Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:11 PM GMT

PDB ID	:	4QWU
Title	:	yCP beta5-C52F mutant in complex with bortezomib
Authors	:	Huber, E.M.; Heinemeyer, W.; Groll, M.
Deposited on	:	2014-07-17
Resolution	:	3.00 Å(reported)

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

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

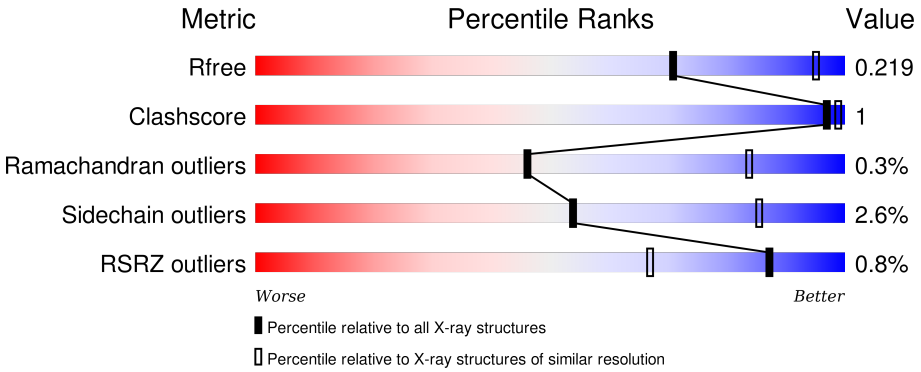
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	97%
1	O	250	97%
2	B	258	90% 5% 5%
2	P	258	90% 5% 5%
3	C	254	87% 7% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	Q	254	3% 88% 6% 6%
4	D	260	87% 10%
4	R	260	86% 10%
5	E	234	% 97%
5	S	234	% 95%
6	F	288	% 82% 16%
6	T	288	82% 16%
7	G	252	91% 5%
7	U	252	% 90% 5%
8	H	232	94%
8	V	232	% 93%
9	I	205	96%
9	W	205	95% 5%
10	J	198	% 91% 7%
10	X	198	% 90% 7%
11	K	212	90% 8%
11	Y	212	88% 10%
12	L	222	95%
12	Z	222	94%
13	M	246	92% 5%
13	a	246	92% 5%
14	N	196	97%
14	b	196	% 98%

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	b	201	-	-	-	X

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 49776 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	52	PHE	CYS	ENGINEERED MUTATION	UNP P30656
Y	52	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			

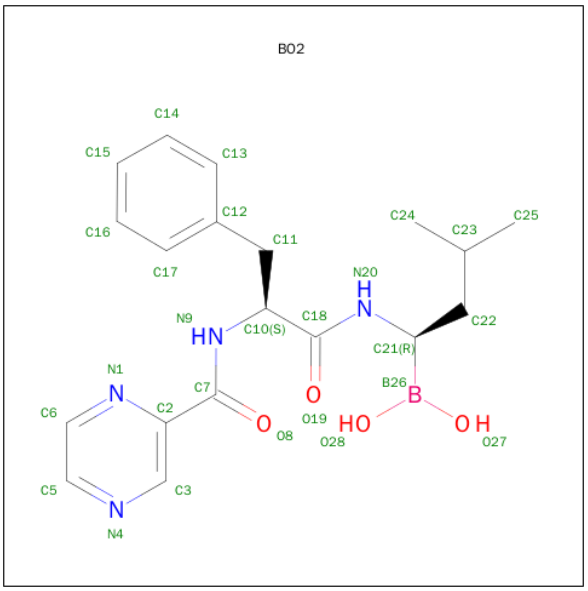
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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	K	1	Total Mg 1 1	0	0
15	V	1	Total Mg 1 1	0	0
15	Z	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0
15	Y	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: $C_{19}H_{25}BN_4O_4$).



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	6	Total	O	0	0
			6	6		
18	B	9	Total	O	0	0
			9	9		
18	C	8	Total	O	0	0
			8	8		
18	D	4	Total	O	0	0
			4	4		
18	E	5	Total	O	0	0
			5	5		
18	F	11	Total	O	0	0
			11	11		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	G	6	Total O 6 6	0	0
18	H	9	Total O 9 9	0	0
18	I	5	Total O 5 5	0	0
18	J	9	Total O 9 9	0	0
18	K	9	Total O 9 9	0	0
18	L	10	Total O 10 10	0	0
18	M	13	Total O 13 13	0	0
18	N	8	Total O 8 8	0	0
18	O	7	Total O 7 7	0	0
18	P	9	Total O 9 9	0	0
18	Q	5	Total O 5 5	0	0
18	R	4	Total O 4 4	0	0
18	S	5	Total O 5 5	0	0
18	T	4	Total O 4 4	0	0
18	U	13	Total O 13 13	0	0
18	V	8	Total O 8 8	0	0
18	W	4	Total O 4 4	0	0
18	X	9	Total O 9 9	0	0
18	Y	13	Total O 13 13	0	0
18	Z	9	Total O 9 9	0	0
18	a	15	Total O 15 15	0	0

Continued on next page...

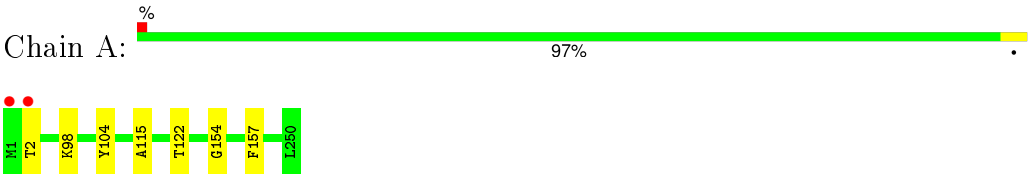
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	b	4	Total O 4 4	0	0

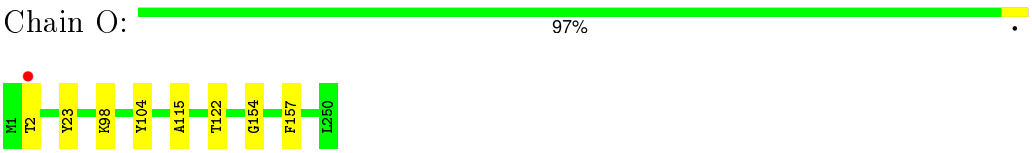
3 Residue-property plots (i)

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

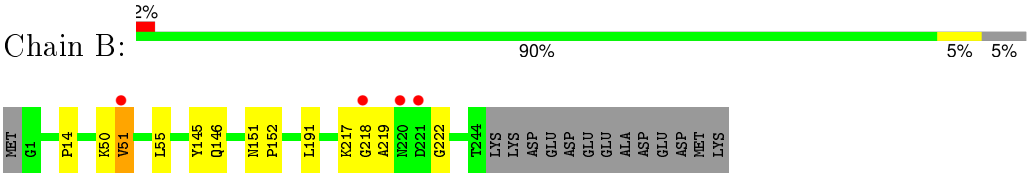
- Molecule 1: Proteasome subunit alpha type-2



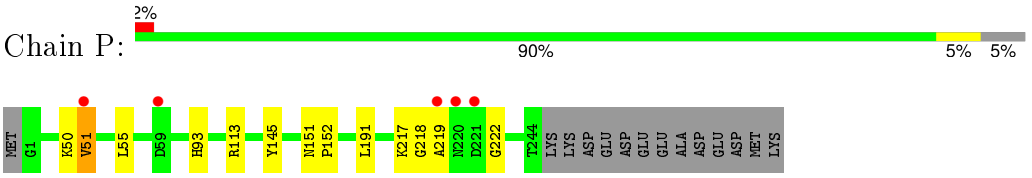
- Molecule 1: Proteasome subunit alpha type-2



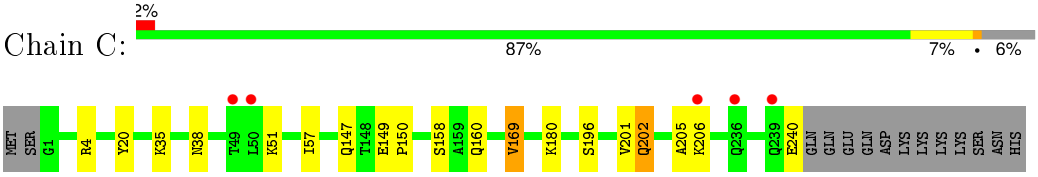
- Molecule 2: Proteasome subunit alpha type-3



- Molecule 2: Proteasome subunit alpha type-3

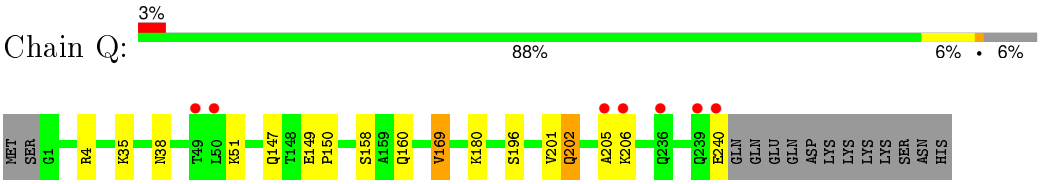


- Molecule 3: Proteasome subunit alpha type-4



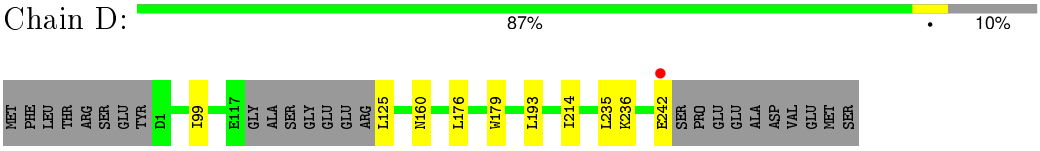
- Molecule 3: Proteasome subunit alpha type-4

Chain Q:



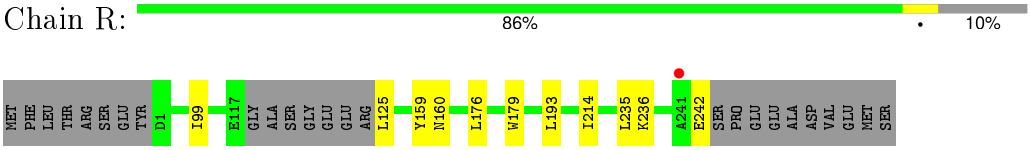
• Molecule 4: Proteasome subunit alpha type-5

Chain D:



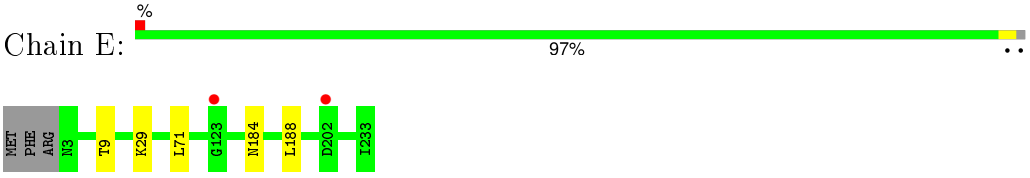
• Molecule 4: Proteasome subunit alpha type-5

Chain R:



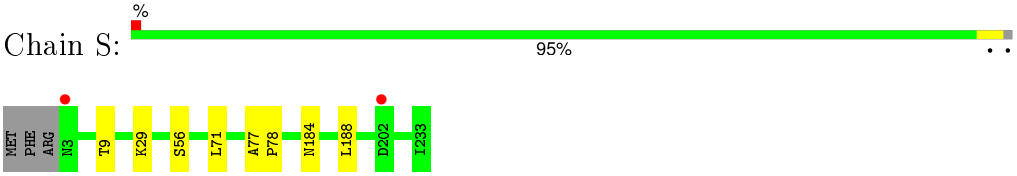
• Molecule 5: Proteasome subunit alpha type-6

Chain E:



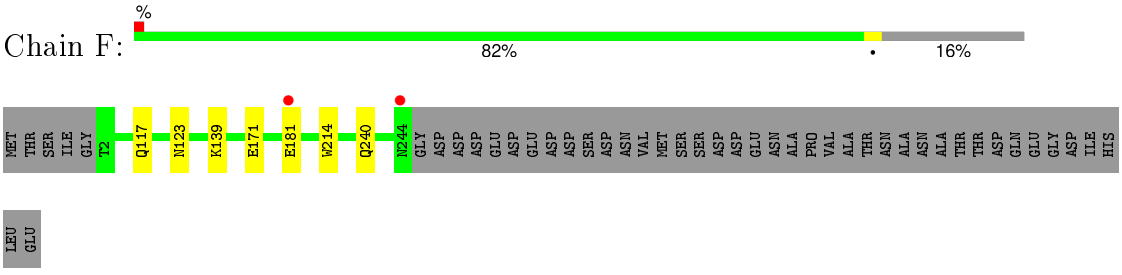
• Molecule 5: Proteasome subunit alpha type-6

Chain S:



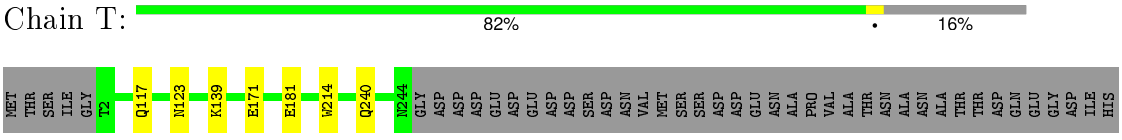
• Molecule 6: Probable proteasome subunit alpha type-7

Chain F:



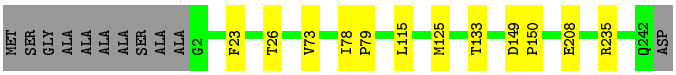
• Molecule 6: Probable proteasome subunit alpha type-7

Chain T:



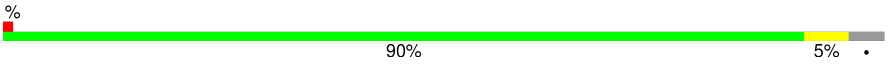
• Molecule 7: Proteasome subunit alpha type-1

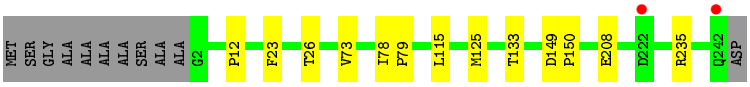
Chain G:



• Molecule 7: Proteasome subunit alpha type-1

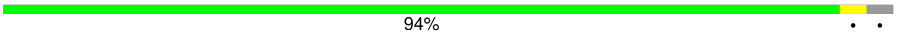
Chain U:

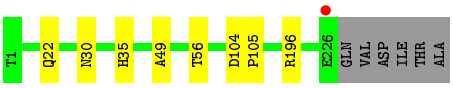




• Molecule 8: Proteasome subunit beta type-2

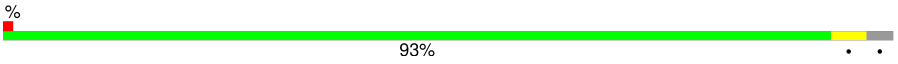
Chain H:

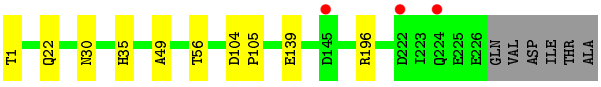




• Molecule 8: Proteasome subunit beta type-2

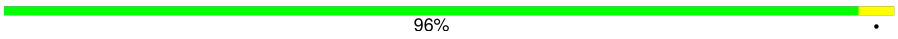
Chain V:

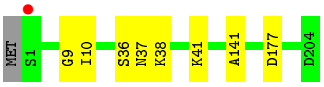




• Molecule 9: Proteasome subunit beta type-3

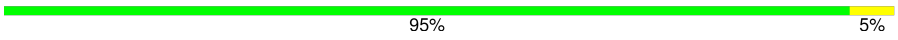
Chain I:

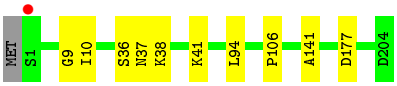




• Molecule 9: Proteasome subunit beta type-3

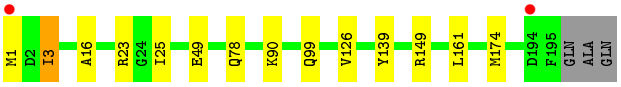
Chain W:





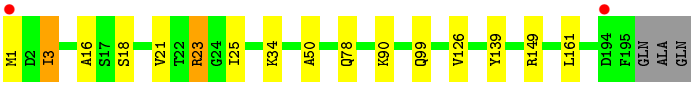
• Molecule 10: Proteasome subunit beta type-4

Chain J:



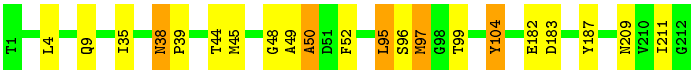
• Molecule 10: Proteasome subunit beta type-4

Chain X:



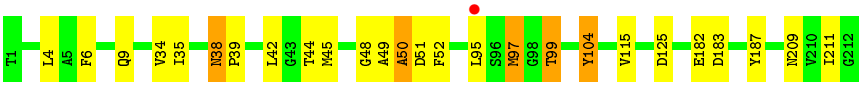
• Molecule 11: Proteasome subunit beta type-5

Chain K:



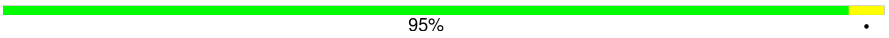
• Molecule 11: Proteasome subunit beta type-5

Chain Y:



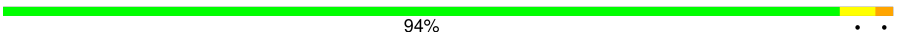
• Molecule 12: Proteasome subunit beta type-6

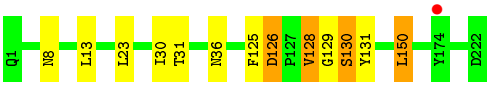
Chain L:



• Molecule 12: Proteasome subunit beta type-6

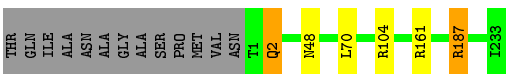
Chain Z:





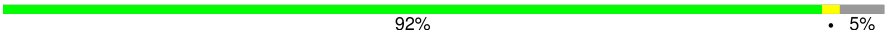
• Molecule 13: Proteasome subunit beta type-7

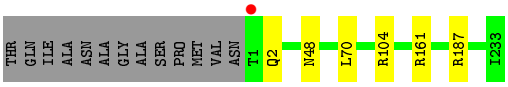
Chain M:



• Molecule 13: Proteasome subunit beta type-7

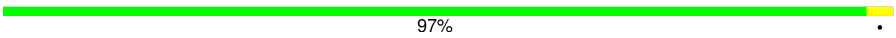
Chain a:





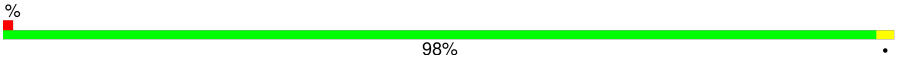
• Molecule 14: Proteasome subunit beta type-1

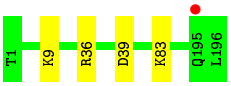
Chain N:



• Molecule 14: Proteasome subunit beta type-1

Chain b:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	135.20Å 299.25Å 144.85Å 90.00° 113.01° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00 15.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.6 (15.00-3.00) 97.7 (15.00-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.17 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.181 , 0.218 0.186 , 0.219	Depositor DCC
R_{free} test set	10215 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	57.5	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 41.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 204308 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	49776	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.27	0/1952	0.46	0/2642
1	O	0.27	0/1952	0.46	0/2642
2	B	0.27	0/1934	0.48	0/2618
2	P	0.27	0/1934	0.48	0/2618
3	C	0.27	0/1910	0.50	0/2586
3	Q	0.27	0/1910	0.49	0/2586
4	D	0.26	0/1837	0.46	0/2475
4	R	0.26	0/1837	0.46	0/2475
5	E	0.26	0/1800	0.45	0/2433
5	S	0.26	0/1800	0.45	0/2433
6	F	0.27	0/1932	0.44	0/2609
6	T	0.27	0/1932	0.44	0/2609
7	G	0.27	0/1945	0.47	0/2634
7	U	0.27	0/1945	0.46	0/2634
8	H	0.24	0/1750	0.46	0/2373
8	V	0.24	0/1750	0.46	0/2373
9	I	0.27	0/1611	0.47	0/2174
9	W	0.27	0/1611	0.47	0/2174
10	J	0.31	0/1589	0.49	0/2142
10	X	0.27	0/1589	0.48	0/2142
11	K	0.31	0/1687	0.54	0/2282
11	Y	0.37	0/1687	0.56	0/2282
12	L	0.28	0/1795	0.46	0/2420
12	Z	0.35	0/1795	0.49	1/2420 (0.0%)
13	M	0.27	0/1855	0.50	0/2514
13	a	0.27	0/1855	0.49	0/2514
14	N	0.24	0/1541	0.46	0/2087
14	b	0.25	0/1541	0.46	0/2087
All	All	0.27	0/50276	0.48	1/67978 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	Z	126	ASP	C-N-CD	5.43	139.80	128.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	2	0
1	O	1915	0	1929	3	0
2	B	1904	0	1904	7	0
2	P	1904	0	1904	6	0
3	C	1881	0	1895	7	0
3	Q	1881	0	1895	5	0
4	D	1813	0	1797	1	0
4	R	1813	0	1797	2	0
5	E	1773	0	1775	0	0
5	S	1773	0	1775	2	0
6	F	1892	0	1883	0	0
6	T	1892	0	1883	0	0
7	G	1907	0	1901	4	0
7	U	1907	0	1901	5	0
8	H	1719	0	1718	4	0
8	V	1719	0	1718	6	0
9	I	1581	0	1574	5	0
9	W	1581	0	1574	6	0
10	J	1561	0	1569	8	0
10	X	1561	0	1569	8	0
11	K	1649	0	1598	20	0
11	Y	1649	0	1598	24	0
12	L	1757	0	1711	6	0
12	Z	1757	0	1711	9	0
13	M	1824	0	1832	2	0
13	a	1824	0	1832	0	0
14	N	1512	0	1480	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	b	1512	0	1480	0	0
15	G	1	0	0	0	0
15	J	1	0	0	0	0
15	K	1	0	0	0	0
15	N	1	0	0	0	0
15	V	1	0	0	0	0
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	1	0
17	K	28	0	25	6	0
17	N	28	0	25	0	0
17	V	28	0	25	2	0
17	Y	28	0	25	4	0
17	b	28	0	25	0	0
18	A	6	0	0	0	0
18	B	9	0	0	0	0
18	C	8	0	0	0	0
18	D	4	0	0	0	0
18	E	5	0	0	0	0
18	F	11	0	0	0	0
18	G	6	0	0	0	0
18	H	9	0	0	0	0
18	I	5	0	0	0	0
18	J	9	0	0	0	0
18	K	9	0	0	0	0
18	L	10	0	0	0	0
18	M	13	0	0	1	0
18	N	8	0	0	0	0
18	O	7	0	0	0	0
18	P	9	0	0	2	0
18	Q	5	0	0	0	0
18	R	4	0	0	0	0
18	S	5	0	0	0	0
18	T	4	0	0	0	0
18	U	13	0	0	0	0
18	V	8	0	0	0	0
18	W	4	0	0	0	0
18	X	9	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	Y	13	0	0	0	0
18	Z	9	0	0	0	0
18	a	15	0	0	0	0
18	b	4	0	0	0	0
All	All	49776	0	49282	128	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 (128) 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:48:GLY:HA2	17:K:301:BO2:H10	1.36	1.05
11:K:48:GLY:CA	17:K:301:BO2:H13	1.93	0.98
11:K:97:MET:SD	11:K:97:MET:N	2.42	0.93
11:K:52:PHE:CE1	11:K:97:MET:HB3	2.14	0.82
11:Y:50:ALA:HB1	12:Z:130:SER:HB2	1.63	0.79
11:Y:49:ALA:HB2	11:Y:97:MET:CG	2.13	0.78
11:Y:49:ALA:HB2	11:Y:97:MET:HG3	1.66	0.78
11:K:48:GLY:HA2	17:K:301:BO2:H13	1.66	0.77
2:P:93:HIS:HB3	18:P:301:HOH:O	1.88	0.74
10:J:1:MET:HG2	10:J:174:MET:HG3	1.70	0.74
11:K:49:ALA:CB	11:K:97:MET:HG3	2.18	0.73
11:Y:34:VAL:CG1	11:Y:42:LEU:HD22	2.20	0.71
11:Y:97:MET:HE2	11:Y:97:MET:N	2.05	0.71
13:M:2:GLN:NE2	18:M:313:HOH:O	2.27	0.68
11:Y:48:GLY:CA	17:Y:301:BO2:H13	2.24	0.67
10:J:1:MET:HG3	10:J:1:MET:O	1.94	0.66
11:Y:48:GLY:HA2	17:Y:301:BO2:H13	1.80	0.64
10:J:3:ILE:O	10:J:3:ILE:HD13	1.98	0.64
11:Y:104:TYR:CD1	11:Y:182:GLU:HB3	2.34	0.63
11:Y:52:PHE:CE1	11:Y:97:MET:HB3	2.33	0.62
11:Y:50:ALA:HB1	12:Z:130:SER:CB	2.29	0.62
11:K:49:ALA:HB2	11:K:97:MET:HG3	1.82	0.61
11:K:104:TYR:CD1	11:K:182:GLU:HB3	2.34	0.61
11:K:35:ILE:HD11	11:K:45:MET:SD	2.39	0.61
11:K:48:GLY:HA3	17:K:301:BO2:H13	1.81	0.60
12:Z:126:ASP:OD2	12:Z:128:VAL:HG23	2.04	0.57
11:Y:97:MET:H	11:Y:97:MET:HE2	1.70	0.57
11:Y:48:GLY:HA2	17:Y:301:BO2:H10	1.87	0.56
11:Y:44:THR:O	11:Y:99:THR:OG1	2.20	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:99:THR:HG22	11:Y:115:VAL:HB	1.88	0.55
11:Y:49:ALA:CB	11:Y:97:MET:CG	2.85	0.53
11:K:49:ALA:HB1	11:K:97:MET:HG3	1.90	0.53
11:Y:48:GLY:N	17:Y:301:BO2:H13	2.24	0.53
3:C:201:VAL:O	3:C:202:GLN:HB3	2.10	0.52
3:Q:201:VAL:O	3:Q:202:GLN:HB3	2.10	0.52
12:Z:126:ASP:OD1	12:Z:129:GLY:N	2.43	0.51
11:K:209:ASN:O	9:W:38:LYS:NZ	2.44	0.51
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.47	0.50
3:C:201:VAL:O	3:C:202:GLN:CB	2.59	0.50
2:B:217:LYS:O	2:B:219:ALA:N	2.43	0.50
11:K:48:GLY:N	17:K:301:BO2:H13	2.27	0.50
13:M:187:ARG:NH1	8:V:139:GLU:OE1	2.40	0.50
11:K:38:ASN:HB2	11:K:39:PRO:CD	2.42	0.50
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.41	0.50
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.93	0.50
10:J:25:ILE:O	10:X:139:TYR:OH	2.31	0.49
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.95	0.49
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.59	0.49
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.94	0.49
7:U:23:PHE:O	7:U:26:THR:HB	2.13	0.49
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.96	0.48
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.95	0.48
10:X:21:VAL:CG1	10:X:23:ARG:NH1	2.77	0.48
2:P:217:LYS:O	2:P:219:ALA:N	2.44	0.48
7:G:23:PHE:O	7:G:26:THR:HB	2.13	0.48
11:K:44:THR:O	11:K:99:THR:OG1	2.26	0.48
11:Y:35:ILE:HD11	11:Y:45:MET:SD	2.55	0.47
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.95	0.47
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.15	0.46
3:C:35:LYS:HG2	3:C:158:SER:O	2.15	0.46
2:B:50:LYS:O	2:B:51:VAL:C	2.54	0.46
2:P:50:LYS:O	2:P:51:VAL:C	2.54	0.46
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.98	0.46
9:I:38:LYS:NZ	11:Y:209:ASN:O	2.49	0.45
7:G:73:VAL:HG12	7:G:133:THR:HB	1.97	0.45
11:Y:34:VAL:HG11	11:Y:42:LEU:HD22	1.97	0.45
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.47	0.45
7:U:73:VAL:HG12	7:U:133:THR:HB	1.98	0.45
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.47	0.45
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:49:ALA:O	11:Y:50:ALA:HB3	2.17	0.45
11:K:50:ALA:HB1	12:L:130:SER:CB	2.47	0.45
11:Y:49:ALA:HB2	11:Y:97:MET:SD	2.57	0.45
8:H:35:HIS:CB	8:H:56:THR:HG21	2.48	0.44
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.99	0.44
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.98	0.44
11:K:48:GLY:H	17:K:301:BO2:H20	1.66	0.44
11:K:50:ALA:HB1	12:L:130:SER:HB2	2.00	0.44
11:K:96:SER:C	11:K:97:MET:SD	2.94	0.44
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.98	0.44
9:I:10:ILE:HG21	9:I:141:ALA:HB3	2.00	0.44
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.98	0.44
9:I:36:SER:HB2	10:J:126:VAL:HG11	2.00	0.44
10:X:3:ILE:HG23	10:X:18:SER:HB3	2.00	0.43
14:N:152:VAL:HA	14:N:175:MET:HE1	2.00	0.43
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.84	0.43
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.53	0.43
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.84	0.43
7:U:78:ILE:N	7:U:79:PRO:CD	2.81	0.43
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	0.43
10:J:139:TYR:OH	10:X:25:ILE:O	2.36	0.43
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.01	0.42
8:V:35:HIS:CB	8:V:56:THR:HG21	2.48	0.42
12:L:13:LEU:HD11	12:L:150:LEU:HD21	2.00	0.42
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.55	0.42
10:X:23:ARG:NH2	10:X:50:ALA:HB2	2.35	0.42
12:Z:13:LEU:HD11	12:Z:150:LEU:HD21	2.01	0.42
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.02	0.42
2:B:145:TYR:OH	2:B:217:LYS:N	2.53	0.42
8:V:49:ALA:HA	17:V:301:BO2:H241	2.01	0.42
8:H:49:ALA:HA	17:H:301:BO2:H241	2.01	0.42
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.54	0.42
1:O:115:ALA:HB1	1:O:154:GLY:O	2.20	0.42
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.55	0.42
12:Z:126:ASP:CG	12:Z:128:VAL:HG23	2.40	0.42
1:A:115:ALA:HB1	1:A:154:GLY:O	2.20	0.42
12:L:8:ASN:HA	12:L:30:ILE:O	2.20	0.41
2:B:50:LYS:HA	2:B:50:LYS:HD3	1.97	0.41
2:P:145:TYR:OH	2:P:217:LYS:N	2.53	0.41
8:V:1:THR:OG1	17:V:301:BO2:C22	2.68	0.41
9:I:141:ALA:HB2	9:I:177:ASP:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.55	0.41
2:B:146:GLN:HG2	3:C:57:ILE:HG21	2.02	0.41
2:P:113:ARG:NE	18:P:301:HOH:O	2.35	0.41
1:O:98:LYS:HE3	1:O:104:TYR:CZ	2.55	0.41
9:W:94:LEU:HD11	9:W:106:PRO:HG2	2.03	0.41
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.20	0.41
5:S:77:ALA:N	5:S:78:PRO:CD	2.84	0.41
9:W:141:ALA:HB2	9:W:177:ASP:HB2	2.03	0.41
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.56	0.41
9:W:36:SER:HB2	10:X:126:VAL:HG11	2.01	0.41
10:J:23:ARG:HA	10:J:23:ARG:HD3	1.64	0.41
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.51	0.40
1:A:98:LYS:HE3	1:A:104:TYR:CZ	2.56	0.40
11:K:49:ALA:O	11:K:50:ALA:CB	2.69	0.40
11:Y:6:PHE:HA	11:Y:125:ASP:O	2.22	0.40
11:Y:49:ALA:O	11:Y:50:ALA:CB	2.70	0.40
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.51	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%)	238 (96%)	9 (4%)	1 (0%)	39	80
1	O	248/250 (99%)	238 (96%)	9 (4%)	1 (0%)	39	80
2	B	242/258 (94%)	232 (96%)	7 (3%)	3 (1%)	16	56
2	P	242/258 (94%)	232 (96%)	7 (3%)	3 (1%)	16	56
3	C	238/254 (94%)	231 (97%)	5 (2%)	2 (1%)	24	66
3	Q	238/254 (94%)	231 (97%)	5 (2%)	2 (1%)	24	66
4	D	231/260 (89%)	225 (97%)	6 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	R	231/260 (89%)	225 (97%)	6 (3%)	0	100	100
5	E	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
5	S	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
6	F	241/288 (84%)	237 (98%)	4 (2%)	0	100	100
6	T	241/288 (84%)	237 (98%)	4 (2%)	0	100	100
7	G	239/252 (95%)	235 (98%)	4 (2%)	0	100	100
7	U	239/252 (95%)	235 (98%)	4 (2%)	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%)	192 (95%)	10 (5%)	0	100	100
9	W	202/205 (98%)	192 (95%)	10 (5%)	0	100	100
10	J	193/198 (98%)	190 (98%)	3 (2%)	0	100	100
10	X	193/198 (98%)	189 (98%)	4 (2%)	0	100	100
11	K	210/212 (99%)	202 (96%)	5 (2%)	3 (1%)	14	51
11	Y	210/212 (99%)	202 (96%)	6 (3%)	2 (1%)	19	61
12	L	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
12	Z	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
13	M	231/246 (94%)	222 (96%)	9 (4%)	0	100	100
13	a	231/246 (94%)	222 (96%)	9 (4%)	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%)	6098 (97%)	169 (3%)	17 (0%)	46	84

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
2	B	218	GLY
3	C	202	GLN
11	K	50	ALA
11	K	95	LEU
2	P	51	VAL
2	P	218	GLY
3	Q	202	GLN
1	A	2	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	222	GLY
1	O	2	THR
2	P	222	GLY
3	C	205	ALA
3	Q	205	ALA
11	Y	50	ALA
11	Y	38	ASN
11	K	38	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	207 (99%)	2 (1%)	82	95
1	O	209/209 (100%)	207 (99%)	2 (1%)	82	95
2	B	203/216 (94%)	201 (99%)	2 (1%)	82	95
2	P	203/216 (94%)	201 (99%)	2 (1%)	82	95
3	C	212/226 (94%)	203 (96%)	9 (4%)	36	76
3	Q	212/226 (94%)	203 (96%)	9 (4%)	36	76
4	D	194/215 (90%)	186 (96%)	8 (4%)	37	76
4	R	194/215 (90%)	186 (96%)	8 (4%)	37	76
5	E	190/193 (98%)	185 (97%)	5 (3%)	54	85
5	S	190/193 (98%)	185 (97%)	5 (3%)	54	85
6	F	201/239 (84%)	194 (96%)	7 (4%)	43	80
6	T	201/239 (84%)	194 (96%)	7 (4%)	43	80
7	G	206/210 (98%)	202 (98%)	4 (2%)	65	90
7	U	206/210 (98%)	202 (98%)	4 (2%)	65	90
8	H	185/190 (97%)	182 (98%)	3 (2%)	70	92
8	V	185/190 (97%)	182 (98%)	3 (2%)	70	92
9	I	172/173 (99%)	171 (99%)	1 (1%)	90	97

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	W	172/173 (99%)	171 (99%)	1 (1%)	90 97
10	J	173/175 (99%)	167 (96%)	6 (4%)	43 80
10	X	173/175 (99%)	167 (96%)	6 (4%)	43 80
11	K	169/169 (100%)	161 (95%)	8 (5%)	32 72
11	Y	169/169 (100%)	159 (94%)	10 (6%)	24 63
12	L	185/185 (100%)	183 (99%)	2 (1%)	80 94
12	Z	185/185 (100%)	181 (98%)	4 (2%)	60 88
13	M	199/208 (96%)	193 (97%)	6 (3%)	48 83
13	a	199/208 (96%)	193 (97%)	6 (3%)	48 83
14	N	162/162 (100%)	158 (98%)	4 (2%)	55 86
14	b	162/162 (100%)	158 (98%)	4 (2%)	55 86
All	All	5320/5540 (96%)	5182 (97%)	138 (3%)	54 85

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	THR
1	A	157	PHE
2	B	55	LEU
2	B	191	LEU
3	C	4	ARG
3	C	38	ASN
3	C	51	LYS
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	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	29	LYS
5	E	71	LEU
5	E	184	ASN
5	E	188	LEU
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	171	GLU
6	F	181	GLU
6	F	214	TRP
6	F	240	GLN
7	G	115	LEU
7	G	125	MET
7	G	208	GLU
7	G	235	ARG
8	H	22	GLN
8	H	30	ASN
8	H	196	ARG
9	I	37	ASN
10	J	3	ILE
10	J	49	GLU
10	J	78	GLN
10	J	90	LYS
10	J	99	GLN
10	J	149	ARG
11	K	4	LEU
11	K	9	GLN
11	K	95	LEU
11	K	97	MET
11	K	104	TYR
11	K	183	ASP
11	K	187	TYR
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	N	36	ARG
14	N	39	ASP
14	N	83	LYS
1	O	122	THR
1	O	157	PHE
2	P	55	LEU
2	P	191	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	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	71	LEU
5	S	184	ASN
5	S	188	LEU
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	171	GLU
6	T	181	GLU
6	T	214	TRP
6	T	240	GLN
7	U	115	LEU
7	U	125	MET
7	U	208	GLU
7	U	235	ARG
8	V	22	GLN
8	V	30	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	V	196	ARG
9	W	37	ASN
10	X	3	ILE
10	X	23	ARG
10	X	78	GLN
10	X	90	LYS
10	X	99	GLN
10	X	149	ARG
11	Y	4	LEU
11	Y	9	GLN
11	Y	51	ASP
11	Y	95	LEU
11	Y	97	MET
11	Y	99	THR
11	Y	104	TYR
11	Y	183	ASP
11	Y	187	TYR
11	Y	211	ILE
12	Z	23	LEU
12	Z	128	VAL
12	Z	130	SER
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
14	b	39	ASP
14	b	83	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	38	ASN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
4	D	146	GLN
5	E	68	HIS
5	E	92	ASN
5	E	116	GLN
5	E	120	GLN
5	E	184	ASN
6	F	19	GLN
6	F	117	GLN
6	F	191	GLN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
10	J	55	GLN
11	K	85	ASN
11	K	176	ASN
12	L	3	ASN
12	L	70	ASN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
1	O	94	HIS
2	P	20	GLN
2	P	58	GLN
2	P	119	GLN
2	P	123	GLN
3	Q	38	ASN
3	Q	147	GLN
3	Q	160	GLN
4	R	91	HIS
4	R	146	GLN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	S	120	GLN
5	S	184	ASN
6	T	19	GLN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
10	X	55	GLN
11	Y	85	ASN
11	Y	176	ASN
12	Z	3	ASN
12	Z	70	ASN
12	Z	79	HIS
12	Z	158	ASN
13	a	48	ASN
13	a	102	GLN
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 11 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	28,29,29	1.52	5 (17%)	31,38,38	1.31	5 (16%)
17	BO2	K	301	11	28,29,29	1.48	5 (17%)	31,38,38	1.15	3 (9%)
17	BO2	N	201	14	28,29,29	1.56	5 (17%)	31,38,38	1.20	4 (12%)
17	BO2	V	301	8	28,29,29	1.53	5 (17%)	31,38,38	1.30	5 (16%)
17	BO2	Y	301	11	28,29,29	1.47	5 (17%)	31,38,38	1.15	3 (9%)
17	BO2	b	201	14	28,29,29	1.54	4 (14%)	31,38,38	1.21	4 (12%)

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 (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	201	BO2	C2-C7	-5.18	1.38	1.50
17	b	201	BO2	C2-C7	-5.09	1.38	1.50
17	V	301	BO2	C2-C7	-4.82	1.39	1.50
17	H	301	BO2	C2-C7	-4.81	1.39	1.50
17	Y	301	BO2	C2-C7	-4.54	1.40	1.50
17	K	301	BO2	C2-C7	-4.48	1.40	1.50
17	b	201	BO2	C11-C12	-4.44	1.40	1.51
17	N	201	BO2	C11-C12	-4.43	1.40	1.51
17	K	301	BO2	C11-C12	-4.11	1.41	1.51
17	H	301	BO2	C11-C12	-4.09	1.41	1.51
17	V	301	BO2	C11-C12	-4.05	1.41	1.51
17	Y	301	BO2	C11-C12	-4.01	1.41	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	201	BO2	C5-N4	2.00	1.39	1.33
17	b	201	BO2	C6-N1	2.19	1.39	1.34
17	Y	301	BO2	C5-N4	2.20	1.40	1.33
17	K	301	BO2	C5-N4	2.21	1.40	1.33
17	N	201	BO2	C6-N1	2.22	1.39	1.34
17	V	301	BO2	C5-N4	2.28	1.40	1.33
17	H	301	BO2	C5-N4	2.31	1.40	1.33
17	b	201	BO2	C3-N4	2.58	1.39	1.34
17	N	201	BO2	C3-N4	2.58	1.39	1.34
17	H	301	BO2	C6-N1	2.58	1.40	1.34
17	V	301	BO2	C6-N1	2.67	1.40	1.34
17	Y	301	BO2	C3-N4	2.71	1.40	1.34
17	K	301	BO2	C3-N4	2.73	1.40	1.34
17	K	301	BO2	C6-N1	2.75	1.40	1.34
17	Y	301	BO2	C6-N1	2.81	1.40	1.34
17	V	301	BO2	C3-N4	2.82	1.40	1.34
17	H	301	BO2	C3-N4	2.83	1.40	1.34

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	b	201	BO2	C11-C10-N9	-3.23	104.04	110.80
17	N	201	BO2	C11-C10-N9	-3.10	104.31	110.80
17	H	301	BO2	C2-C3-N4	-2.72	119.23	122.11
17	V	301	BO2	C2-C3-N4	-2.67	119.29	122.11
17	H	301	BO2	C5-C6-N1	-2.46	119.19	122.25
17	Y	301	BO2	C18-C10-N9	-2.46	104.34	111.26
17	K	301	BO2	C18-C10-N9	-2.44	104.37	111.26
17	V	301	BO2	C5-C6-N1	-2.44	119.23	122.25
17	H	301	BO2	C12-C11-C10	-2.37	106.50	113.41
17	V	301	BO2	C12-C11-C10	-2.37	106.52	113.41
17	H	301	BO2	B26-C21-C22	-2.26	106.92	112.79
17	V	301	BO2	B26-C21-C22	-2.24	106.97	112.79
17	N	201	BO2	C2-C3-N4	-2.15	119.84	122.11
17	b	201	BO2	C2-C3-N4	-2.06	119.93	122.11
17	N	201	BO2	C18-C10-N9	-2.03	105.54	111.26
17	b	201	BO2	C18-C10-N9	-2.00	105.62	111.26
17	Y	301	BO2	C3-C2-C7	2.05	121.64	119.55
17	K	301	BO2	C3-C2-C7	2.08	121.66	119.55
17	b	201	BO2	C6-N1-C2	2.49	120.26	116.92
17	N	201	BO2	C6-N1-C2	2.51	120.29	116.92
17	Y	301	BO2	C6-N1-C2	3.11	121.10	116.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	K	301	BO2	C6-N1-C2	3.14	121.13	116.92
17	V	301	BO2	C6-N1-C2	3.42	121.51	116.92
17	H	301	BO2	C6-N1-C2	3.44	121.54	116.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	H	301	BO2	1	0
17	K	301	BO2	6	0
17	V	301	BO2	2	0
17	Y	301	BO2	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	250/250 (100%)	-0.61	2 (0%)	87	67	33, 52, 89, 123	0
1	O	250/250 (100%)	-0.56	1 (0%)	93	80	39, 60, 102, 135	0
2	B	244/258 (94%)	-0.57	4 (1%)	74	47	35, 57, 103, 157	0
2	P	244/258 (94%)	-0.53	5 (2%)	68	39	41, 61, 103, 152	0
3	C	240/254 (94%)	-0.42	5 (2%)	67	36	37, 61, 123, 148	0
3	Q	240/254 (94%)	-0.30	7 (2%)	55	26	45, 73, 153, 182	0
4	D	235/260 (90%)	-0.56	1 (0%)	93	80	46, 65, 96, 132	0
4	R	235/260 (90%)	-0.46	1 (0%)	93	80	50, 72, 114, 144	0
5	E	231/234 (98%)	-0.49	2 (0%)	85	64	44, 68, 107, 140	0
5	S	231/234 (98%)	-0.48	2 (0%)	85	64	43, 70, 113, 146	0
6	F	243/288 (84%)	-0.61	2 (0%)	87	67	37, 61, 108, 138	0
6	T	243/288 (84%)	-0.56	0	100	100	38, 67, 121, 148	0
7	G	241/252 (95%)	-0.66	0	100	100	34, 53, 90, 134	0
7	U	241/252 (95%)	-0.62	2 (0%)	87	67	34, 56, 90, 133	0
8	H	226/232 (97%)	-0.67	1 (0%)	93	80	29, 48, 87, 134	0
8	V	226/232 (97%)	-0.62	3 (1%)	79	53	31, 51, 82, 155	0
9	I	204/205 (99%)	-0.80	1 (0%)	91	76	27, 47, 78, 104	0
9	W	204/205 (99%)	-0.78	1 (0%)	91	76	33, 50, 77, 109	0
10	J	195/198 (98%)	-0.68	2 (1%)	84	60	25, 50, 79, 115	0
10	X	195/198 (98%)	-0.68	2 (1%)	84	60	36, 53, 81, 135	0
11	K	212/212 (100%)	-0.61	0	100	100	40, 59, 89, 108	0
11	Y	212/212 (100%)	-0.61	1 (0%)	91	76	41, 58, 87, 112	0
12	L	222/222 (100%)	-0.64	1 (0%)	91	76	41, 55, 102, 129	0
12	Z	222/222 (100%)	-0.64	1 (0%)	91	76	31, 54, 103, 129	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%)	-0.75	0 100 100	31, 51, 73, 95	0
13	a	233/246 (94%)	-0.74	1 (0%) 93 80	29, 49, 73, 90	0
14	N	196/196 (100%)	-0.81	0 100 100	28, 45, 73, 106	0
14	b	196/196 (100%)	-0.76	1 (0%) 91 76	29, 47, 78, 109	0
All	All	6344/6614 (95%)	-0.61	49 (0%) 87 67	25, 57, 103, 182	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	49	THR	5.5
5	E	202	ASP	3.7
3	Q	236	GLN	3.6
2	B	51	VAL	3.6
3	Q	206	LYS	3.5
3	Q	50	LEU	3.4
3	C	206	LYS	3.4
5	S	202	ASP	3.3
10	X	194	ASP	3.2
8	V	222	ASP	3.2
2	B	221	ASP	3.2
10	X	1	MET	3.0
2	P	51	VAL	3.0
9	W	1	SER	3.0
3	Q	239	GLN	2.9
3	C	50	LEU	2.9
3	Q	205	ALA	2.9
3	C	49	THR	2.9
8	V	224	GLN	2.9
2	P	59	ASP	2.7
3	Q	240	GLU	2.7
2	P	221	ASP	2.7
2	B	218	GLY	2.6
1	A	2	THR	2.5
7	U	242	GLN	2.4
12	L	174	TYR	2.4
12	Z	174	TYR	2.4
1	A	1	MET	2.4
6	F	244	ASN	2.4
3	C	239	GLN	2.3
10	J	194	ASP	2.3
8	H	226	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	220	ASN	2.2
10	J	1	MET	2.2
11	Y	95	LEU	2.2
2	P	219	ALA	2.2
13	a	1	THR	2.1
9	I	1	SER	2.1
1	O	2	THR	2.1
3	C	236	GLN	2.1
2	P	220	ASN	2.1
4	R	241	ALA	2.1
4	D	242	GLU	2.1
7	U	222	ASP	2.1
8	V	145	ASP	2.1
5	S	3	ASN	2.1
5	E	123	GLY	2.0
14	b	195	GLN	2.0
6	F	181	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
15	MG	J	201	1/1	0.98	0.15	3.92	45,45,45,45	0
17	BO2	N	201	28/28	0.92	0.22	3.06	29,45,63,67	0
17	BO2	b	201	28/28	0.92	0.21	2.85	36,46,58,60	0
17	BO2	V	301	28/28	0.93	0.22	1.81	45,52,68,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
17	BO2	H	301	28/28	0.92	0.21	1.64	39,48,59,63	0
15	MG	Z	301	1/1	0.95	0.18	0.75	45,45,45,45	0
17	BO2	Y	301	28/28	0.94	0.19	0.53	59,64,69,72	0
17	BO2	K	301	28/28	0.94	0.18	0.17	56,61,65,68	0
15	MG	Y	302	1/1	1.00	0.10	-0.96	55,55,55,55	0
15	MG	K	302	1/1	0.98	0.08	-1.15	59,59,59,59	0
15	MG	N	202	1/1	0.99	0.08	-1.26	29,29,29,29	0
16	CL	N	203	1/1	0.97	0.08	-1.51	38,38,38,38	0
15	MG	G	301	1/1	0.98	0.06	-1.84	56,56,56,56	0
16	CL	b	202	1/1	0.98	0.08	-1.86	51,51,51,51	0
15	MG	V	302	1/1	0.98	0.06	-2.57	53,53,53,53	0
16	CL	U	301	1/1	0.99	0.20	-	41,41,41,41	0
16	CL	G	302	1/1	0.99	0.15	-	35,35,35,35	0

6.5 Other polymers

There are no such residues in this entry.