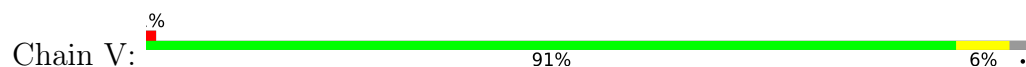
- Molecule 7: Proteasome subunit alpha type-1



- 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

Chain W: 95% 5%



- Molecule 10: Proteasome subunit beta type-4

Chain J: 89% 9% ..



- Molecule 10: Proteasome subunit beta type-4

Chain X: 90% 8% ..



- Molecule 11: Proteasome subunit beta type-5

Chain K: 95% 5%



- Molecule 11: Proteasome subunit beta type-5

Chain Y: 95% 5%



- Molecule 12: Proteasome subunit beta type-6

Chain L: 90% 8% .

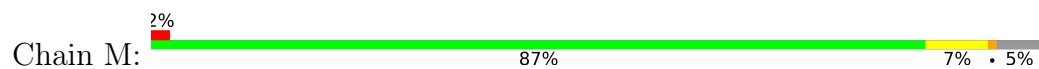


- Molecule 12: Proteasome subunit beta type-6

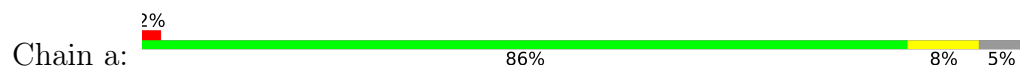
Chain Z: 90% 8% .



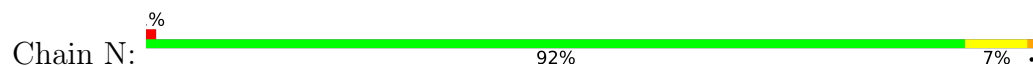
• Molecule 13: Proteasome subunit beta type-7



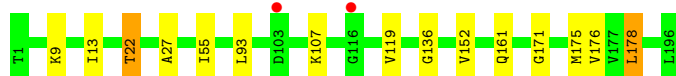
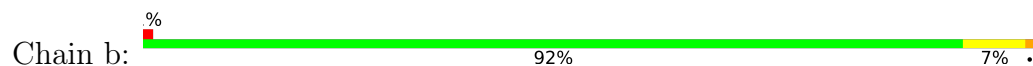
• Molecule 13: Proteasome subunit beta type-7



• 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	136.63Å 299.66Å 145.15Å 90.00° 113.39° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 15.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.2 (15.00-2.50) 97.1 (15.00-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.189 , 0.216 0.194 , 0.219	Depositor DCC
R_{free} test set	17869 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	49.4	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	50758	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GQK, CL, MG, MES

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	0.54	0/1952	0.81	0/2642
1	O	0.54	0/1952	0.82	0/2642
2	B	0.56	0/1934	0.84	0/2618
2	P	0.55	0/1934	0.85	1/2618 (0.0%)
3	C	0.55	0/1910	0.84	0/2586
3	Q	0.55	0/1910	0.84	0/2586
4	D	0.53	0/1837	0.83	0/2475
4	R	0.54	0/1837	0.82	0/2475
5	E	0.55	0/1800	0.78	0/2433
5	S	0.55	0/1800	0.78	0/2433
6	F	0.55	0/1932	0.80	0/2609
6	T	0.55	0/1932	0.81	0/2609
7	G	0.52	0/1945	0.80	0/2634
7	U	0.52	0/1945	0.79	0/2634
8	H	0.50	0/1751	0.79	0/2375
8	V	0.51	1/1751 (0.1%)	0.79	0/2375
9	I	0.49	0/1611	0.78	0/2174
9	W	0.50	0/1611	0.79	0/2174
10	J	0.52	0/1589	0.80	0/2142
10	X	0.52	0/1589	0.81	0/2142
11	K	0.48	0/1681	0.86	3/2274 (0.1%)
11	Y	0.47	0/1681	0.88	3/2274 (0.1%)
12	L	0.51	0/1795	0.79	0/2420
12	Z	0.51	0/1795	0.79	0/2420
13	M	0.53	0/1855	0.81	1/2514 (0.0%)
13	a	0.53	0/1855	0.81	1/2514 (0.0%)
14	N	0.49	0/1541	0.79	0/2087
14	b	0.48	0/1541	0.80	0/2087
All	All	0.52	1/50266 (0.0%)	0.81	9/67966 (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
12	L	0	1
12	Z	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	V	35	HIS	CE1-NE2	5.10	1.37	1.32

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Y	73	ARG	NE-CZ-NH2	11.09	129.18	119.20
11	Y	73	ARG	CD-NE-CZ	10.19	138.66	124.40
11	Y	73	ARG	NE-CZ-NH1	-10.07	111.43	121.50
11	K	73	ARG	CD-NE-CZ	9.79	138.11	124.40
11	K	73	ARG	NE-CZ-NH2	-8.88	111.21	119.20
11	K	73	ARG	NE-CZ-NH1	8.00	129.50	121.50
13	M	10	SER	N-CA-C	5.25	117.06	110.24
13	a	10	SER	N-CA-C	5.23	117.04	110.24
2	P	224	VAL	N-CA-C	5.02	115.70	108.48

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	L	135	GLN	Peptide
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	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	1915	0	1929	3	0
2	B	1904	0	1904	10	0
2	P	1904	0	1904	8	0
3	C	1881	0	1895	6	0
3	Q	1881	0	1895	5	0
4	D	1813	0	1797	7	0
4	R	1813	0	1797	6	0
5	E	1773	0	1775	8	0
5	S	1773	0	1775	7	0
6	F	1892	0	1883	5	0
6	T	1892	0	1883	4	0
7	G	1907	0	1901	6	0
7	U	1907	0	1901	6	0
8	H	1720	0	1719	4	0
8	V	1720	0	1719	4	0
9	I	1581	0	1574	6	0
9	W	1581	0	1574	5	0
10	J	1561	0	1569	5	0
10	X	1561	0	1569	5	0
11	K	1644	0	1593	4	0
11	Y	1644	0	1593	5	0
12	L	1757	0	1711	14	0
12	Z	1757	0	1711	14	0
13	M	1824	0	1832	8	0
13	a	1824	0	1832	9	0
14	N	1512	0	1479	8	0
14	b	1512	0	1479	8	0
15	G	1	0	0	0	0
15	I	2	0	0	0	0
15	K	1	0	0	0	0
15	L	1	0	0	0	0
15	N	1	0	0	0	0
15	W	1	0	0	0	0
15	Z	1	0	0	0	0
16	G	1	0	0	0	0
16	U	1	0	0	0	0
17	H	42	0	0	0	0
17	K	42	0	0	2	0
17	N	42	0	0	0	0
17	V	42	0	0	0	0
17	Y	42	0	0	2	0
17	b	42	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	H	12	0	13	0	0
18	K	12	0	13	0	0
18	V	12	0	13	0	0
18	Y	12	0	13	0	0
19	N	5	0	0	0	0
19	b	5	0	0	0	0
20	A	49	0	0	0	0
20	B	41	0	0	0	0
20	C	35	0	0	0	0
20	D	25	0	0	0	0
20	E	19	0	0	0	0
20	F	32	0	0	0	0
20	G	47	0	0	0	0
20	H	42	0	0	0	0
20	I	36	0	0	0	0
20	J	48	0	0	0	0
20	K	64	0	0	0	0
20	L	52	0	0	0	0
20	M	41	0	0	1	0
20	N	35	0	0	0	0
20	O	25	0	0	0	0
20	P	25	0	0	0	0
20	Q	22	0	0	0	0
20	R	16	0	0	0	0
20	S	21	0	0	0	0
20	T	32	0	0	0	0
20	U	39	0	0	0	0
20	V	43	0	0	0	0
20	W	35	0	0	0	0
20	X	43	0	0	0	0
20	Y	53	0	0	0	0
20	Z	47	0	0	0	0
20	a	64	0	0	1	0
20	b	39	0	0	0	0
All	All	50758	0	49174	151	0

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

All (151) 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)
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.50	0.76
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.51	0.75
5:S:12:PHE:H	6:T:19:GLN:HE22	1.37	0.73
2:B:12:PHE:H	3:C:17:GLN:HE22	1.37	0.70
5:E:12:PHE:H	6:F:19:GLN:HE22	1.38	0.69
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.39	0.68
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.59	0.68
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.59	0.67
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.42	0.67
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.78	0.66
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.77	0.66
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.44	0.65
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.45	0.63
14:b:13:ILE:HG21	14:b:175:MET:HE2	1.80	0.63
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.82	0.61
14:N:13:ILE:HG21	14:N:175:MET:HE2	1.81	0.61
14:N:136:GLY:HA2	14:b:161:GLN:HE21	1.65	0.61
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.82	0.61
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.49	0.61
14:N:161:GLN:HE21	14:b:136:GLY:HA2	1.65	0.61
12:Z:42:LYS:HD2	12:Z:55:ASN:HD22	1.66	0.60
12:L:42:LYS:HD2	12:L:55:ASN:HD22	1.67	0.60
13:a:190:ARG:NH2	20:a:301:HOH:O	2.36	0.59
2:P:145:TYR:OH	2:P:217:LYS:N	2.37	0.58
1:O:12:PHE:H	2:P:20:GLN:HE22	1.50	0.58
4:R:99:ILE:HD11	4:R:104:LEU:HB2	1.86	0.58
2:B:145:TYR:OH	2:B:217:LYS:N	2.37	0.57
7:G:23:PHE:O	7:G:26:THR:HB	2.04	0.57
14:N:152:VAL:HA	14:N:175:MET:HE1	1.86	0.57
7:U:23:PHE:O	7:U:26:THR:HB	2.04	0.57
14:b:152:VAL:HA	14:b:175:MET:HE1	1.86	0.56
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.88	0.56
4:D:99:ILE:HD11	4:D:104:LEU:HB2	1.88	0.56
2:P:95:GLN:NE2	9:W:71:ASN:HD22	2.04	0.55
4:R:32:ILE:HD12	4:R:192:VAL:HG23	1.88	0.55
1:A:12:PHE:H	2:B:20:GLN:HE22	1.55	0.54
7:G:83:ASN:C	7:G:83:ASN:HD22	2.16	0.54
11:K:176:ASN:ND2	11:K:190:ASN:HD22	2.06	0.54
4:D:32:ILE:HD12	4:D:192:VAL:HG23	1.88	0.54
2:B:95:GLN:NE2	9:I:71:ASN:HD22	2.06	0.54
13:M:156:ARG:HH11	8:V:165:ASN:HD22	1.56	0.54
5:S:92:ASN:ND2	12:Z:70:ASN:HD21	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:176:ASN:ND2	11:Y:190:ASN:HD22	2.05	0.53
6:T:123:ASN:C	6:T:123:ASN:HD22	2.17	0.53
9:W:36:SER:HB2	10:X:126:VAL:HG11	1.90	0.53
12:Z:31:THR:CG2	12:Z:36:ASN:HD21	2.21	0.53
3:C:9:PHE:H	4:D:15:GLN:HE22	1.56	0.52
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.57	0.52
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.92	0.52
12:Z:23:LEU:HD13	12:Z:43:VAL:HG13	1.91	0.52
12:L:23:LEU:HD13	12:L:43:VAL:HG13	1.90	0.52
13:M:27:LEU:HD21	13:M:34:LEU:HD22	1.92	0.51
7:U:83:ASN:C	7:U:83:ASN:HD22	2.18	0.51
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.92	0.51
6:T:123:ASN:HD22	6:T:124:SER:N	2.07	0.51
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.92	0.51
6:F:123:ASN:HD22	6:F:124:SER:N	2.08	0.51
8:V:20:SER:HB3	8:V:31:CYS:SG	2.51	0.51
6:F:123:ASN:HD22	6:F:123:ASN:C	2.19	0.51
8:H:165:ASN:HD22	13:a:156:ARG:HH11	1.58	0.50
12:L:31:THR:CG2	12:L:36:ASN:HD21	2.21	0.50
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.92	0.50
13:a:27:LEU:HD21	13:a:34:LEU:HD22	1.92	0.50
14:b:176:VAL:HG12	14:b:178:LEU:HD13	1.93	0.50
5:E:118:ASN:HD22	5:E:118:ASN:N	2.10	0.50
5:S:92:ASN:HD21	12:Z:70:ASN:ND2	2.08	0.50
11:K:176:ASN:HD21	11:K:190:ASN:HD22	1.59	0.49
13:M:219:TRP:CH2	14:b:171:GLY:HA2	2.48	0.49
5:S:118:ASN:N	5:S:118:ASN:HD22	2.11	0.49
12:Z:136:CYS:SG	12:Z:150:LEU:HB3	2.52	0.49
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.93	0.49
11:Y:176:ASN:HD21	11:Y:190:ASN:HD22	1.60	0.48
14:N:171:GLY:HA2	13:a:219:TRP:CH2	2.48	0.48
3:Q:38:ASN:HD22	3:Q:38:ASN:C	2.22	0.48
14:b:22:THR:OG1	14:b:27:ALA:HB2	2.14	0.48
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.49	0.47
12:L:8:ASN:HA	12:L:30:ILE:O	2.14	0.47
12:L:136:CYS:SG	12:L:150:LEU:HB3	2.55	0.47
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.14	0.47
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.50	0.47
2:B:145:TYR:HH	2:B:217:LYS:N	2.12	0.47
8:H:20:SER:HB3	8:H:31:CYS:SG	2.54	0.47
5:E:92:ASN:ND2	12:L:70:ASN:HD21	2.11	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:22:THR:OG1	14:N:27:ALA:HB2	2.14	0.47
10:X:152:MET:HE1	10:X:160:LEU:HD22	1.98	0.46
14:N:55:ILE:HD11	14:N:93:LEU:HD13	1.96	0.46
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.45	0.46
5:E:92:ASN:HD21	12:L:70:ASN:ND2	2.14	0.46
14:b:55:ILE:HD11	14:b:93:LEU:HD13	1.96	0.46
2:P:145:TYR:OH	2:P:217:LYS:HB2	2.16	0.46
3:C:38:ASN:C	3:C:38:ASN:HD22	2.22	0.46
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.81	0.46
7:G:83:ASN:C	7:G:83:ASN:ND2	2.74	0.46
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.46	0.45
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.46	0.45
10:J:152:MET:HE1	10:J:160:LEU:HD22	1.98	0.45
13:M:127:LEU:HG	13:M:142:LEU:HD12	1.99	0.45
7:G:167:GLN:HE21	7:G:171:THR:HG23	1.82	0.45
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.82	0.45
12:Z:146:ILE:HG22	12:Z:150:LEU:HD22	1.99	0.45
8:H:196:ARG:NH2	9:I:150:GLU:O	2.49	0.44
4:D:113:LEU:HD12	5:E:78:PRO:HB2	2.00	0.44
2:B:143:TYR:O	3:C:56:ARG:NH1	2.46	0.44
2:B:145:TYR:OH	2:B:217:LYS:HB2	2.17	0.44
7:U:167:GLN:HE21	7:U:171:THR:HG23	1.83	0.44
9:I:65:MET:HE1	9:I:93:SER:HB3	2.00	0.44
12:L:146:ILE:HG22	12:L:150:LEU:HD22	1.99	0.44
1:O:83:ARG:HE	7:U:114:ASN:ND2	2.15	0.43
13:a:179:ASN:HD22	13:a:182:ARG:HH11	1.65	0.43
13:M:179:ASN:HD22	13:M:182:ARG:HH11	1.65	0.43
9:W:65:MET:HE1	9:W:93:SER:HB3	1.99	0.43
3:C:51:LYS:O	3:C:52:LEU:HB2	2.18	0.43
9:I:10:ILE:HG21	9:I:141:ALA:HB3	2.01	0.43
7:U:83:ASN:C	7:U:83:ASN:ND2	2.76	0.43
11:K:31:VAL:HG11	17:K:301:GQK:C3	2.49	0.43
13:a:127:LEU:HG	13:a:142:LEU:HD12	1.99	0.43
10:J:3:ILE:HG23	10:J:18:SER:HB3	2.01	0.42
11:K:31:VAL:HG11	17:K:301:GQK:C4	2.50	0.42
1:A:55:LEU:HD12	7:G:170:THR:HG23	2.02	0.42
10:J:126:VAL:HG12	10:J:128:LEU:HG	2.01	0.42
6:T:172:LEU:HD13	6:T:195:ILE:HD13	2.01	0.42
10:X:3:ILE:HG23	10:X:18:SER:HB3	2.01	0.42
13:M:179:ASN:HD22	13:M:182:ARG:NH1	2.17	0.42
12:L:13:LEU:CD1	12:L:150:LEU:HD21	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.19	0.42
5:S:68:HIS:HE1	5:S:102:LEU:O	2.02	0.42
8:V:4:VAL:HG22	8:V:159:ILE:HD11	2.01	0.42
13:a:150:MET:HE1	13:a:187:ARG:HG2	2.02	0.42
13:M:2:GLN:NE2	20:M:301:HOH:O	2.52	0.42
1:O:83:ARG:HE	7:U:114:ASN:HD21	1.67	0.41
10:X:126:VAL:HG12	10:X:128:LEU:HG	2.01	0.41
11:Y:31:VAL:HG11	17:Y:301:GQK:C3	2.50	0.41
13:M:150:MET:HE1	13:M:187:ARG:HG2	2.02	0.41
13:a:179:ASN:HD22	13:a:182:ARG:NH1	2.18	0.41
6:F:172:LEU:HD13	6:F:195:ILE:HD13	2.01	0.41
9:W:10:ILE:HG21	9:W:141:ALA:HB3	2.02	0.41
12:Z:18:GLU:HG3	12:Z:174:TYR:CD2	2.55	0.41
13:a:97:ALA:HA	13:a:130:VAL:HG21	2.02	0.41
2:B:47:ALA:HB1	2:B:64:LYS:HD2	2.02	0.41
7:G:34:LEU:C	7:G:34:LEU:HD23	2.46	0.41
8:H:4:VAL:HG22	8:H:159:ILE:HD11	2.01	0.41
12:L:18:GLU:HG3	12:L:174:TYR:CD2	2.56	0.41
2:P:47:ALA:HB1	2:P:64:LYS:HD2	2.02	0.41
6:F:240:GLN:HE21	6:F:240:GLN:HA	1.85	0.41
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.51	0.41
8:V:112:SER:HB3	8:V:125:LEU:HD13	2.03	0.41
5:E:68:HIS:HE1	5:E:102:LEU:O	2.03	0.41
11:Y:31:VAL:HG11	17:Y:301:GQK:C4	2.51	0.41
1:A:75:TYR:HB3	1:A:82:TYR:CD1	2.56	0.40
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.51	0.40
11:Y:86:LEU:HD13	11:Y:86:LEU:C	2.47	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%)	241 (97%)	6 (2%)	1 (0%)	30	49
1	O	248/250 (99%)	241 (97%)	6 (2%)	1 (0%)	30	49
2	B	242/258 (94%)	233 (96%)	8 (3%)	1 (0%)	30	49
2	P	242/258 (94%)	233 (96%)	8 (3%)	1 (0%)	30	49
3	C	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	16	31
3	Q	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	16	31
4	D	231/260 (89%)	225 (97%)	5 (2%)	1 (0%)	30	49
4	R	231/260 (89%)	226 (98%)	4 (2%)	1 (0%)	30	49
5	E	229/234 (98%)	220 (96%)	9 (4%)	0	100	100
5	S	229/234 (98%)	220 (96%)	9 (4%)	0	100	100
6	F	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
6	T	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
7	G	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
7	U	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
8	H	224/232 (97%)	220 (98%)	4 (2%)	0	100	100
8	V	224/232 (97%)	220 (98%)	4 (2%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
10	J	193/198 (98%)	190 (98%)	3 (2%)	0	100	100
10	X	193/198 (98%)	190 (98%)	3 (2%)	0	100	100
11	K	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
11	Y	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
12	L	220/222 (99%)	212 (96%)	7 (3%)	1 (0%)	24	43
12	Z	220/222 (99%)	212 (96%)	7 (3%)	1 (0%)	24	43
13	M	231/246 (94%)	221 (96%)	9 (4%)	1 (0%)	30	49
13	a	231/246 (94%)	221 (96%)	9 (4%)	1 (0%)	30	49
14	N	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
14	b	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
All	All	6284/6614 (95%)	6116 (97%)	154 (2%)	14 (0%)	43	63

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	221	ASP
4	D	2	ARG
2	P	221	ASP
4	R	2	ARG
1	A	166	LYS
1	O	166	LYS
3	C	183	PRO
3	Q	183	PRO
13	M	229	GLY
13	a	229	GLY
12	L	166	GLY
12	Z	166	GLY
3	C	204	GLY
3	Q	204	GLY

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%)	202 (97%)	7 (3%)	33	61
1	O	209/209 (100%)	202 (97%)	7 (3%)	33	61
2	B	203/216 (94%)	193 (95%)	10 (5%)	22	45
2	P	203/216 (94%)	193 (95%)	10 (5%)	22	45
3	C	212/226 (94%)	197 (93%)	15 (7%)	13	29
3	Q	212/226 (94%)	197 (93%)	15 (7%)	13	29
4	D	194/215 (90%)	181 (93%)	13 (7%)	15	31
4	R	194/215 (90%)	181 (93%)	13 (7%)	15	31
5	E	190/193 (98%)	181 (95%)	9 (5%)	23	47
5	S	190/193 (98%)	181 (95%)	9 (5%)	23	47
6	F	201/239 (84%)	186 (92%)	15 (8%)	12	26
6	T	201/239 (84%)	186 (92%)	15 (8%)	12	26
7	G	206/210 (98%)	196 (95%)	10 (5%)	22	45
7	U	206/210 (98%)	196 (95%)	10 (5%)	22	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	185/190 (97%)	176 (95%)	9 (5%)	22	45
8	V	185/190 (97%)	176 (95%)	9 (5%)	22	45
9	I	172/173 (99%)	168 (98%)	4 (2%)	44	72
9	W	172/173 (99%)	168 (98%)	4 (2%)	44	72
10	J	173/175 (99%)	162 (94%)	11 (6%)	16	33
10	X	173/175 (99%)	163 (94%)	10 (6%)	18	38
11	K	169/169 (100%)	163 (96%)	6 (4%)	31	58
11	Y	169/169 (100%)	162 (96%)	7 (4%)	27	53
12	L	185/185 (100%)	175 (95%)	10 (5%)	20	41
12	Z	185/185 (100%)	176 (95%)	9 (5%)	22	45
13	M	199/208 (96%)	192 (96%)	7 (4%)	32	58
13	a	199/208 (96%)	192 (96%)	7 (4%)	32	58
14	N	162/162 (100%)	157 (97%)	5 (3%)	35	62
14	b	162/162 (100%)	157 (97%)	5 (3%)	35	62
All	All	5320/5540 (96%)	5059 (95%)	261 (5%)	22	45

All (261) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	SER
1	A	61	LEU
1	A	122	THR
1	A	157	PHE
1	A	184	GLU
1	A	201	GLU
1	A	250	LEU
2	B	51	VAL
2	B	52	THR
2	B	55	LEU
2	B	58	GLN
2	B	102	ASN
2	B	180	LYS
2	B	191	LEU
2	B	224	VAL
2	B	237	ILE
2	B	238	LEU
3	C	4	ARG

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Mol	Chain	Res	Type
3	C	38	ASN
3	C	48	SER
3	C	49	THR
3	C	51	LYS
3	C	52	LEU
3	C	61	LYS
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	187	GLU
3	C	203	THR
3	C	216	ASP
3	C	240	GLU
4	D	20	LEU
4	D	40	LEU
4	D	51	LEU
4	D	99	ILE
4	D	117	GLU
4	D	176	LEU
4	D	190	LEU
4	D	193	LEU
4	D	202	GLU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	10	VAL
5	E	25	LEU
5	E	29	LYS
5	E	55	LEU
5	E	71	LEU
5	E	118	ASN
5	E	153	THR
5	E	188	LEU
6	F	68	ARG
6	F	94	SER
6	F	117	GLN
6	F	123	ASN
6	F	165	ARG
6	F	171	GLU

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Mol	Chain	Res	Type
6	F	172	LEU
6	F	181	GLU
6	F	187	GLU
6	F	201	GLU
6	F	203	ASN
6	F	205	GLU
6	F	207	ASP
6	F	221	ASN
6	F	240	GLN
7	G	13	GLU
7	G	26	THR
7	G	34	LEU
7	G	83	ASN
7	G	115	LEU
7	G	122	ARG
7	G	125	MET
7	G	208	GLU
7	G	235	ARG
7	G	236	LEU
8	H	22	GLN
8	H	30	ASN
8	H	31	CYS
8	H	34	LEU
8	H	55	VAL
8	H	68	LEU
8	H	84	LYS
8	H	127	LEU
8	H	196	ARG
9	I	31	GLN
9	I	37	ASN
9	I	171	LEU
9	I	182	TRP
10	J	2	ASP
10	J	3	ILE
10	J	7	ILE
10	J	35	THR
10	J	49	GLU
10	J	90	LYS
10	J	99	GLN
10	J	110	LYS
10	J	136	SER
10	J	143	LEU

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Mol	Chain	Res	Type
10	J	172	MET
11	K	9	GLN
11	K	41	LEU
11	K	118	ASP
11	K	148	LEU
11	K	177	LEU
11	K	209	ASN
12	L	13	LEU
12	L	18	GLU
12	L	23	LEU
12	L	31	THR
12	L	49	ASN
12	L	106	TYR
12	L	136	CYS
12	L	150	LEU
12	L	172	LEU
12	L	173	LYS
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
13	M	212	LEU
14	N	9	LYS
14	N	22	THR
14	N	107	LYS
14	N	119	VAL
14	N	178	LEU
1	O	51	SER
1	O	61	LEU
1	O	122	THR
1	O	157	PHE
1	O	184	GLU
1	O	201	GLU
1	O	250	LEU
2	P	51	VAL
2	P	52	THR
2	P	55	LEU
2	P	58	GLN
2	P	102	ASN
2	P	180	LYS

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Mol	Chain	Res	Type
2	P	191	LEU
2	P	224	VAL
2	P	237	ILE
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	48	SER
3	Q	49	THR
3	Q	51	LYS
3	Q	52	LEU
3	Q	61	LYS
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	187	GLU
3	Q	203	THR
3	Q	216	ASP
3	Q	240	GLU
4	R	20	LEU
4	R	40	LEU
4	R	51	LEU
4	R	99	ILE
4	R	117	GLU
4	R	176	LEU
4	R	190	LEU
4	R	193	LEU
4	R	202	GLU
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	10	VAL
5	S	25	LEU
5	S	29	LYS
5	S	55	LEU
5	S	71	LEU
5	S	118	ASN
5	S	153	THR
5	S	188	LEU
6	T	68	ARG

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Mol	Chain	Res	Type
6	T	94	SER
6	T	117	GLN
6	T	123	ASN
6	T	165	ARG
6	T	171	GLU
6	T	172	LEU
6	T	181	GLU
6	T	187	GLU
6	T	201	GLU
6	T	203	ASN
6	T	205	GLU
6	T	207	ASP
6	T	221	ASN
6	T	240	GLN
7	U	13	GLU
7	U	26	THR
7	U	34	LEU
7	U	83	ASN
7	U	115	LEU
7	U	122	ARG
7	U	125	MET
7	U	208	GLU
7	U	235	ARG
7	U	236	LEU
8	V	22	GLN
8	V	30	ASN
8	V	31	CYS
8	V	34	LEU
8	V	55	VAL
8	V	68	LEU
8	V	84	LYS
8	V	127	LEU
8	V	196	ARG
9	W	31	GLN
9	W	37	ASN
9	W	171	LEU
9	W	182	TRP
10	X	3	ILE
10	X	7	ILE
10	X	35	THR
10	X	49	GLU
10	X	90	LYS

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Mol	Chain	Res	Type
10	X	99	GLN
10	X	110	LYS
10	X	136	SER
10	X	143	LEU
10	X	172	MET
11	Y	9	GLN
11	Y	41	LEU
11	Y	73	ARG
11	Y	118	ASP
11	Y	148	LEU
11	Y	177	LEU
11	Y	209	ASN
12	Z	13	LEU
12	Z	18	GLU
12	Z	23	LEU
12	Z	31	THR
12	Z	49	ASN
12	Z	106	TYR
12	Z	150	LEU
12	Z	172	LEU
12	Z	173	LYS
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
13	a	212	LEU
14	b	9	LYS
14	b	22	THR
14	b	107	LYS
14	b	119	VAL
14	b	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (182) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	94	HIS
1	A	190	HIS
2	B	20	GLN
2	B	58	GLN

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Mol	Chain	Res	Type
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	124	HIS
2	B	155	ASN
2	B	176	GLN
2	B	232	GLN
3	C	17	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
3	C	165	ASN
3	C	207	ASN
4	D	15	GLN
4	D	91	HIS
4	D	100	ASN
4	D	106	GLN
4	D	146	GLN
4	D	160	ASN
4	D	198	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	151	ASN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	143	HIS
6	F	191	GLN
6	F	240	GLN
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN

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Mol	Chain	Res	Type
7	G	121	GLN
7	G	167	GLN
7	G	175	ASN
7	G	212	ASN
7	G	231	ASN
8	H	30	ASN
8	H	66	HIS
8	H	165	ASN
8	H	172	ASN
8	H	189	ASN
9	I	37	ASN
9	I	63	ASN
9	I	88	GLN
9	I	168	GLN
10	J	55	GLN
10	J	63	ASN
11	K	9	GLN
11	K	85	ASN
11	K	143	ASN
11	K	176	ASN
11	K	188	HIS
11	K	209	ASN
12	L	3	ASN
12	L	36	ASN
12	L	49	ASN
12	L	70	ASN
12	L	76	HIS
12	L	79	HIS
12	L	80	ASN
12	L	152	ASN
12	L	153	GLN
12	L	155	ASN
12	L	158	ASN
12	L	197	GLN
13	M	48	ASN
13	M	102	GLN
13	M	108	ASN
13	M	179	ASN
13	M	194	ASN
13	M	203	ASN
13	M	213	GLN
14	N	53	GLN

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Mol	Chain	Res	Type
14	N	69	GLN
14	N	141	ASN
14	N	161	GLN
1	O	30	GLN
1	O	94	HIS
1	O	190	HIS
2	P	20	GLN
2	P	58	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	124	HIS
2	P	176	GLN
2	P	232	GLN
3	Q	17	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
3	Q	165	ASN
3	Q	207	ASN
3	Q	233	GLN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	146	GLN
4	R	160	ASN
4	R	225	ASN
5	S	68	HIS
5	S	90	GLN
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	151	ASN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN

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Mol	Chain	Res	Type
6	T	143	HIS
6	T	191	GLN
6	T	240	GLN
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	167	GLN
7	U	175	ASN
8	V	30	ASN
8	V	35	HIS
8	V	66	HIS
8	V	165	ASN
8	V	172	ASN
8	V	189	ASN
9	W	37	ASN
9	W	63	ASN
9	W	88	GLN
9	W	168	GLN
10	X	55	GLN
10	X	63	ASN
10	X	86	GLN
10	X	146	HIS
11	Y	9	GLN
11	Y	85	ASN
11	Y	176	ASN
11	Y	188	HIS
11	Y	209	ASN
12	Z	3	ASN
12	Z	36	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	76	HIS
12	Z	79	HIS
12	Z	80	ASN
12	Z	152	ASN
12	Z	153	GLN
12	Z	155	ASN
12	Z	158	ASN
13	a	48	ASN
13	a	102	GLN

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Mol	Chain	Res	Type
13	a	108	ASN
13	a	149	HIS
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN
14	b	53	GLN
14	b	69	GLN
14	b	141	ASN
14	b	161	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 10 are monoatomic - leaving 12 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

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%)	-0.30	4 (1%) 70 67	35, 51, 84, 131	0
1	O	250/250 (100%)	-0.22	4 (1%) 70 67	36, 56, 96, 135	0
2	B	244/258 (94%)	-0.08	7 (2%) 53 49	35, 55, 108, 164	0
2	P	244/258 (94%)	0.01	7 (2%) 53 49	41, 60, 105, 168	0
3	C	240/254 (94%)	-0.00	6 (2%) 58 54	38, 61, 122, 146	0
3	Q	240/254 (94%)	0.32	14 (5%) 29 25	40, 74, 153, 183	0
4	D	235/260 (90%)	-0.11	6 (2%) 57 52	40, 60, 91, 133	0
4	R	235/260 (90%)	-0.04	7 (2%) 52 48	39, 63, 98, 132	0
5	E	231/234 (98%)	-0.15	0 100 100	42, 63, 99, 134	0
5	S	231/234 (98%)	0.12	5 (2%) 62 58	41, 67, 109, 138	0
6	F	243/288 (84%)	-0.15	4 (1%) 70 67	36, 56, 103, 132	0
6	T	243/288 (84%)	-0.07	8 (3%) 49 45	37, 58, 109, 139	0
7	G	241/252 (95%)	-0.24	1 (0%) 88 86	35, 52, 86, 131	0
7	U	241/252 (95%)	-0.22	2 (0%) 82 80	35, 52, 87, 115	0
8	H	226/232 (97%)	-0.30	3 (1%) 75 71	35, 49, 76, 147	0
8	V	226/232 (97%)	-0.28	3 (1%) 75 71	36, 51, 82, 175	0
9	I	204/205 (99%)	-0.48	0 100 100	32, 46, 74, 95	0
9	W	204/205 (99%)	-0.44	1 (0%) 87 85	28, 49, 76, 106	0
10	J	195/198 (98%)	-0.37	2 (1%) 79 76	34, 47, 74, 121	0
10	X	195/198 (98%)	-0.38	1 (0%) 87 85	34, 50, 76, 140	0
11	K	212/212 (100%)	-0.46	0 100 100	29, 47, 73, 104	0
11	Y	212/212 (100%)	-0.42	0 100 100	28, 49, 73, 105	0
12	L	222/222 (100%)	-0.44	2 (0%) 81 78	33, 49, 74, 93	0
12	Z	222/222 (100%)	-0.43	0 100 100	34, 48, 75, 101	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.31	5 (2%) 63 59	33, 48, 88, 149	0
13	a	233/246 (94%)	-0.38	6 (2%) 57 52	30, 46, 85, 136	0
14	N	196/196 (100%)	-0.38	1 (0%) 87 85	29, 46, 73, 104	0
14	b	196/196 (100%)	-0.40	2 (1%) 79 76	30, 47, 75, 100	0
All	All	6344/6614 (95%)	-0.23	101 (1%) 70 67	28, 53, 99, 183	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	J	1	MET	6.2
3	Q	50	LEU	5.4
4	R	113	LEU	4.7
2	B	51	VAL	4.5
1	A	1	MET	4.5
13	M	233	ILE	4.4
10	X	1	MET	4.2
2	P	51	VAL	4.1
13	M	230	THR	4.0
8	V	223	ILE	3.9
13	a	233	ILE	3.9
1	O	1	MET	3.9
8	H	223	ILE	3.8
6	T	204	LYS	3.8
13	M	228	TYR	3.7
3	Q	49	THR	3.5
3	Q	51	LYS	3.2
3	Q	48	SER	3.2
2	P	219	ALA	3.2
8	V	224	GLN	3.1
4	D	242	GLU	3.1
3	Q	234	ILE	3.0
2	B	219	ALA	3.0
7	U	203	ASP	3.0
6	T	244	ASN	3.0
3	Q	223	SER	3.0
3	C	49	THR	2.9
6	T	178	HIS	2.9
3	C	240	GLU	2.9
13	a	230	THR	2.9
6	F	203	ASN	2.8
13	a	1	THR	2.8

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Mol	Chain	Res	Type	RSRZ
14	N	103	ASP	2.8
2	P	93	HIS	2.8
2	B	217	LYS	2.8
2	P	222	GLY	2.8
3	Q	207	ASN	2.8
3	C	238	LYS	2.7
6	T	243	ILE	2.7
3	C	50	LEU	2.7
13	a	227	GLY	2.7
10	J	174	MET	2.7
3	C	204	GLY	2.7
14	b	103	ASP	2.6
2	B	218	GLY	2.6
2	B	52	THR	2.6
4	R	112	ALA	2.6
6	F	215	CYS	2.6
3	Q	52	LEU	2.6
2	P	218	GLY	2.6
3	Q	204	GLY	2.6
3	Q	206	LYS	2.5
13	M	1	THR	2.5
6	F	178	HIS	2.5
6	T	205	GLU	2.5
4	D	236	LYS	2.5
5	S	52	ALA	2.5
1	O	2	THR	2.5
1	A	249	ALA	2.4
6	T	14	ASP	2.4
4	D	238	LYS	2.4
4	R	114	ARG	2.4
6	T	215	CYS	2.4
3	Q	216	ASP	2.3
2	B	220	ASN	2.3
3	Q	205	ALA	2.3
4	D	240	ALA	2.3
1	O	209	ILE	2.3
4	D	99	ILE	2.3
7	G	242	GLN	2.3
12	L	106	TYR	2.3
1	A	2	THR	2.3
5	S	209	ASN	2.3
13	M	229	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	201	GLU	2.3
3	C	48	SER	2.2
6	F	202	ASP	2.2
8	V	222	ASP	2.2
4	R	242	GLU	2.2
4	R	157	TYR	2.2
5	S	29	LYS	2.2
1	O	53	SER	2.2
2	P	59	ASP	2.2
3	Q	208	ILE	2.2
4	D	224	ASP	2.2
5	S	49	LYS	2.2
4	R	99	ILE	2.1
9	W	130	ASP	2.1
13	a	69	ASP	2.1
7	U	242	GLN	2.1
2	P	113	ARG	2.1
3	Q	240	GLU	2.1
5	S	58	TYR	2.1
4	R	125	LEU	2.1
2	B	221	ASP	2.1
6	T	53	LYS	2.1
12	L	136	CYS	2.1
8	H	224	GLN	2.1
13	a	228	TYR	2.1
8	H	120	ASP	2.0
14	b	116	GLY	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 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	B-factors(Å ²)	Q<0.9
15	MG	Z	301	1/1	0.90	0.05	70,70,70,70	0
17	GQK	N	201	42/42	0.91	0.10	31,47,66,69	0
18	MES	V	302	12/12	0.91	0.13	58,67,71,71	12
17	GQK	b	201	42/42	0.92	0.09	27,48,71,74	0
17	GQK	H	301	42/42	0.92	0.09	35,41,67,68	0
17	GQK	V	301	42/42	0.93	0.09	36,40,74,74	0
17	GQK	Y	301	42/42	0.94	0.08	24,38,55,57	0
19	SO4	N	203	5/5	0.94	0.13	53,60,69,70	5
18	MES	H	302	12/12	0.95	0.11	51,62,72,72	12
15	MG	W	301	1/1	0.95	0.06	57,57,57,57	0
17	GQK	K	301	42/42	0.95	0.07	25,39,53,54	0
19	SO4	b	202	5/5	0.95	0.14	50,58,66,67	5
15	MG	G	301	1/1	0.96	0.03	52,52,52,52	0
15	MG	I	301	1/1	0.96	0.05	59,59,59,59	0
18	MES	K	303	12/12	0.97	0.10	35,39,39,43	12
18	MES	Y	302	12/12	0.97	0.11	38,41,41,43	12
15	MG	N	202	1/1	0.98	0.03	51,51,51,51	0
15	MG	K	302	1/1	0.98	0.08	58,58,58,58	0
15	MG	L	301	1/1	0.98	0.09	54,54,54,54	0
15	MG	I	302	1/1	0.99	0.04	59,59,59,59	0
16	CL	G	302	1/1	0.99	0.04	43,43,43,43	0
16	CL	U	301	1/1	0.99	0.06	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.