



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 07:41 am GMT

PDB ID : 4QW3
Title : yCP beta5-C63F mutant in complex with bortezomib
Authors : Huber, E.M.; Heinemeyer, W.; Groll, M.
Deposited on : 2014-07-16
Resolution : 2.90 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

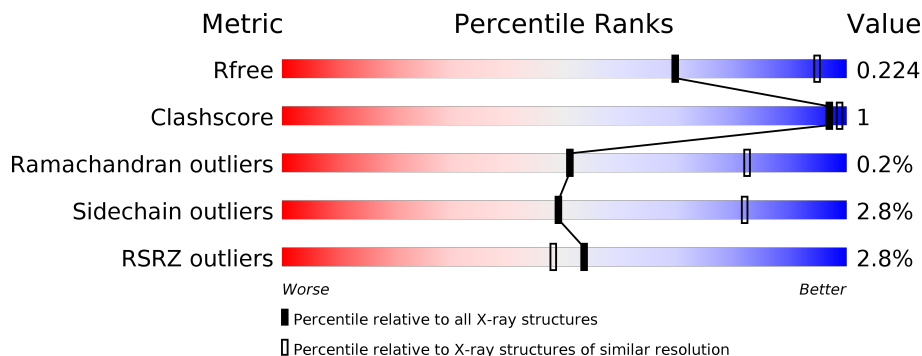
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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.



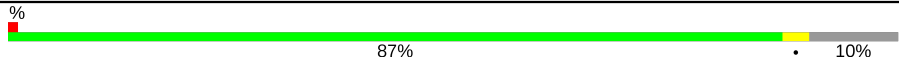

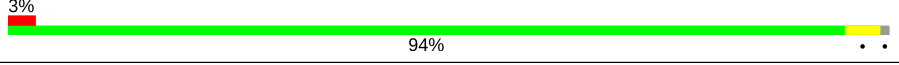
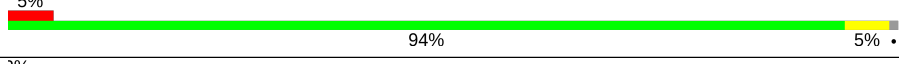
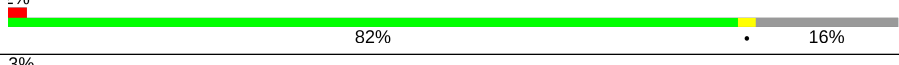
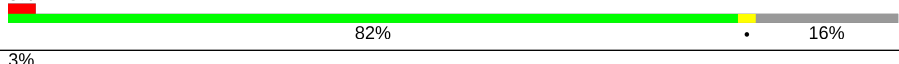
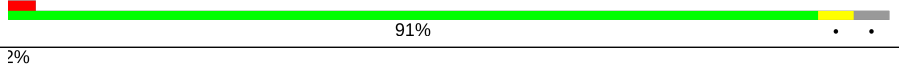
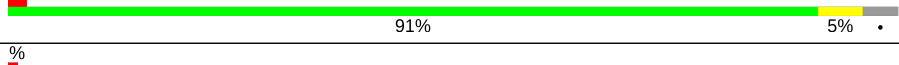
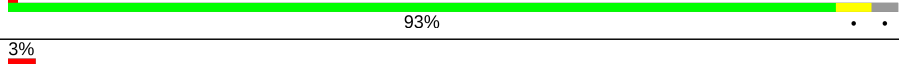
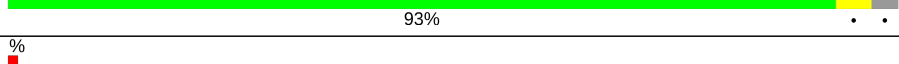
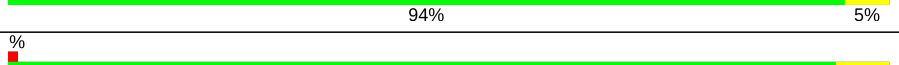
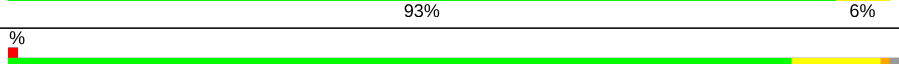

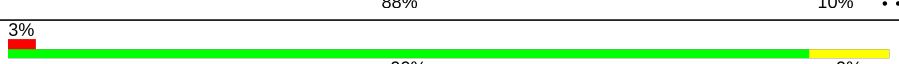
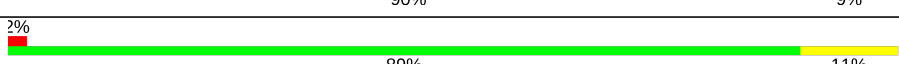
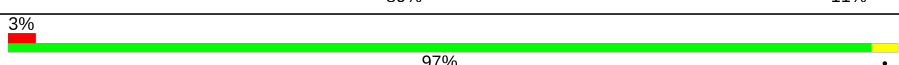
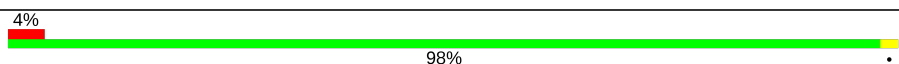
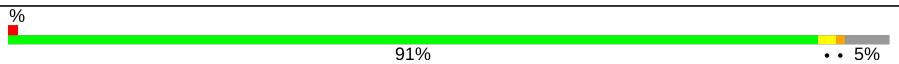
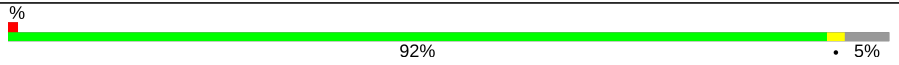
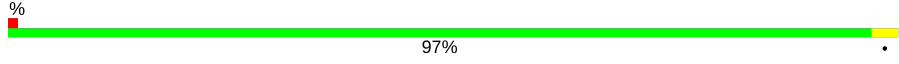
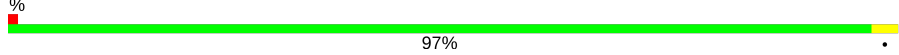
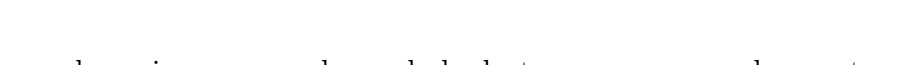
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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>98%</div> <div>•</div> </div>
1	O	250	<div> <div>4%</div> <div>98%</div> <div>•</div> </div>
2	B	258	<div> <div>3%</div> <div>90%</div> <div>• 5%</div> </div>
2	P	258	<div> <div>3%</div> <div>91%</div> <div>• 5%</div> </div>
3	C	254	<div> <div>7%</div> <div>88%</div> <div>6% • 6%</div> </div>
3	Q	254	<div> <div>7%</div> <div>89%</div> <div>5% • 6%</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	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	MG	J	201	-	-	-	X
17	BO2	N	201	-	-	-	X
17	BO2	V	301	-	-	-	X
17	BO2	b	201	-	-	-	X

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 49806 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	226	Total	C	N	O	S	0	0	0
			1719	1082	298	332	7			
8	V	226	Total	C	N	O	S	0	0	0
			1719	1082	298	332	7			

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1649	1051	280	312	6			
11	Y	212	Total	C	N	O	S	0	0	0
			1649	1051	280	312	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	63	PHE	CYS	ENGINEERED MUTATION	UNP P30656
Y	63	PHE	CYS	ENGINEERED MUTATION	UNP P30656

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

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

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

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

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

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

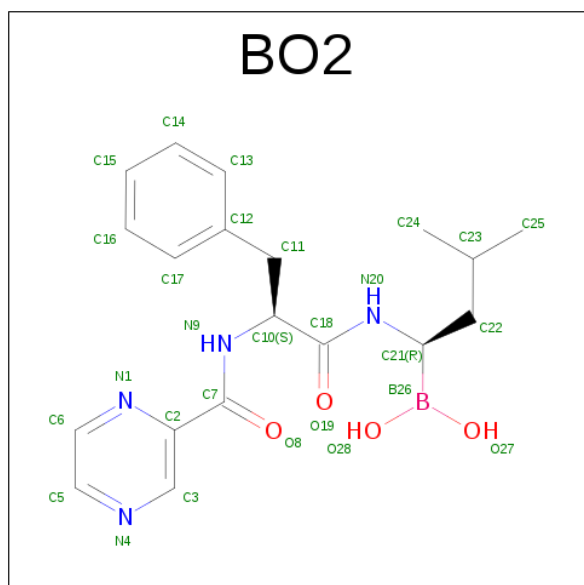
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	G	1	Total Mg 1 1	0	0
15	J	1	Total Mg 1 1	0	0
15	Y	1	Total Mg 1 1	0	0
15	Z	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0

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

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

- Molecule 17 is N-[(1R)-1-(DIHYDROXYBORYL)-3-METHYLBUTYL]-N-(PYRAZIN-2-YLCARBONYL)-L-PHENYLALANINAMIDE (three-letter code: BO2) (formula: C₁₉H₂₅BN₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	H	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
17	K	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
17	N	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
17	V	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
17	Y	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
17	b	1	Total	B	C	N	O	0	0
			28	1	19	4	4		

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	7	Total	O	0	0
			7	7		
18	B	8	Total	O	0	0
			8	8		
18	C	5	Total	O	0	0
			5	5		
18	D	5	Total	O	0	0
			5	5		
18	E	2	Total	O	0	0
			2	2		
18	F	11	Total	O	0	0
			11	11		
18	G	13	Total	O	0	0
			13	13		
18	H	14	Total	O	0	0
			14	14		
18	I	9	Total	O	0	0
			9	9		
18	J	9	Total	O	0	0
			9	9		
18	K	12	Total	O	0	0
			12	12		
18	L	10	Total	O	0	0
			10	10		
18	M	18	Total	O	0	0
			18	18		
18	N	5	Total	O	0	0
			5	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	O	8	Total O 8 8	0	0
18	P	8	Total O 8 8	0	0
18	Q	8	Total O 8 8	0	0
18	R	5	Total O 5 5	0	0
18	S	3	Total O 3 3	0	0
18	T	4	Total O 4 4	0	0
18	U	8	Total O 8 8	0	0
18	V	11	Total O 11 11	0	0
18	W	4	Total O 4 4	0	0
18	X	11	Total O 11 11	0	0
18	Y	8	Total O 8 8	0	0
18	Z	14	Total O 14 14	0	0
18	a	25	Total O 25 25	0	0
18	b	8	Total O 8 8	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.

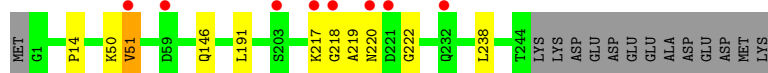
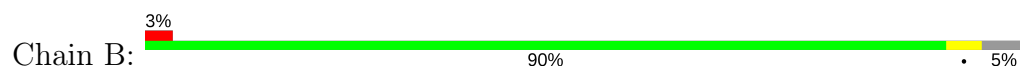
- Molecule 1: Proteasome subunit alpha type-2



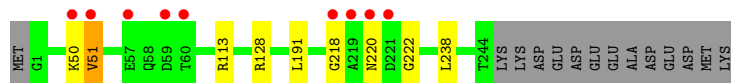
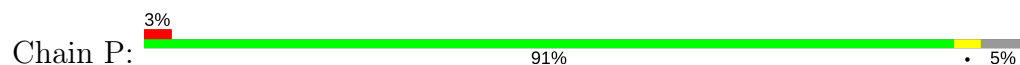
- Molecule 1: Proteasome subunit alpha type-2



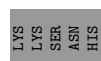
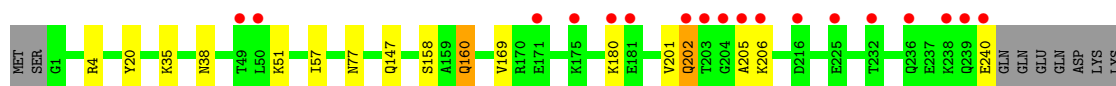
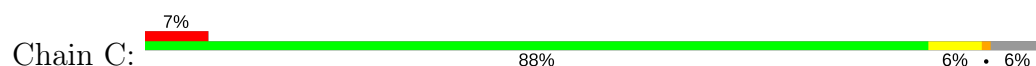
- Molecule 2: Proteasome subunit alpha type-3



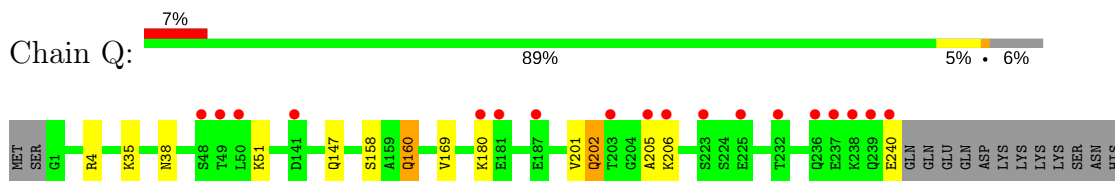
- Molecule 2: Proteasome subunit alpha type-3



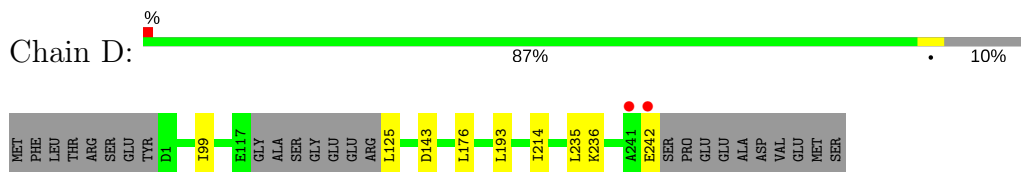
- Molecule 3: Proteasome subunit alpha type-4



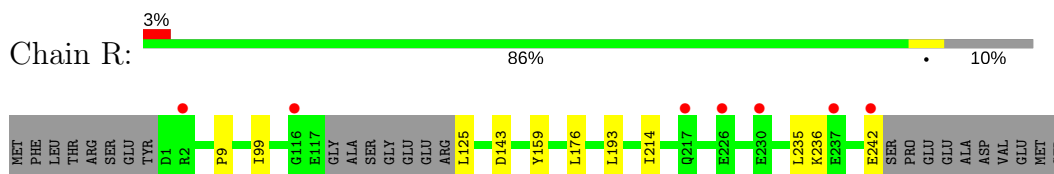
- Molecule 3: Proteasome subunit alpha type-4



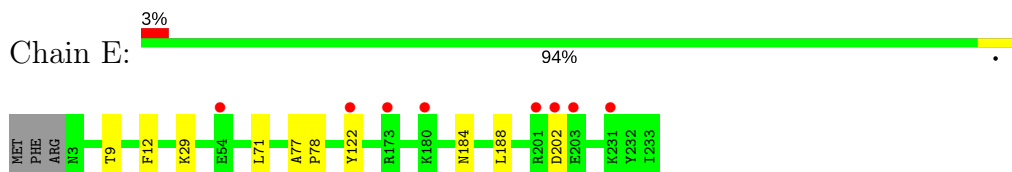
- Molecule 4: Proteasome subunit alpha type-5



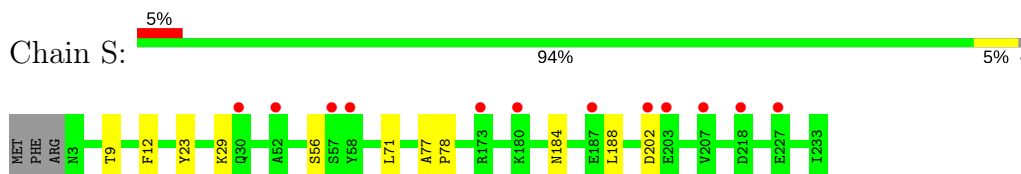
- Molecule 4: Proteasome subunit alpha type-5



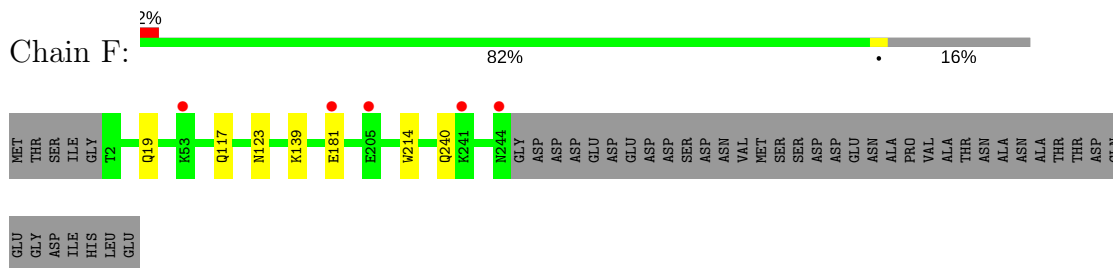
- Molecule 5: Proteasome subunit alpha type-6



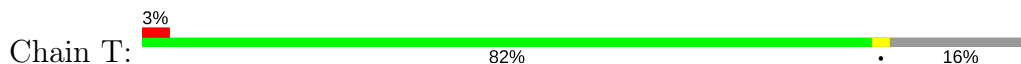
- Molecule 5: Proteasome subunit alpha type-6



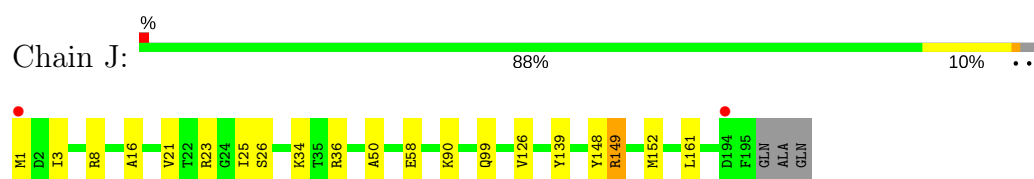
- Molecule 6: Probable proteasome subunit alpha type-7



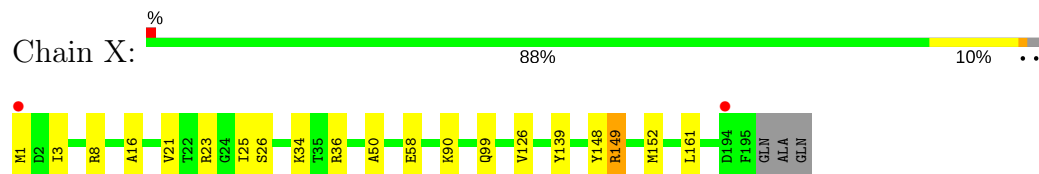
- Molecule 6: Probable proteasome subunit alpha type-7



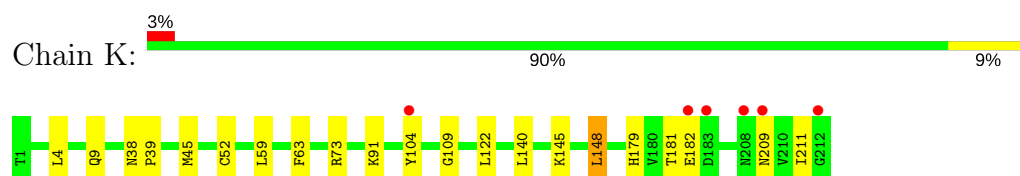




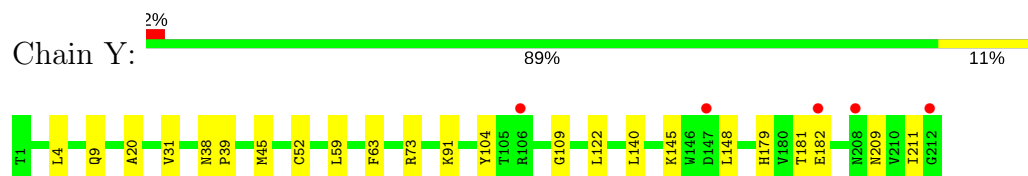
- Molecule 10: Proteasome subunit beta type-4



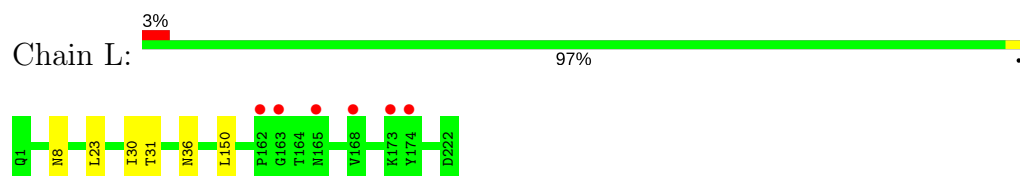
- Molecule 11: Proteasome subunit beta type-5



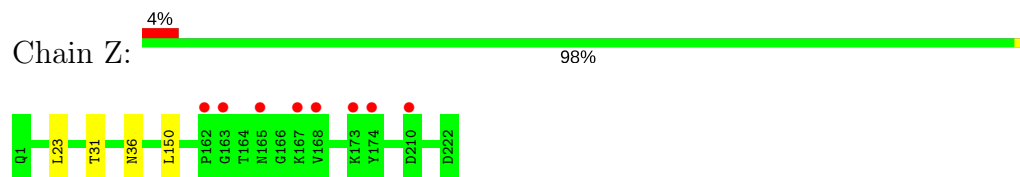
- Molecule 11: Proteasome subunit beta type-5



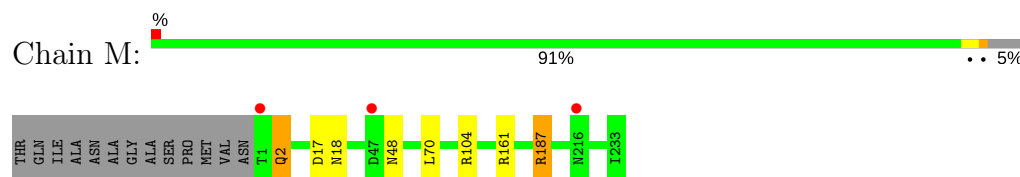
- Molecule 12: Proteasome subunit beta type-6



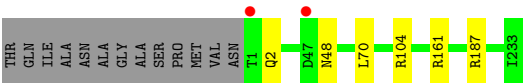
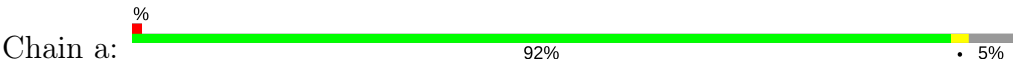
- Molecule 12: Proteasome subunit beta type-6



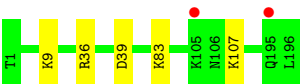
- Molecule 13: Proteasome subunit beta type-7



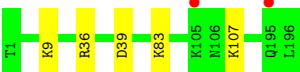
- Molecule 13: Proteasome subunit beta type-7



• Molecule 14: Proteasome subunit beta type-1



• Molecule 14: Proteasome subunit beta type-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	138.14Å 299.96Å 146.57Å 90.00° 113.18° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 15.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.7 (15.00-2.90) 98.7 (15.00-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.25 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.183 , 0.217 0.192 , 0.224	Depositor DCC
R_{free} test set	11833 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	65.2	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.6	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	0.94	EDS
Total number of atoms	49806	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% 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: BO2, MG, CL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.28	0/1952	0.47	0/2642
1	O	0.27	0/1952	0.46	0/2642
2	B	0.28	0/1934	0.49	0/2618
2	P	0.27	0/1934	0.49	0/2618
3	C	0.27	0/1910	0.50	0/2586
3	Q	0.27	0/1910	0.50	0/2586
4	D	0.27	0/1837	0.47	0/2475
4	R	0.27	0/1837	0.47	0/2475
5	E	0.27	0/1800	0.46	0/2433
5	S	0.27	0/1800	0.46	0/2433
6	F	0.28	0/1932	0.44	0/2609
6	T	0.27	0/1932	0.44	0/2609
7	G	0.28	0/1945	0.46	0/2634
7	U	0.27	0/1945	0.46	0/2634
8	H	0.26	0/1750	0.46	0/2373
8	V	0.25	0/1750	0.46	0/2373
9	I	0.28	0/1611	0.48	0/2174
9	W	0.28	0/1611	0.48	0/2174
10	J	0.34	0/1589	0.49	0/2142
10	X	0.36	0/1589	0.48	0/2142
11	K	0.27	0/1687	0.50	0/2282
11	Y	0.27	0/1687	0.50	0/2282
12	L	0.28	0/1795	0.47	0/2420
12	Z	0.28	0/1795	0.47	0/2420
13	M	0.28	0/1855	0.50	0/2514
13	a	0.28	0/1855	0.51	0/2514
14	N	0.26	0/1541	0.47	0/2087
14	b	0.26	0/1541	0.47	0/2087
All	All	0.28	0/50276	0.48	0/67978

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	2	0
1	O	1915	0	1929	2	0
2	B	1904	0	1904	5	0
2	P	1904	0	1904	3	0
3	C	1881	0	1895	6	0
3	Q	1881	0	1895	4	0
4	D	1813	0	1797	0	0
4	R	1813	0	1797	2	0
5	E	1773	0	1775	4	0
5	S	1773	0	1775	4	0
6	F	1892	0	1883	1	0
6	T	1892	0	1883	1	0
7	G	1907	0	1901	2	0
7	U	1907	0	1901	3	0
8	H	1719	0	1718	5	0
8	V	1719	0	1718	6	0
9	I	1581	0	1574	7	0
9	W	1581	0	1574	7	0
10	J	1561	0	1569	14	0
10	X	1561	0	1569	13	0
11	K	1649	0	1598	18	0
11	Y	1649	0	1598	18	0
12	L	1757	0	1711	2	0
12	Z	1757	0	1711	1	0
13	M	1824	0	1832	3	0
13	a	1824	0	1832	0	0
14	N	1512	0	1480	0	0
14	b	1512	0	1480	0	0
15	G	1	0	0	0	0
15	J	1	0	0	0	0
15	N	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	Y	1	0	0	0	0
15	Z	1	0	0	0	0
16	G	1	0	0	0	0
16	N	1	0	0	0	0
16	U	1	0	0	0	0
16	b	1	0	0	0	0
17	H	28	0	25	0	0
17	K	28	0	25	0	0
17	N	28	0	25	1	0
17	V	28	0	25	0	0
17	Y	28	0	25	0	0
17	b	28	0	25	0	0
18	A	7	0	0	0	0
18	B	8	0	0	0	0
18	C	5	0	0	0	0
18	D	5	0	0	0	0
18	E	2	0	0	0	0
18	F	11	0	0	0	0
18	G	13	0	0	0	0
18	H	14	0	0	0	0
18	I	9	0	0	0	0
18	J	9	0	0	0	0
18	K	12	0	0	0	0
18	L	10	0	0	0	0
18	M	18	0	0	1	0
18	N	5	0	0	0	0
18	O	8	0	0	0	0
18	P	8	0	0	0	0
18	Q	8	0	0	0	0
18	R	5	0	0	0	0
18	S	3	0	0	0	0
18	T	4	0	0	0	0
18	U	8	0	0	0	0
18	V	11	0	0	0	0
18	W	4	0	0	0	0
18	X	11	0	0	0	0
18	Y	8	0	0	0	0
18	Z	14	0	0	0	0
18	a	25	0	0	0	0
18	b	8	0	0	0	0
All	All	49806	0	49282	109	0

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

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

All (109) 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:K:104:TYR:CE2	11:K:182:GLU:HA	2.00	0.95
11:Y:104:TYR:CE2	11:Y:182:GLU:HA	2.00	0.94
10:J:149:ARG:O	10:J:152:MET:HG3	1.78	0.83
10:X:149:ARG:HG3	10:X:149:ARG:HH21	1.45	0.81
10:X:149:ARG:NH2	10:X:149:ARG:HG3	2.00	0.77
11:K:104:TYR:CD2	11:K:182:GLU:HA	2.20	0.76
11:Y:104:TYR:CD2	11:Y:182:GLU:HA	2.20	0.75
11:K:104:TYR:HE2	11:K:182:GLU:HA	1.51	0.74
11:Y:104:TYR:HE2	11:Y:182:GLU:HA	1.53	0.72
10:J:25:ILE:O	10:X:139:TYR:OH	2.11	0.68
11:K:104:TYR:HE2	11:K:182:GLU:CA	2.08	0.66
11:Y:104:TYR:HE1	11:Y:109:GLY:HA2	1.60	0.66
11:Y:104:TYR:HE2	11:Y:182:GLU:CA	2.09	0.66
11:K:104:TYR:HE1	11:K:109:GLY:HA2	1.60	0.66
10:J:139:TYR:OH	10:X:25:ILE:O	2.13	0.65
10:X:149:ARG:O	10:X:152:MET:HG3	1.99	0.62
10:J:149:ARG:CG	10:J:149:ARG:HH21	2.13	0.61
10:X:8:ARG:O	10:X:148:TYR:OH	2.12	0.60
11:K:104:TYR:CE2	11:K:182:GLU:CA	2.78	0.59
11:Y:104:TYR:CE2	11:Y:182:GLU:CA	2.78	0.58
10:X:149:ARG:CG	10:X:149:ARG:HH21	2.12	0.58
11:Y:104:TYR:CE1	11:Y:109:GLY:HA2	2.40	0.57
10:X:50:ALA:O	11:Y:91:LYS:NZ	2.38	0.56
11:K:104:TYR:CE1	11:K:109:GLY:HA2	2.40	0.55
10:J:149:ARG:HG3	10:J:149:ARG:NH2	2.21	0.55
11:K:209:ASN:O	9:W:38:LYS:NZ	2.39	0.55
11:K:73:ARG:NH2	11:K:104:TYR:O	2.36	0.55
11:Y:45:MET:HG2	11:Y:52:CYS:HB3	1.90	0.54
8:H:196:ARG:NH2	9:I:150:GLU:O	2.41	0.54
11:Y:59:LEU:HG	11:Y:63:PHE:CZ	2.43	0.53
13:M:2:GLN:NE2	18:M:318:HOH:O	2.41	0.53
11:K:45:MET:HG2	11:K:52:CYS:HB3	1.91	0.53
11:K:59:LEU:HG	11:K:63:PHE:CZ	2.44	0.53
9:I:125:LEU:HG	9:I:126:ILE:HG22	1.91	0.52
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	1.92	0.52
9:W:125:LEU:HG	9:W:126:ILE:HG22	1.92	0.52
11:Y:73:ARG:NH2	11:Y:104:TYR:O	2.36	0.52
10:J:50:ALA:O	11:K:91:LYS:NZ	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:23:PHE:O	7:U:26:THR:HB	2.09	0.51
7:G:23:PHE:O	7:G:26:THR:HB	2.11	0.51
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.58	0.51
8:V:196:ARG:NH2	9:W:150:GLU:O	2.44	0.51
9:I:38:LYS:NZ	11:Y:209:ASN:O	2.44	0.51
3:C:201:VAL:O	3:C:202:GLN:CB	2.58	0.50
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.93	0.50
10:J:149:ARG:HG3	10:J:149:ARG:HH21	1.77	0.49
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.48	0.49
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.97	0.47
10:X:36:ARG:NH1	10:X:58:GLU:OE2	2.48	0.47
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.97	0.46
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.50	0.46
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.98	0.46
10:J:8:ARG:O	10:J:148:TYR:OH	2.21	0.46
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.80	0.46
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.81	0.46
10:J:36:ARG:NH1	10:J:58:GLU:OE2	2.49	0.45
3:C:35:LYS:HG2	3:C:158:SER:O	2.16	0.44
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.99	0.44
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.82	0.44
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.17	0.44
11:K:179:HIS:CE1	11:K:181:THR:HG23	2.53	0.44
8:V:104:ASP:HB2	8:V:105:PRO:HD2	2.00	0.44
11:Y:179:HIS:CE1	11:Y:181:THR:HG23	2.53	0.44
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.99	0.44
9:W:36:SER:HB2	10:X:126:VAL:HG11	2.00	0.43
2:B:146:GLN:HG2	3:C:57:ILE:HG21	1.99	0.43
2:B:50:LYS:O	2:B:51:VAL:C	2.57	0.43
2:P:50:LYS:O	2:P:51:VAL:C	2.57	0.43
8:H:104:ASP:HB2	8:H:105:PRO:HD2	2.01	0.42
2:P:50:LYS:HD3	2:P:50:LYS:HA	1.88	0.42
8:V:84:LYS:HE2	8:V:119:THR:HG23	2.01	0.42
8:V:35:HIS:HB3	8:V:56:THR:HG21	2.00	0.42
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.53	0.42
13:M:17:ASP:OD1	13:M:18:ASN:N	2.52	0.42
9:I:10:ILE:HG21	9:I:141:ALA:HB3	2.02	0.42
10:X:1:MET:HG2	10:X:34:LYS:HE3	2.00	0.42
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	2.02	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.83	0.42
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ARG:HD3	5:E:122:TYR:HD2	1.85	0.42
8:H:84:LYS:HE2	8:H:119:THR:HG23	2.01	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.42
2:B:217:LYS:O	2:B:219:ALA:N	2.46	0.42
11:K:104:TYR:CE2	11:K:182:GLU:HG3	2.55	0.42
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.85	0.41
9:W:10:ILE:HG21	9:W:141:ALA:HB3	2.01	0.41
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.51	0.41
5:S:12:PHE:H	6:T:19:GLN:HE22	1.67	0.41
13:M:187:ARG:NH1	8:V:139:GLU:OE1	2.50	0.41
5:E:77:ALA:N	5:E:78:PRO:CD	2.84	0.41
11:K:145:LYS:HB2	11:K:148:LEU:HD13	2.02	0.41
11:K:38:ASN:HB2	11:K:39:PRO:CD	2.51	0.41
4:R:9:PRO:HA	5:S:23:TYR:CD1	2.56	0.41
2:B:14:PRO:HA	3:C:20:TYR:CE1	2.55	0.41
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.41
10:J:25:ILE:HG12	10:J:25:ILE:O	2.21	0.41
8:H:114:HIS:CD2	17:N:201:BO2:H5	2.56	0.41
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.51	0.41
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	2.03	0.41
5:E:12:PHE:H	6:F:19:GLN:HE22	1.68	0.40
11:K:104:TYR:HE2	11:K:182:GLU:CB	2.34	0.40
12:L:8:ASN:HA	12:L:30:ILE:O	2.21	0.40
3:Q:201:VAL:O	3:Q:202:GLN:HB3	2.21	0.40
1:A:4:ARG:NH1	5:E:122:TYR:O	2.55	0.40
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.04	0.40
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.04	0.40
9:W:9:GLY:HA3	9:W:41:LYS:HE2	2.04	0.40
11:Y:104:TYR:HE2	11:Y:182:GLU:CB	2.34	0.40
9:I:98:ARG:CD	9:I:126:ILE:HD12	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	38	72
1	O	248/250 (99%)	241 (97%)	6 (2%)	1 (0%)	38	72
2	B	242/258 (94%)	232 (96%)	6 (2%)	4 (2%)	11	36
2	P	242/258 (94%)	232 (96%)	6 (2%)	4 (2%)	11	36
3	C	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	22	57
3	Q	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	22	57
4	D	231/260 (89%)	228 (99%)	3 (1%)	0	100	100
4	R	231/260 (89%)	228 (99%)	3 (1%)	0	100	100
5	E	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
5	S	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
6	F	241/288 (84%)	238 (99%)	3 (1%)	0	100	100
6	T	241/288 (84%)	238 (99%)	3 (1%)	0	100	100
7	G	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
7	U	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
8	H	224/232 (97%)	216 (96%)	8 (4%)	0	100	100
8	V	224/232 (97%)	216 (96%)	8 (4%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	189 (98%)	4 (2%)	0	100	100
10	X	193/198 (98%)	189 (98%)	4 (2%)	0	100	100
11	K	210/212 (99%)	207 (99%)	3 (1%)	0	100	100
11	Y	210/212 (99%)	207 (99%)	3 (1%)	0	100	100
12	L	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
12	Z	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
13	M	231/246 (94%)	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
All	All	6284/6614 (95%)	6130 (98%)	140 (2%)	14 (0%)	51	82

All (14) Ramachandran outliers are listed below:

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

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%)	206 (99%)	3 (1%)	71	91
1	O	209/209 (100%)	206 (99%)	3 (1%)	71	91
2	B	203/216 (94%)	201 (99%)	2 (1%)	80	95
2	P	203/216 (94%)	200 (98%)	3 (2%)	70	91
3	C	212/226 (94%)	202 (95%)	10 (5%)	30	65
3	Q	212/226 (94%)	203 (96%)	9 (4%)	34	69
4	D	194/215 (90%)	185 (95%)	9 (5%)	31	65
4	R	194/215 (90%)	185 (95%)	9 (5%)	31	65
5	E	190/193 (98%)	184 (97%)	6 (3%)	44	78
5	S	190/193 (98%)	184 (97%)	6 (3%)	44	78
6	F	201/239 (84%)	195 (97%)	6 (3%)	46	80
6	T	201/239 (84%)	195 (97%)	6 (3%)	46	80
7	G	206/210 (98%)	199 (97%)	7 (3%)	42	76
7	U	206/210 (98%)	199 (97%)	7 (3%)	42	76

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	185/190 (97%)	181 (98%)	4 (2%)	57	86
8	V	185/190 (97%)	181 (98%)	4 (2%)	57	86
9	I	172/173 (99%)	169 (98%)	3 (2%)	66	89
9	W	172/173 (99%)	169 (98%)	3 (2%)	66	89
10	J	173/175 (99%)	167 (96%)	6 (4%)	41	75
10	X	173/175 (99%)	167 (96%)	6 (4%)	41	75
11	K	169/169 (100%)	164 (97%)	5 (3%)	46	80
11	Y	169/169 (100%)	165 (98%)	4 (2%)	54	84
12	L	185/185 (100%)	183 (99%)	2 (1%)	78	94
12	Z	185/185 (100%)	183 (99%)	2 (1%)	78	94
13	M	199/208 (96%)	193 (97%)	6 (3%)	46	80
13	a	199/208 (96%)	193 (97%)	6 (3%)	46	80
14	N	162/162 (100%)	157 (97%)	5 (3%)	45	79
14	b	162/162 (100%)	157 (97%)	5 (3%)	45	79
All	All	5320/5540 (96%)	5173 (97%)	147 (3%)	49	82

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	51	LYS
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	206	LYS
3	C	240	GLU
4	D	99	ILE
4	D	125	LEU
4	D	143	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	71	LEU
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	181	GLU
6	F	214	TRP
6	F	240	GLN
7	G	115	LEU
7	G	117	GLN
7	G	122	ARG
7	G	125	MET
7	G	208	GLU
7	G	235	ARG
7	G	236	LEU
8	H	30	ASN
8	H	68	LEU
8	H	113	ILE
8	H	196	ARG
9	I	37	ASN
9	I	126	ILE
9	I	171	LEU
10	J	3	ILE
10	J	23	ARG
10	J	26	SER
10	J	90	LYS
10	J	99	GLN
10	J	149	ARG
11	K	4	LEU
11	K	9	GLN
11	K	140	LEU
11	K	148	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	K	211	ILE
12	L	23	LEU
12	L	150	LEU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
14	N	9	LYS
14	N	36	ARG
14	N	39	ASP
14	N	83	LYS
14	N	107	LYS
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	113	ARG
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	51	LYS
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	206	LYS
3	Q	240	GLU
4	R	99	ILE
4	R	125	LEU
4	R	143	ASP
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	71	LEU
5	S	184	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	S	188	LEU
5	S	202	ASP
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	181	GLU
6	T	214	TRP
6	T	240	GLN
7	U	115	LEU
7	U	117	GLN
7	U	122	ARG
7	U	125	MET
7	U	208	GLU
7	U	235	ARG
7	U	236	LEU
8	V	30	ASN
8	V	68	LEU
8	V	113	ILE
8	V	196	ARG
9	W	37	ASN
9	W	126	ILE
9	W	171	LEU
10	X	3	ILE
10	X	23	ARG
10	X	26	SER
10	X	90	LYS
10	X	99	GLN
10	X	149	ARG
11	Y	4	LEU
11	Y	9	GLN
11	Y	140	LEU
11	Y	211	ILE
12	Z	23	LEU
12	Z	150	LEU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
14	b	9	LYS
14	b	36	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	b	39	ASP
14	b	83	LYS
14	b	107	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	20	GLN
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
3	C	147	GLN
3	C	160	GLN
4	D	91	HIS
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
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
8	H	66	HIS
10	J	55	GLN
11	K	9	GLN
11	K	85	ASN
11	K	176	ASN
12	L	3	ASN
12	L	79	HIS
13	M	48	ASN
13	M	102	GLN
1	O	94	HIS
2	P	20	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	58	GLN
2	P	119	GLN
2	P	123	GLN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS
4	R	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
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
10	X	55	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	176	ASN
12	Z	3	ASN
12	Z	79	HIS
13	a	48	ASN
13	a	102	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 9 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BO2	H	301	8	27,29,29	1.56	5 (18%)	30,38,38	1.22	3 (10%)
17	BO2	K	301	11	27,29,29	1.58	5 (18%)	30,38,38	1.25	4 (13%)
17	BO2	N	201	14	27,29,29	1.54	4 (14%)	30,38,38	1.15	4 (13%)
17	BO2	V	301	8	27,29,29	1.52	5 (18%)	30,38,38	1.22	4 (13%)
17	BO2	Y	301	11	27,29,29	1.58	5 (18%)	30,38,38	1.23	4 (13%)
17	BO2	b	201	14	27,29,29	1.55	4 (14%)	30,38,38	1.15	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BO2	H	301	8	-	0/22/28/28	0/2/2/2
17	BO2	K	301	11	-	0/22/28/28	0/2/2/2
17	BO2	N	201	14	-	0/22/28/28	0/2/2/2
17	BO2	V	301	8	-	0/22/28/28	0/2/2/2
17	BO2	Y	301	11	-	0/22/28/28	0/2/2/2
17	BO2	b	201	14	-	0/22/28/28	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	201	BO2	C2-C7	-4.72	1.39	1.50
17	N	201	BO2	C2-C7	-4.66	1.39	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	H	301	BO2	C2-C7	-4.66	1.39	1.50
17	Y	301	BO2	C2-C7	-4.61	1.39	1.50
17	K	301	BO2	C2-C7	-4.60	1.39	1.50
17	V	301	BO2	C2-C7	-4.55	1.39	1.50
17	K	301	BO2	C11-C12	-4.47	1.40	1.51
17	Y	301	BO2	C11-C12	-4.41	1.40	1.51
17	H	301	BO2	C11-C12	-4.31	1.41	1.51
17	b	201	BO2	C11-C12	-4.25	1.41	1.51
17	V	301	BO2	C11-C12	-4.15	1.41	1.51
17	N	201	BO2	C11-C12	-4.15	1.41	1.51
17	H	301	BO2	C5-N4	2.19	1.40	1.33
17	V	301	BO2	C5-N4	2.20	1.40	1.33
17	Y	301	BO2	C5-N4	2.23	1.40	1.33
17	K	301	BO2	C5-N4	2.26	1.40	1.33
17	b	201	BO2	C6-N1	2.42	1.39	1.34
17	N	201	BO2	C6-N1	2.57	1.40	1.34
17	V	301	BO2	C6-N1	2.63	1.40	1.34
17	H	301	BO2	C6-N1	2.65	1.40	1.34
17	b	201	BO2	C3-N4	2.67	1.39	1.34
17	K	301	BO2	C6-N1	2.74	1.40	1.34
17	V	301	BO2	C3-N4	2.76	1.40	1.34
17	Y	301	BO2	C6-N1	2.78	1.40	1.34
17	N	201	BO2	C3-N4	2.79	1.40	1.34
17	H	301	BO2	C3-N4	2.86	1.40	1.34
17	Y	301	BO2	C3-N4	2.92	1.40	1.34
17	K	301	BO2	C3-N4	2.94	1.40	1.34

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	H	301	BO2	C12-C11-C10	-2.66	105.98	113.41
17	V	301	BO2	C12-C11-C10	-2.56	106.26	113.41
17	b	201	BO2	C11-C10-N9	-2.45	105.62	110.80
17	N	201	BO2	C11-C10-N9	-2.39	105.74	110.80
17	Y	301	BO2	C18-C10-N9	-2.37	104.69	111.20
17	K	301	BO2	C18-C10-N9	-2.34	104.76	111.20
17	K	301	BO2	C6-C5-N4	-2.18	119.24	121.97
17	b	201	BO2	C6-C5-N4	-2.17	119.25	121.97
17	N	201	BO2	C18-C10-N9	-2.13	105.33	111.20
17	N	201	BO2	C6-C5-N4	-2.13	119.30	121.97
17	Y	301	BO2	C6-C5-N4	-2.11	119.33	121.97
17	V	301	BO2	C5-C6-N1	-2.06	119.45	122.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Y	301	BO2	C2-C3-N4	-2.04	119.66	122.04
17	H	301	BO2	C5-C6-N1	-2.04	119.47	122.17
17	b	201	BO2	C18-C10-N9	-2.02	105.64	111.20
17	V	301	BO2	C6-C5-N4	-2.01	119.45	121.97
17	K	301	BO2	C2-C3-N4	-2.00	119.70	122.04
17	b	201	BO2	C6-N1-C2	2.79	120.64	116.94
17	N	201	BO2	C6-N1-C2	2.87	120.73	116.94
17	Y	301	BO2	C6-N1-C2	3.29	121.29	116.94
17	H	301	BO2	C6-N1-C2	3.34	121.36	116.94
17	V	301	BO2	C6-N1-C2	3.38	121.41	116.94
17	K	301	BO2	C6-N1-C2	3.41	121.45	116.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	N	201	BO2	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.38	5 (2%) 65 62	45, 62, 101, 145	0
1	O	250/250 (100%)	-0.27	9 (3%) 43 37	51, 72, 117, 155	0
2	B	244/258 (94%)	-0.27	8 (3%) 47 40	46, 68, 114, 163	0
2	P	244/258 (94%)	-0.23	9 (3%) 42 37	52, 74, 114, 163	0
3	C	240/254 (94%)	-0.10	18 (7%) 15 11	47, 75, 143, 170	0
3	Q	240/254 (94%)	0.15	18 (7%) 15 11	57, 90, 174, 201	0
4	D	235/260 (90%)	-0.37	2 (0%) 84 83	51, 73, 107, 145	0
4	R	235/260 (90%)	-0.19	7 (2%) 51 44	59, 80, 123, 153	0
5	E	231/234 (98%)	-0.18	8 (3%) 44 38	54, 79, 121, 156	0
5	S	231/234 (98%)	-0.09	12 (5%) 28 23	54, 84, 132, 165	0
6	F	243/288 (84%)	-0.42	5 (2%) 64 60	47, 70, 116, 142	0
6	T	243/288 (84%)	-0.30	9 (3%) 42 37	49, 74, 128, 163	0
7	G	241/252 (95%)	-0.41	7 (2%) 52 46	46, 65, 107, 157	0
7	U	241/252 (95%)	-0.38	6 (2%) 58 53	50, 66, 102, 146	0
8	H	226/232 (97%)	-0.42	3 (1%) 77 76	41, 59, 97, 149	0
8	V	226/232 (97%)	-0.38	7 (3%) 49 43	39, 61, 100, 168	0
9	I	204/205 (99%)	-0.67	2 (0%) 82 81	41, 57, 88, 124	0
9	W	204/205 (99%)	-0.59	2 (0%) 82 81	41, 61, 90, 118	0
10	J	195/198 (98%)	-0.47	2 (1%) 82 81	37, 63, 96, 141	0
10	X	195/198 (98%)	-0.47	2 (1%) 82 81	48, 66, 95, 143	0
11	K	212/212 (100%)	-0.39	6 (2%) 53 48	43, 62, 102, 123	0
11	Y	212/212 (100%)	-0.39	5 (2%) 59 55	45, 62, 104, 125	0
12	L	222/222 (100%)	-0.38	6 (2%) 55 50	43, 62, 119, 151	0
12	Z	222/222 (100%)	-0.43	8 (3%) 43 37	34, 61, 112, 143	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%)	-0.56	3 (1%)	77	76	40, 60, 86, 104	0
13	a	233/246 (94%)	-0.55	2 (0%)	84	83	41, 60, 85, 102	0
14	N	196/196 (100%)	-0.61	2 (1%)	82	81	42, 56, 90, 117	0
14	b	196/196 (100%)	-0.61	2 (1%)	82	81	41, 57, 91, 121	0
All	All	6344/6614 (95%)	-0.36	175 (2%)	53	48	34, 67, 117, 201	0

All (175) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	49	THR	8.0
3	C	49	THR	7.5
3	Q	206	LYS	6.9
12	L	174	TYR	6.8
3	Q	236	GLN	6.8
3	Q	239	GLN	6.7
3	Q	50	LEU	6.6
12	Z	174	TYR	5.8
10	X	1	MET	5.3
5	E	202	ASP	5.2
3	C	205	ALA	5.2
2	B	218	GLY	5.1
2	B	221	ASP	5.0
10	J	1	MET	4.8
2	P	51	VAL	4.7
1	O	249	ALA	4.6
8	V	224	GLN	4.4
10	J	194	ASP	4.2
1	O	248	GLU	4.2
8	H	224	GLN	4.1
6	F	241	LYS	4.1
5	S	202	ASP	4.1
2	P	219	ALA	4.1
3	C	206	LYS	4.0
10	X	194	ASP	3.9
2	P	221	ASP	3.9
2	P	218	GLY	3.9
2	P	59	ASP	3.8
14	b	195	GLN	3.8
3	Q	223	SER	3.8
3	Q	48	SER	3.8
12	Z	173	LYS	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	Q	240	GLU	3.7
5	S	173	ARG	3.6
3	C	236	GLN	3.6
12	Z	167	LYS	3.5
12	L	162	PRO	3.5
3	C	225	GLU	3.5
5	E	180	LYS	3.4
3	C	50	LEU	3.4
12	L	165	ASN	3.4
6	F	244	ASN	3.4
7	U	242	GLN	3.4
1	O	201	GLU	3.4
2	B	220	ASN	3.4
3	Q	205	ALA	3.4
9	W	1	SER	3.3
6	T	237	ASP	3.3
7	U	203	ASP	3.3
2	B	203	SER	3.3
3	Q	180	LYS	3.3
11	K	212	GLY	3.3
7	G	241	GLU	3.2
8	V	226	GLU	3.2
8	V	222	ASP	3.2
6	T	244	ASN	3.2
3	Q	225	GLU	3.2
11	K	182	GLU	3.2
6	T	230	ASP	3.1
3	C	239	GLN	3.1
5	S	203	GLU	3.1
1	A	249	ALA	3.1
13	a	1	THR	3.1
3	Q	237	GLU	3.1
3	C	238	LYS	3.1
12	L	163	GLY	3.1
5	S	227	GLU	3.1
9	I	1	SER	3.1
6	T	205	GLU	3.1
14	b	105	LYS	3.0
5	E	54	GLU	3.0
1	A	1	MET	3.0
3	C	180	LYS	3.0
8	H	222	ASP	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	O	1	MET	3.0
3	C	202	GLN	3.0
14	N	105	LYS	3.0
2	B	51	VAL	2.9
12	Z	163	GLY	2.9
7	G	2	GLY	2.9
1	A	250	LEU	2.8
8	V	221	CYS	2.8
3	Q	238	LYS	2.8
11	K	209	ASN	2.8
11	Y	212	GLY	2.8
3	Q	203	THR	2.8
12	L	173	LYS	2.7
7	G	3	TYR	2.7
3	Q	187	GLU	2.7
5	E	203	GLU	2.7
5	S	187	GLU	2.7
3	Q	232	THR	2.7
7	G	181	LYS	2.7
1	A	248	GLU	2.7
1	O	231	LYS	2.6
2	P	220	ASN	2.6
8	H	145	ASP	2.6
2	B	217	LYS	2.6
2	P	60	THR	2.6
6	T	241	LYS	2.6
3	C	240	GLU	2.6
5	S	57	SER	2.6
5	E	201	ARG	2.6
5	E	173	ARG	2.6
2	B	232	GLN	2.6
11	Y	182	GLU	2.6
4	R	242	GLU	2.5
3	Q	181	GLU	2.5
1	O	182	GLU	2.5
8	V	145	ASP	2.5
7	G	242	GLN	2.5
1	O	241	GLN	2.5
11	K	104	TYR	2.5
11	K	208	ASN	2.5
3	C	232	THR	2.5
4	R	116	GLY	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	U	222	ASP	2.5
1	O	2	THR	2.5
1	A	182	GLU	2.4
4	R	217	GLN	2.4
5	E	231	LYS	2.4
12	Z	162	PRO	2.4
12	L	168	VAL	2.4
11	K	183	ASP	2.4
4	R	230	GLU	2.4
5	S	180	LYS	2.4
11	Y	106	ARG	2.3
4	D	242	GLU	2.3
5	S	207	VAL	2.3
5	S	58	TYR	2.3
11	Y	147	ASP	2.3
3	C	204	GLY	2.3
3	C	181	GLU	2.3
7	U	192	LYS	2.3
13	M	1	THR	2.3
13	M	47	ASP	2.3
5	S	30	GLN	2.3
4	R	2	ARG	2.2
12	Z	210	ASP	2.2
3	Q	141	ASP	2.2
4	R	237	GLU	2.2
5	E	122	TYR	2.2
9	W	192	ASP	2.2
12	Z	168	VAL	2.2
7	G	179	LYS	2.2
8	V	217	ILE	2.2
2	B	59	ASP	2.2
6	F	181	GLU	2.2
6	F	205	GLU	2.2
7	G	186	ASN	2.2
7	U	181	LYS	2.2
2	P	50	LYS	2.1
11	Y	208	ASN	2.1
3	C	171	GLU	2.1
4	D	241	ALA	2.1
13	M	216	ASN	2.1
3	C	216	ASP	2.1
14	N	195	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	T	243	ILE	2.1
4	R	226	GLU	2.1
5	S	52	ALA	2.1
6	T	229	GLY	2.1
6	T	201	GLU	2.1
6	F	53	LYS	2.1
9	I	192	ASP	2.1
8	V	9	ASN	2.1
3	C	203	THR	2.0
6	T	215	CYS	2.0
7	U	241	GLU	2.0
12	Z	165	ASN	2.0
2	P	57	GLU	2.0
5	S	218	ASP	2.0
13	a	47	ASP	2.0
1	O	52	SER	2.0
3	C	175	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
15	MG	J	201	1/1	0.98	0.28	7.80	43,43,43,43	0
17	BO2	N	201	28/28	0.90	0.23	3.42	41,54,70,70	0
17	BO2	b	201	28/28	0.92	0.20	2.77	47,54,67,69	0
17	BO2	V	301	28/28	0.92	0.20	2.08	54,59,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
17	BO2	Y	301	28/28	0.95	0.18	1.41	50,61,66,69	0
17	BO2	H	301	28/28	0.94	0.18	1.36	50,55,70,71	0
17	BO2	K	301	28/28	0.94	0.16	0.96	47,58,62,63	0
15	MG	Z	301	1/1	0.95	0.15	0.64	66,66,66,66	0
15	MG	N	202	1/1	0.97	0.10	-0.82	39,39,39,39	0
15	MG	Y	302	1/1	0.98	0.08	-1.01	66,66,66,66	0
15	MG	G	301	1/1	0.98	0.04	-2.18	65,65,65,65	0
16	CL	N	203	1/1	0.98	0.08	-2.31	47,47,47,47	0
16	CL	b	202	1/1	0.98	0.06	-3.37	51,51,51,51	0
16	CL	G	302	1/1	0.97	0.17	-	55,55,55,55	0
16	CL	U	301	1/1	0.98	0.20	-	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.