



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:17 PM GMT

PDB ID : 4QVY
Title : yCP beta5-A49T-mutant in complex with bortezomib
Authors : Huber, E.M.; Heinemeyer, W.; Groll, M.
Deposited on : 2014-07-16
Resolution : 2.51 Å(reported)

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

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

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

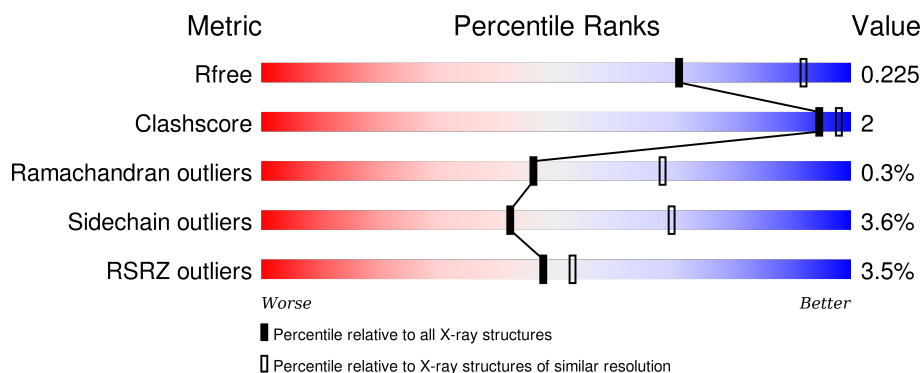
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	250	<div> <div>5%</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>5%</div> <div>86%</div> <div>8% • 5%</div> </div>
2	P	258	<div> <div>4%</div> <div>86%</div> <div>8% • 5%</div> </div>
3	C	254	<div> <div>7%</div> <div>86%</div> <div>7% • 6%</div> </div>

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Mol	Chain	Length	Quality of chain
3	Q	254	
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	MG	J	201	-	-	-	X
15	MG	K	303	-	-	-	X
15	MG	Z	301	-	-	-	X
17	BO2	N	201	-	-	-	X
17	BO2	Y	301	-	-	-	X
17	BO2	b	201	-	-	-	X

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 49977 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-2.

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

- Molecule 2 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-3.

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

- Molecule 3 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-4.

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

- Molecule 4 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-5.

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

- Molecule 5 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-6.

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

- Molecule 6 is a protein called PROBABLE PROTEASOME SUBUNIT ALPHA TYPE-7.

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

- Molecule 7 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-1.

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

- Molecule 8 is a protein called PROTEASOME SUBUNIT BETA TYPE-2.

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

- Molecule 9 is a protein called PROTEASOME SUBUNIT BETA TYPE-3.

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

- Molecule 10 is a protein called PROTEASOME SUBUNIT BETA TYPE-4.

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

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

- Molecule 11 is a protein called PROTEASOME SUBUNIT BETA TYPE-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1646	1046	280	313	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1646	1046	280	313	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	49	THR	ALA	ENGINEERED MUTATION	UNP P30656
Y	49	THR	ALA	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			

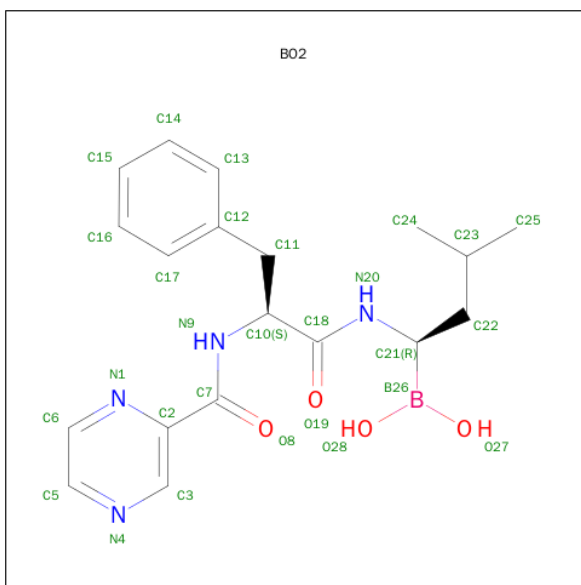
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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	2	Total Mg 2 2	0	0
15	I	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: 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	12	Total	O	0	0
			12	12		
18	B	14	Total	O	0	0
			14	14		
18	C	12	Total	O	0	0
			12	12		
18	D	7	Total	O	0	0
			7	7		
18	E	6	Total	O	0	0
			6	6		
18	F	15	Total	O	0	0
			15	15		

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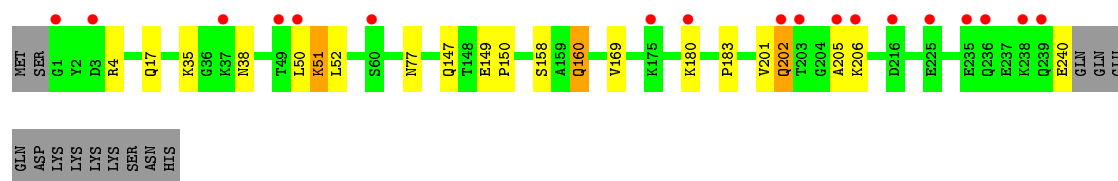
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	G	18	Total O 18 18	0	0
18	H	31	Total O 31 31	0	0
18	I	13	Total O 13 13	0	0
18	J	13	Total O 13 13	0	0
18	K	19	Total O 19 19	0	0
18	L	24	Total O 24 24	0	0
18	M	24	Total O 24 24	0	0
18	N	13	Total O 13 13	0	0
18	O	15	Total O 15 15	0	0
18	P	12	Total O 12 12	0	0
18	Q	6	Total O 6 6	0	0
18	R	7	Total O 7 7	0	0
18	S	5	Total O 5 5	0	0
18	T	13	Total O 13 13	0	0
18	U	15	Total O 15 15	0	0
18	V	23	Total O 23 23	0	0
18	W	7	Total O 7 7	0	0
18	X	19	Total O 19 19	0	0
18	Y	18	Total O 18 18	0	0
18	Z	15	Total O 15 15	0	0
18	a	30	Total O 30 30	0	0

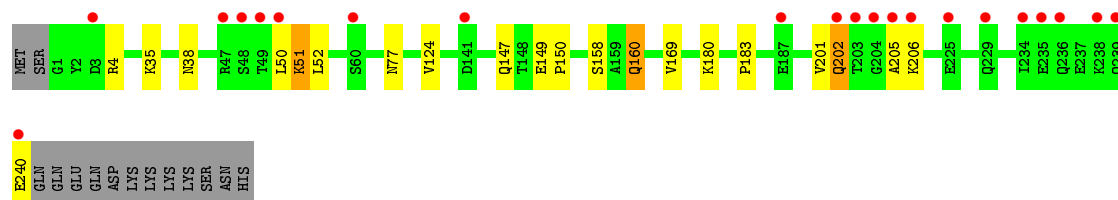
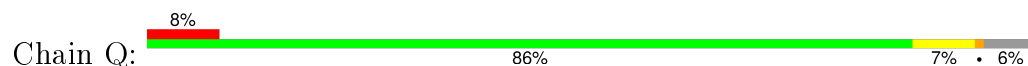
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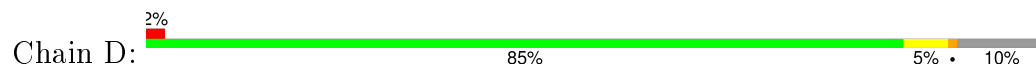
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	b	20	Total	O	0	0
			20	20		



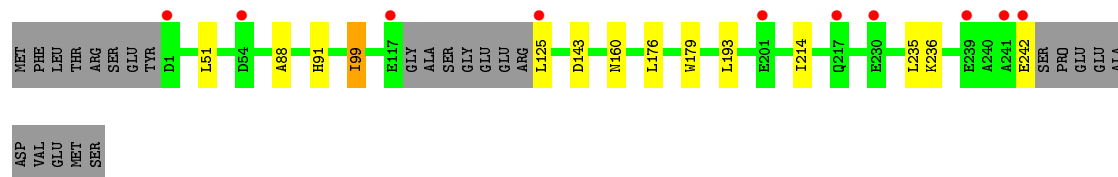
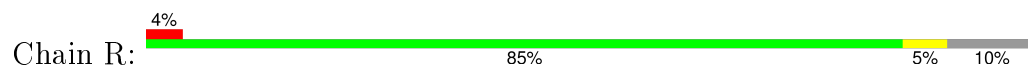
• Molecule 3: PROTEASOME SUBUNIT ALPHA TYPE-4



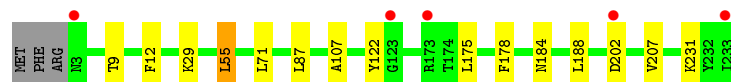
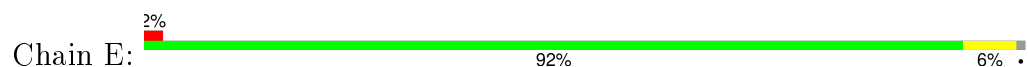
• Molecule 4: PROTEASOME SUBUNIT ALPHA TYPE-5



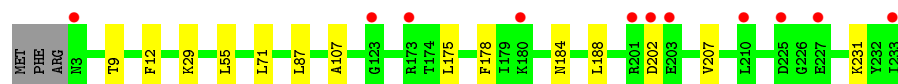
• Molecule 4: PROTEASOME SUBUNIT ALPHA TYPE-5



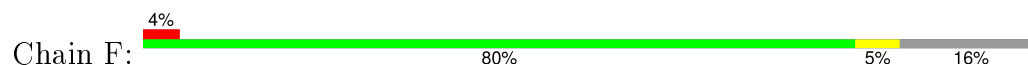
• Molecule 5: PROTEASOME SUBUNIT ALPHA TYPE-6

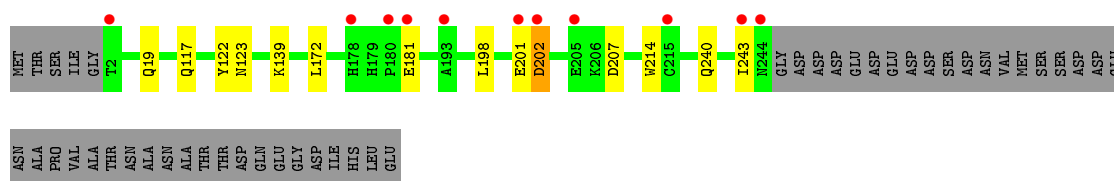


• Molecule 5: PROTEASOME SUBUNIT ALPHA TYPE-6

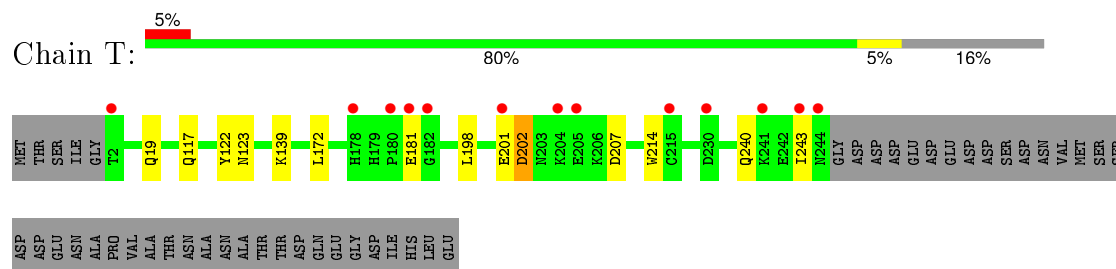


• Molecule 6: PROBABLE PROTEASOME SUBUNIT ALPHA TYPE-7

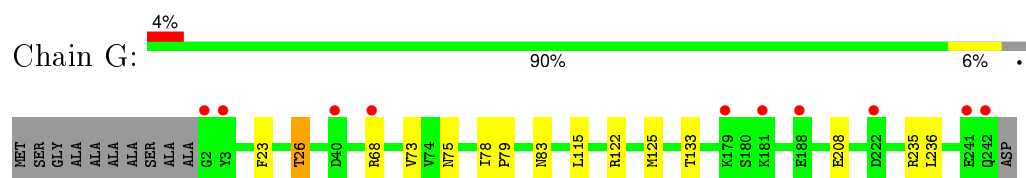




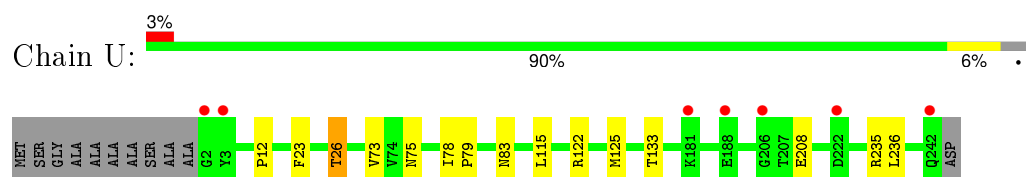
• Molecule 6: PROBABLE PROTEASOME SUBUNIT ALPHA TYPE-7



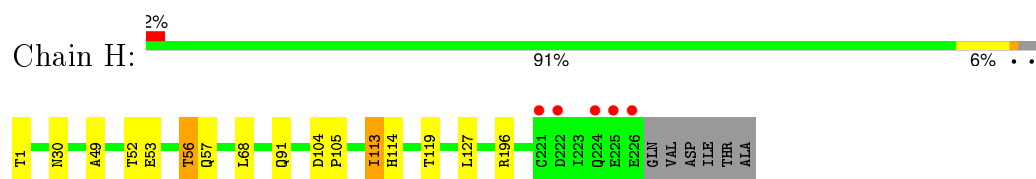
• Molecule 7: PROTEASOME SUBUNIT ALPHA TYPE-1



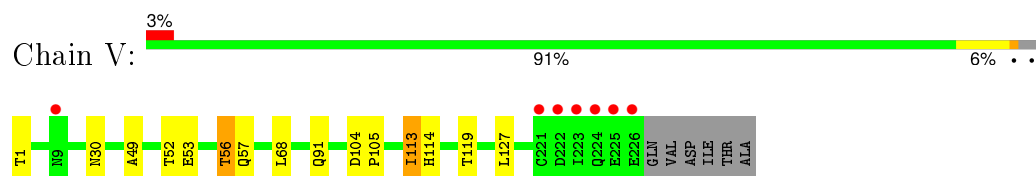
• Molecule 7: PROTEASOME SUBUNIT ALPHA TYPE-1



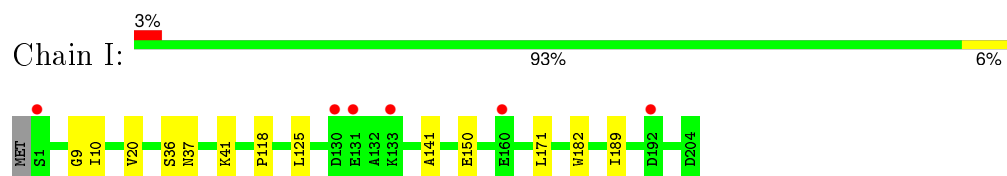
• Molecule 8: PROTEASOME SUBUNIT BETA TYPE-2



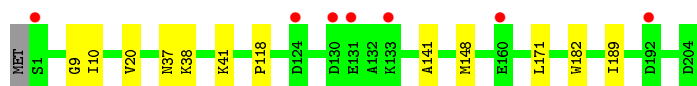
• Molecule 8: PROTEASOME SUBUNIT BETA TYPE-2



• Molecule 9: PROTEASOME SUBUNIT BETA TYPE-3



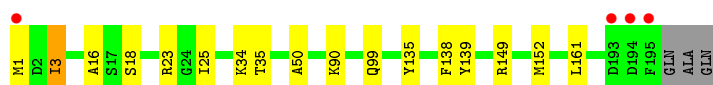
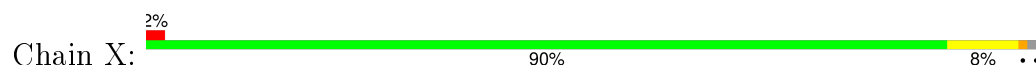
- Molecule 9: PROTEASOME SUBUNIT BETA TYPE-3



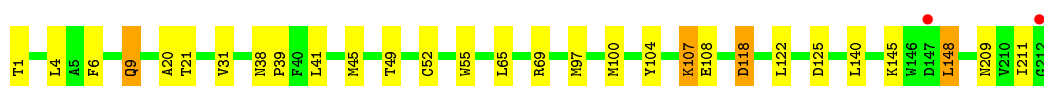
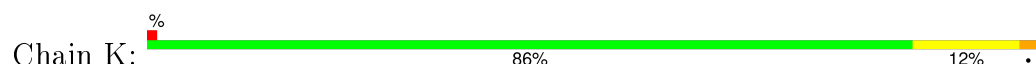
- Molecule 10: PROTEASOME SUBUNIT BETA TYPE-4



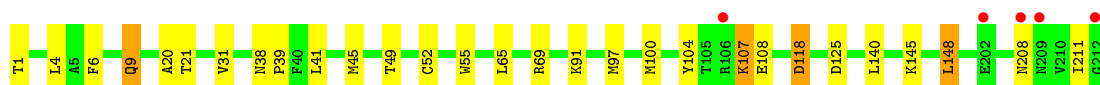
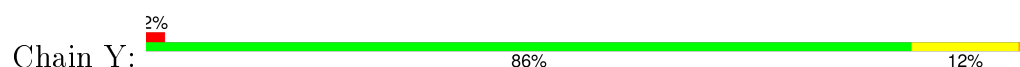
- Molecule 10: PROTEASOME SUBUNIT BETA TYPE-4



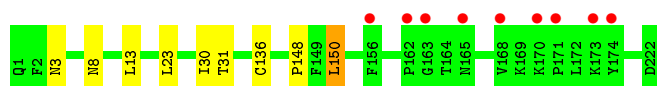
- Molecule 11: PROTEASOME SUBUNIT BETA TYPE-5



- Molecule 11: PROTEASOME SUBUNIT BETA TYPE-5



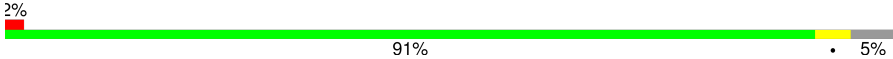
- Molecule 12: PROTEASOME SUBUNIT BETA TYPE-6

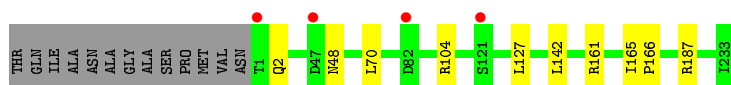


- Molecule 12: PROTEASOME SUBUNIT BETA TYPE-6



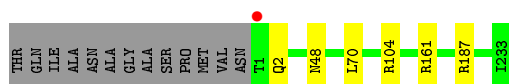
- Molecule 13: PROTEASOME SUBUNIT BETA TYPE-7

Chain M:  91% 2% 5%



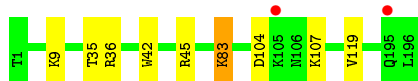
- Molecule 13: PROTEASOME SUBUNIT BETA TYPE-7

Chain a:  92% 5%



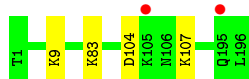
- Molecule 14: PROTEASOME SUBUNIT BETA TYPE-1

Chain N:  95% 2% 3%



- Molecule 14: PROTEASOME SUBUNIT BETA TYPE-1

Chain b:  98% 1% 1%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.32Å 300.90Å 144.92Å 90.00° 112.81° 90.00°	Depositor
Resolution (Å)	15.00 – 2.51 15.00 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.6 (15.00-2.51) 99.6 (15.00-2.51)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.01 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.193 , 0.219 0.198 , 0.225	Depositor DCC
R_{free} test set	18005 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	50.3	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 361260 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	49977	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.50	0/2618
2	P	0.27	0/1934	0.50	0/2618
3	C	0.27	0/1910	0.50	0/2586
3	Q	0.27	0/1910	0.50	0/2586
4	D	0.26	0/1837	0.48	0/2475
4	R	0.27	0/1837	0.47	0/2475
5	E	0.27	0/1800	0.47	0/2433
5	S	0.27	0/1800	0.47	0/2433
6	F	0.27	0/1932	0.45	0/2609
6	T	0.27	0/1932	0.45	0/2609
7	G	0.27	0/1945	0.47	0/2634
7	U	0.27	0/1945	0.47	0/2634
8	H	0.27	0/1750	0.50	0/2373
8	V	0.27	0/1750	0.49	0/2373
9	I	0.29	0/1611	0.49	0/2174
9	W	0.29	0/1611	0.49	0/2174
10	J	0.41	0/1589	0.50	0/2142
10	X	0.49	1/1589 (0.1%)	0.51	0/2142
11	K	0.27	0/1683	0.51	0/2277
11	Y	0.27	0/1683	0.51	0/2277
12	L	0.28	0/1795	0.48	0/2420
12	Z	0.27	0/1795	0.48	0/2420
13	M	0.28	0/1855	0.50	0/2514
13	a	0.27	0/1855	0.50	0/2514
14	N	0.25	0/1541	0.48	0/2087
14	b	0.26	0/1541	0.48	0/2087
All	All	0.29	1/50268 (0.0%)	0.48	0/67968

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	X	139	TYR	CB-CG	-5.67	1.43	1.51

There are no bond angle outliers.

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	11	0
2	P	1904	0	1904	11	0
3	C	1881	0	1895	6	0
3	Q	1881	0	1895	6	0
4	D	1813	0	1797	5	0
4	R	1813	0	1797	4	0
5	E	1773	0	1775	5	0
5	S	1773	0	1775	3	0
6	F	1892	0	1883	4	0
6	T	1892	0	1883	4	0
7	G	1907	0	1901	4	0
7	U	1907	0	1901	4	0
8	H	1719	0	1718	15	0
8	V	1719	0	1718	9	0
9	I	1581	0	1574	6	0
9	W	1581	0	1574	6	0
10	J	1561	0	1569	16	0
10	X	1561	0	1569	10	0
11	K	1646	0	1596	16	0
11	Y	1646	0	1596	17	0
12	L	1757	0	1711	3	0
12	Z	1757	0	1711	2	0
13	M	1824	0	1832	2	0
13	a	1824	0	1832	0	0
14	N	1512	0	1480	5	0
14	b	1512	0	1480	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	G	1	0	0	0	0
15	I	1	0	0	0	0
15	J	1	0	0	0	0
15	K	2	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	2	0
17	K	28	0	25	3	0
17	N	28	0	25	5	0
17	V	28	0	25	2	0
17	Y	28	0	25	3	0
17	b	28	0	25	0	0
18	A	12	0	0	0	0
18	B	14	0	0	0	0
18	C	12	0	0	0	0
18	D	7	0	0	0	0
18	E	6	0	0	0	0
18	F	15	0	0	0	0
18	G	18	0	0	0	0
18	H	31	0	0	0	0
18	I	13	0	0	0	0
18	J	13	0	0	0	0
18	K	19	0	0	0	0
18	L	24	0	0	0	0
18	M	24	0	0	0	0
18	N	13	0	0	0	0
18	O	15	0	0	0	0
18	P	12	0	0	2	0
18	Q	6	0	0	0	0
18	R	7	0	0	0	0
18	S	5	0	0	0	0
18	T	13	0	0	0	0
18	U	15	0	0	0	0
18	V	23	0	0	0	0
18	W	7	0	0	0	0
18	X	19	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	Y	18	0	0	0	0
18	Z	15	0	0	0	0
18	a	30	0	0	0	0
18	b	20	0	0	0	0
All	All	49977	0	49278	158	0

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

All (158) 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)
8:H:114:HIS:CD2	17:N:201:BO2:H5	1.98	0.97
8:H:114:HIS:HD2	17:N:201:BO2:H5	1.33	0.90
10:J:149:ARG:O	10:J:152:MET:HG3	1.77	0.84
8:H:52:THR:O	8:H:56:THR:OG1	2.02	0.77
8:H:114:HIS:HD2	17:N:201:BO2:C5	1.98	0.75
10:J:152:MET:HE3	10:J:156:GLU:HB3	1.68	0.74
8:V:52:THR:O	8:V:56:THR:OG1	2.06	0.73
8:V:113:ILE:HG13	8:V:119:THR:HG22	1.74	0.70
8:H:113:ILE:HG13	8:H:119:THR:HG22	1.75	0.68
11:Y:45:MET:HG2	11:Y:52:CYS:HB3	1.74	0.68
10:J:149:ARG:HD2	11:Y:208:ASN:OD1	1.94	0.68
11:K:45:MET:HG2	11:K:52:CYS:HB3	1.76	0.68
10:X:149:ARG:HD3	18:X:202:HOH:O	1.98	0.63
10:J:149:ARG:CG	10:J:149:ARG:HH21	2.11	0.62
10:J:25:ILE:HG12	10:J:25:ILE:O	2.00	0.61
10:J:149:ARG:HG3	10:J:149:ARG:NH2	2.16	0.60
10:X:149:ARG:O	10:X:152:MET:HG3	2.03	0.59
10:J:149:ARG:HG3	10:J:149:ARG:HH21	1.68	0.58
8:H:113:ILE:CG1	8:H:119:THR:HG22	2.33	0.58
8:V:113:ILE:CG1	8:V:119:THR:HG22	2.33	0.58
11:Y:9:GLN:NE2	11:Y:148:LEU:O	2.38	0.56
11:K:9:GLN:NE2	11:K:148:LEU:O	2.39	0.56
14:N:35:THR:HG21	14:N:45:ARG:HE	1.71	0.56
2:P:93:HIS:HB3	18:P:301:HOH:O	2.06	0.55
10:X:149:ARG:CD	18:X:202:HOH:O	2.55	0.55
8:V:53:GLU:OE2	8:V:57:GLN:NE2	2.35	0.54
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.90	0.54
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.07	0.53
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:51:LYS:O	3:C:52:LEU:HB2	2.07	0.52
2:B:221:ASP:O	2:B:223:GLU:N	2.43	0.52
7:G:23:PHE:O	7:G:26:THR:HB	2.10	0.52
2:P:221:ASP:O	2:P:223:GLU:N	2.43	0.52
11:K:209:ASN:O	9:W:38:LYS:NZ	2.43	0.52
7:U:23:PHE:O	7:U:26:THR:HB	2.10	0.51
8:H:53:GLU:OE2	8:H:57:GLN:NE2	2.35	0.51
2:P:217:LYS:C	2:P:219:ALA:H	2.14	0.51
3:C:201:VAL:O	3:C:202:GLN:CB	2.58	0.51
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.58	0.51
10:J:139:TYR:OH	10:X:25:ILE:HG12	2.11	0.50
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.77	0.50
11:Y:1:THR:OG1	17:Y:301:BO2:C22	2.60	0.50
10:X:135:TYR:O	10:X:138:PHE:HB2	2.13	0.49
2:B:217:LYS:C	2:B:219:ALA:H	2.14	0.49
11:K:55:TRP:HB2	11:K:97:MET:HE1	1.95	0.49
4:D:176:LEU:HD22	5:E:55:LEU:CD2	2.42	0.49
11:K:1:THR:OG1	17:K:301:BO2:C22	2.59	0.49
11:K:21:THR:O	17:K:301:BO2:H3	2.13	0.48
5:S:12:PHE:H	6:T:19:GLN:HE22	1.61	0.48
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	1.96	0.48
11:K:145:LYS:HB2	11:K:148:LEU:HD13	1.96	0.48
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.77	0.48
8:V:49:ALA:HA	17:V:301:BO2:H241	1.96	0.48
2:B:12:PHE:H	3:C:17:GLN:HE22	1.61	0.48
11:Y:21:THR:O	17:Y:301:BO2:H3	2.14	0.47
10:J:91:SER:HG	10:J:98:TYR:H	1.63	0.47
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.97	0.47
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.96	0.47
10:X:149:ARG:NE	18:X:202:HOH:O	2.48	0.46
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.49	0.46
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.46	0.46
10:J:152:MET:HE3	10:J:156:GLU:CB	2.42	0.46
8:H:49:ALA:HA	17:H:301:BO2:H241	1.96	0.46
1:A:1:MET:HG3	6:F:122:TYR:CZ	2.50	0.46
11:Y:118:ASP:OD2	11:Y:118:ASP:N	2.49	0.46
8:H:114:HIS:CD2	17:N:201:BO2:C5	2.80	0.46
1:O:1:MET:HG3	6:T:122:TYR:CZ	2.51	0.46
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.97	0.46
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.98	0.46
11:K:118:ASP:N	11:K:118:ASP:OD2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.96	0.45
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.98	0.45
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.46	0.45
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.46	0.45
2:B:50:LYS:HD3	2:B:50:LYS:HA	1.80	0.45
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.99	0.45
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.98	0.45
6:F:202:ASP:OD1	6:F:202:ASP:N	2.50	0.44
11:Y:55:TRP:HB2	11:Y:97:MET:HE1	1.99	0.44
14:N:35:THR:CG2	14:N:45:ARG:HE	2.30	0.44
7:G:68:ARG:HH12	14:N:36:ARG:HH22	1.64	0.44
6:T:202:ASP:N	6:T:202:ASP:OD1	2.51	0.44
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	2.00	0.44
2:P:113:ARG:NE	18:P:301:HOH:O	2.40	0.44
11:Y:49:THR:HA	17:Y:301:BO2:H241	1.99	0.44
8:H:1:THR:OG1	17:H:301:BO2:C22	2.65	0.44
4:D:91:HIS:HB3	4:D:99:ILE:HG22	2.00	0.44
11:K:49:THR:HA	17:K:301:BO2:H241	2.00	0.44
4:R:91:HIS:HB3	4:R:99:ILE:HG22	2.00	0.44
10:J:21:VAL:HG11	11:K:122:LEU:HD11	2.00	0.43
8:V:1:THR:OG1	17:V:301:BO2:C22	2.65	0.43
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.54	0.43
8:H:114:HIS:HD2	17:N:201:BO2:C6	2.30	0.43
3:C:35:LYS:HG2	3:C:158:SER:O	2.19	0.43
2:B:3:ARG:HB3	5:E:122:TYR:OH	2.17	0.43
11:Y:38:ASN:OD1	11:Y:41:LEU:N	2.50	0.43
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.49	0.43
11:K:20:ALA:HB2	11:K:31:VAL:HG21	2.00	0.43
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.53	0.43
5:S:87:LEU:HD21	5:S:107:ALA:HB1	2.01	0.43
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.42
9:I:36:SER:HB2	10:J:126:VAL:HG11	2.01	0.42
11:Y:65:LEU:HB3	11:Y:69:ARG:HH21	1.84	0.42
8:H:104:ASP:HB2	8:H:105:PRO:HD2	2.01	0.42
5:E:12:PHE:H	6:F:19:GLN:HE22	1.66	0.42
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.83	0.42
8:V:104:ASP:HB2	8:V:105:PRO:HD2	2.01	0.42
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.49	0.42
11:K:38:ASN:OD1	11:K:41:LEU:N	2.51	0.42
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:73:VAL:HG12	7:G:133:THR:HB	2.01	0.42
13:M:127:LEU:HG	13:M:142:LEU:HD12	2.02	0.42
11:K:107:LYS:HG3	11:K:108:GLU:HG3	2.02	0.42
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.02	0.42
6:T:198:LEU:HD12	6:T:243:ILE:HG22	2.01	0.42
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	2.02	0.42
11:K:65:LEU:HB3	11:K:69:ARG:HH21	1.84	0.42
5:E:87:LEU:HD21	5:E:107:ALA:HB1	2.01	0.42
8:H:114:HIS:HE1	8:H:127:LEU:HD11	1.85	0.42
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.55	0.42
11:K:38:ASN:HB2	11:K:39:PRO:CD	2.50	0.41
9:W:20:VAL:HG23	9:W:189:ILE:HB	2.02	0.41
7:U:73:VAL:HG12	7:U:133:THR:HB	2.01	0.41
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.03	0.41
8:H:196:ARG:NH2	9:I:150:GLU:O	2.52	0.41
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.50	0.41
12:L:8:ASN:HA	12:L:30:ILE:O	2.20	0.41
2:B:50:LYS:O	2:B:51:VAL:C	2.58	0.41
2:P:151:ASN:HB2	2:P:152:PRO:HD2	2.03	0.41
6:F:198:LEU:HD12	6:F:243:ILE:HG22	2.01	0.41
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.85	0.41
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.19	0.41
2:P:50:LYS:O	2:P:51:VAL:C	2.58	0.41
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.55	0.41
12:L:148:PRO:HB2	9:W:148:MET:SD	2.61	0.41
9:I:20:VAL:HG13	9:I:118:PRO:HB3	2.03	0.41
2:B:219:ALA:HB2	2:B:225:TYR:HB2	2.02	0.41
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.03	0.41
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.51	0.41
10:J:3:ILE:HG23	10:J:18:SER:HB3	2.02	0.41
11:Y:107:LYS:HG3	11:Y:108:GLU:HG3	2.02	0.41
8:V:114:HIS:HE1	8:V:127:LEU:HD11	1.86	0.41
10:J:149:ARG:CD	11:Y:208:ASN:OD1	2.66	0.41
2:B:151:ASN:HB2	2:B:152:PRO:HD2	2.02	0.41
12:Z:13:LEU:HD11	12:Z:150:LEU:HD21	2.02	0.41
11:K:6:PHE:HA	11:K:125:ASP:O	2.20	0.41
13:M:165:ILE:HB	13:M:166:PRO:HD3	2.03	0.41
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.51	0.41
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.03	0.41
2:P:219:ALA:HB2	2:P:225:TYR:HB2	2.02	0.40
10:X:3:ILE:HG23	10:X:18:SER:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.56	0.40
9:I:20:VAL:HG23	9:I:189:ILE:HB	2.02	0.40
11:Y:6:PHE:HA	11:Y:125:ASP:O	2.20	0.40
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.21	0.40
10:X:50:ALA:O	11:Y:91:LYS:NZ	2.53	0.40
12:L:13:LEU:HD11	12:L:150:LEU:HD21	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	39	61
1	O	248/250 (99%)	239 (96%)	8 (3%)	1 (0%)	39	61
2	B	242/258 (94%)	235 (97%)	3 (1%)	4 (2%)	11	19
2	P	242/258 (94%)	235 (97%)	3 (1%)	4 (2%)	11	19
3	C	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	15	26
3	Q	238/254 (94%)	233 (98%)	2 (1%)	3 (1%)	15	26
4	D	231/260 (89%)	229 (99%)	2 (1%)	0	100	100
4	R	231/260 (89%)	229 (99%)	2 (1%)	0	100	100
5	E	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
5	S	229/234 (98%)	221 (96%)	8 (4%)	0	100	100
6	F	241/288 (84%)	238 (99%)	3 (1%)	0	100	100
6	T	241/288 (84%)	238 (99%)	3 (1%)	0	100	100
7	G	239/252 (95%)	238 (100%)	1 (0%)	0	100	100
7	U	239/252 (95%)	238 (100%)	1 (0%)	0	100	100
8	H	224/232 (97%)	219 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	V	224/232 (97%)	219 (98%)	5 (2%)	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%)	216 (98%)	4 (2%)	0	100	100
13	M	231/246 (94%)	224 (97%)	7 (3%)	0	100	100
13	a	231/246 (94%)	224 (97%)	7 (3%)	0	100	100
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
14	b	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
All	All	6284/6614 (95%)	6144 (98%)	124 (2%)	16 (0%)	46	68

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
2	B	222	GLY
3	C	202	GLN
2	P	51	VAL
2	P	222	GLY
3	Q	202	GLN
1	A	2	THR
2	B	218	GLY
1	O	2	THR
2	P	218	GLY
2	B	220	ASN
3	C	205	ALA
2	P	220	ASN
3	Q	205	ALA
3	Q	183	PRO
3	C	183	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	206 (99%)	3 (1%)	74	91
1	O	209/209 (100%)	206 (99%)	3 (1%)	74	91
2	B	203/216 (94%)	196 (97%)	7 (3%)	44	72
2	P	203/216 (94%)	196 (97%)	7 (3%)	44	72
3	C	212/226 (94%)	201 (95%)	11 (5%)	29	51
3	Q	212/226 (94%)	201 (95%)	11 (5%)	29	51
4	D	194/215 (90%)	184 (95%)	10 (5%)	29	51
4	R	194/215 (90%)	184 (95%)	10 (5%)	29	51
5	E	190/193 (98%)	181 (95%)	9 (5%)	32	56
5	S	190/193 (98%)	181 (95%)	9 (5%)	32	56
6	F	201/239 (84%)	191 (95%)	10 (5%)	30	53
6	T	201/239 (84%)	191 (95%)	10 (5%)	30	53
7	G	206/210 (98%)	197 (96%)	9 (4%)	35	60
7	U	206/210 (98%)	197 (96%)	9 (4%)	35	60
8	H	185/190 (97%)	180 (97%)	5 (3%)	52	79
8	V	185/190 (97%)	180 (97%)	5 (3%)	52	79
9	I	172/173 (99%)	168 (98%)	4 (2%)	58	83
9	W	172/173 (99%)	169 (98%)	3 (2%)	68	89
10	J	173/175 (99%)	168 (97%)	5 (3%)	50	77
10	X	173/175 (99%)	168 (97%)	5 (3%)	50	77
11	K	170/170 (100%)	161 (95%)	9 (5%)	28	50
11	Y	170/170 (100%)	161 (95%)	9 (5%)	28	50
12	L	185/185 (100%)	180 (97%)	5 (3%)	52	79
12	Z	185/185 (100%)	180 (97%)	5 (3%)	52	79
13	M	199/208 (96%)	193 (97%)	6 (3%)	48	76
13	a	199/208 (96%)	193 (97%)	6 (3%)	48	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	162/162 (100%)	158 (98%)	4 (2%)	55	82
14	b	162/162 (100%)	158 (98%)	4 (2%)	55	82
All	All	5322/5542 (96%)	5129 (96%)	193 (4%)	42	69

All (193) 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	50	LYS
2	B	55	LEU
2	B	79	LEU
2	B	113	ARG
2	B	186	ASP
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	50	LEU
3	C	51	LYS
3	C	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	51	LEU
4	D	99	ILE
4	D	125	LEU
4	D	143	ASP
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	55	LEU

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Mol	Chain	Res	Type
5	E	71	LEU
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
5	E	207	VAL
5	E	231	LYS
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	172	LEU
6	F	181	GLU
6	F	201	GLU
6	F	202	ASP
6	F	207	ASP
6	F	214	TRP
6	F	240	GLN
7	G	26	THR
7	G	75	ASN
7	G	83	ASN
7	G	115	LEU
7	G	122	ARG
7	G	125	MET
7	G	208	GLU
7	G	235	ARG
7	G	236	LEU
8	H	30	ASN
8	H	56	THR
8	H	68	LEU
8	H	91	GLN
8	H	113	ILE
9	I	37	ASN
9	I	125	LEU
9	I	171	LEU
9	I	182	TRP
10	J	3	ILE
10	J	35	THR
10	J	90	LYS
10	J	99	GLN
10	J	149	ARG
11	K	4	LEU
11	K	9	GLN
11	K	100	MET

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Mol	Chain	Res	Type
11	K	104	TYR
11	K	107	LYS
11	K	118	ASP
11	K	140	LEU
11	K	148	LEU
11	K	211	ILE
12	L	3	ASN
12	L	23	LEU
12	L	31	THR
12	L	136	CYS
12	L	150	LEU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
14	N	9	LYS
14	N	83	LYS
14	N	104	ASP
14	N	107	LYS
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	50	LYS
2	P	55	LEU
2	P	79	LEU
2	P	113	ARG
2	P	186	ASP
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	50	LEU
3	Q	51	LYS
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	206	LYS
3	Q	240	GLU

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Mol	Chain	Res	Type
4	R	51	LEU
4	R	99	ILE
4	R	125	LEU
4	R	143	ASP
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	55	LEU
5	S	71	LEU
5	S	184	ASN
5	S	188	LEU
5	S	202	ASP
5	S	207	VAL
5	S	231	LYS
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	172	LEU
6	T	181	GLU
6	T	201	GLU
6	T	202	ASP
6	T	207	ASP
6	T	214	TRP
6	T	240	GLN
7	U	26	THR
7	U	75	ASN
7	U	83	ASN
7	U	115	LEU
7	U	122	ARG
7	U	125	MET
7	U	208	GLU
7	U	235	ARG
7	U	236	LEU
8	V	30	ASN
8	V	56	THR
8	V	68	LEU
8	V	91	GLN

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Mol	Chain	Res	Type
8	V	113	ILE
9	W	37	ASN
9	W	171	LEU
9	W	182	TRP
10	X	3	ILE
10	X	23	ARG
10	X	35	THR
10	X	90	LYS
10	X	99	GLN
11	Y	4	LEU
11	Y	9	GLN
11	Y	100	MET
11	Y	104	TYR
11	Y	107	LYS
11	Y	118	ASP
11	Y	140	LEU
11	Y	148	LEU
11	Y	211	ILE
12	Z	3	ASN
12	Z	23	LEU
12	Z	31	THR
12	Z	136	CYS
12	Z	150	LEU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
14	b	9	LYS
14	b	83	LYS
14	b	104	ASP
14	b	107	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN
2	B	58	GLN
2	B	95	GLN
2	B	119	GLN

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Mol	Chain	Res	Type
2	B	123	GLN
2	B	155	ASN
3	C	17	GLN
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	146	GLN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	151	ASN
5	E	184	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
6	F	240	GLN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
8	H	66	HIS
8	H	114	HIS
9	I	37	ASN
10	J	55	GLN
11	K	9	GLN
11	K	85	ASN
11	K	176	ASN
11	K	188	HIS
11	K	190	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
13	M	48	ASN

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Mol	Chain	Res	Type
13	M	102	GLN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	161	GLN
1	O	94	HIS
2	P	20	GLN
2	P	58	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
3	Q	17	GLN
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	146	GLN
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	151	ASN
5	S	184	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
8	V	114	HIS
9	W	37	ASN
10	X	55	GLN
10	X	146	HIS
11	Y	9	GLN
11	Y	85	ASN

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Mol	Chain	Res	Type
11	Y	176	ASN
11	Y	188	HIS
11	Y	190	ASN
12	Z	3	ASN
12	Z	49	ASN
13	a	48	ASN
13	a	102	GLN
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN
14	b	161	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 13 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	1.56	5 (17%)	31,38,38	1.29	6 (19%)
17	BO2	K	301	11	28,29,29	1.51	5 (17%)	31,38,38	1.27	4 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BO2	N	201	14	28,29,29	1.49	3 (10%)	31,38,38	1.17	5 (16%)
17	BO2	V	301	8	28,29,29	1.56	5 (17%)	31,38,38	1.29	6 (19%)
17	BO2	Y	301	11	28,29,29	1.51	5 (17%)	31,38,38	1.29	5 (16%)
17	BO2	b	201	14	28,29,29	1.49	3 (10%)	31,38,38	1.17	5 (16%)

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 (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	201	BO2	C2-C7	-5.24	1.38	1.50
17	b	201	BO2	C2-C7	-5.16	1.38	1.50
17	H	301	BO2	C2-C7	-4.66	1.39	1.50
17	V	301	BO2	C2-C7	-4.58	1.39	1.50
17	Y	301	BO2	C2-C7	-4.51	1.40	1.50
17	K	301	BO2	C2-C7	-4.49	1.40	1.50
17	b	201	BO2	C11-C12	-4.35	1.40	1.51
17	H	301	BO2	C11-C12	-4.31	1.40	1.51
17	N	201	BO2	C11-C12	-4.26	1.40	1.51
17	V	301	BO2	C11-C12	-4.23	1.40	1.51
17	K	301	BO2	C11-C12	-4.17	1.41	1.51
17	Y	301	BO2	C11-C12	-4.11	1.41	1.51
17	b	201	BO2	C3-N4	2.11	1.38	1.34
17	N	201	BO2	C3-N4	2.13	1.38	1.34
17	K	301	BO2	C5-N4	2.21	1.40	1.33
17	Y	301	BO2	C5-N4	2.25	1.40	1.33
17	H	301	BO2	C5-N4	2.26	1.40	1.33
17	V	301	BO2	C5-N4	2.33	1.40	1.33
17	K	301	BO2	C6-N1	2.80	1.40	1.34
17	K	301	BO2	C3-N4	2.82	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Y	301	BO2	C3-N4	2.86	1.40	1.34
17	H	301	BO2	C6-N1	2.87	1.40	1.34
17	Y	301	BO2	C6-N1	2.89	1.40	1.34
17	V	301	BO2	C6-N1	2.91	1.40	1.34
17	H	301	BO2	C3-N4	2.98	1.40	1.34
17	V	301	BO2	C3-N4	3.06	1.40	1.34

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	301	BO2	C18-C10-N9	-2.79	103.41	111.26
17	Y	301	BO2	C18-C10-N9	-2.77	103.46	111.26
17	N	201	BO2	C5-C6-N1	-2.72	118.88	122.25
17	b	201	BO2	C11-C10-N9	-2.59	105.37	110.80
17	K	301	BO2	B26-C21-C22	-2.50	106.29	112.79
17	N	201	BO2	C11-C10-N9	-2.47	105.63	110.80
17	b	201	BO2	C5-C6-N1	-2.46	119.20	122.25
17	V	301	BO2	C12-C11-C10	-2.46	106.25	113.41
17	Y	301	BO2	B26-C21-C22	-2.44	106.46	112.79
17	H	301	BO2	C12-C11-C10	-2.43	106.35	113.41
17	b	201	BO2	B26-C21-C22	-2.42	106.50	112.79
17	b	201	BO2	C18-C10-N9	-2.39	104.52	111.26
17	N	201	BO2	B26-C21-C22	-2.39	106.60	112.79
17	H	301	BO2	C18-C10-N9	-2.31	104.75	111.26
17	N	201	BO2	C18-C10-N9	-2.31	104.77	111.26
17	V	301	BO2	C18-C10-N9	-2.26	104.89	111.26
17	Y	301	BO2	C6-C5-N4	-2.11	119.08	121.94
17	V	301	BO2	C5-C6-N1	-2.10	119.64	122.25
17	H	301	BO2	C5-C6-N1	-2.08	119.67	122.25
17	H	301	BO2	C6-C5-N4	-2.05	119.17	121.94
17	V	301	BO2	C6-C5-N4	-2.03	119.19	121.94
17	N	201	BO2	C6-N1-C2	2.18	119.84	116.92
17	b	201	BO2	C6-N1-C2	2.21	119.89	116.92
17	K	301	BO2	C3-C2-C7	2.22	121.81	119.55
17	Y	301	BO2	C3-C2-C7	2.33	121.92	119.55
17	H	301	BO2	C3-C2-C7	2.37	121.96	119.55
17	V	301	BO2	C3-C2-C7	2.42	122.02	119.55
17	K	301	BO2	C6-N1-C2	3.16	121.16	116.92
17	Y	301	BO2	C6-N1-C2	3.21	121.23	116.92
17	H	301	BO2	C6-N1-C2	3.41	121.50	116.92
17	V	301	BO2	C6-N1-C2	3.50	121.62	116.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	H	301	BO2	2	0
17	K	301	BO2	3	0
17	N	201	BO2	5	0
17	V	301	BO2	2	0
17	Y	301	BO2	3	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%)	-0.15	13 (5%)	31 35	40, 54, 91, 133	0
1	O	250/250 (100%)	-0.10	11 (4%)	38 43	42, 60, 105, 139	0
2	B	244/258 (94%)	-0.11	12 (4%)	33 38	39, 59, 105, 150	0
2	P	244/258 (94%)	-0.03	11 (4%)	37 42	44, 62, 104, 150	0
3	C	240/254 (94%)	0.12	18 (7%)	17 19	39, 63, 123, 156	0
3	Q	240/254 (94%)	0.22	21 (8%)	12 13	45, 74, 153, 183	0
4	D	235/260 (90%)	-0.12	5 (2%)	67 71	43, 63, 94, 138	0
4	R	235/260 (90%)	-0.04	10 (4%)	39 44	48, 69, 107, 149	0
5	E	231/234 (98%)	-0.08	5 (2%)	65 69	46, 65, 104, 151	0
5	S	231/234 (98%)	0.02	11 (4%)	34 39	49, 72, 109, 144	0
6	F	243/288 (84%)	-0.17	11 (4%)	37 42	39, 60, 111, 139	0
6	T	243/288 (84%)	-0.07	13 (5%)	30 34	39, 66, 120, 149	0
7	G	241/252 (95%)	-0.22	10 (4%)	41 46	37, 57, 97, 153	0
7	U	241/252 (95%)	-0.17	7 (2%)	55 60	41, 57, 90, 138	0
8	H	226/232 (97%)	-0.10	5 (2%)	65 69	36, 51, 90, 156	0
8	V	226/232 (97%)	-0.10	7 (3%)	52 57	36, 52, 87, 169	0
9	I	204/205 (99%)	-0.32	6 (2%)	55 60	33, 50, 83, 103	0
9	W	204/205 (99%)	-0.32	7 (3%)	49 54	35, 51, 84, 105	0
10	J	195/198 (98%)	-0.29	3 (1%)	76 79	36, 52, 78, 131	0
10	X	195/198 (98%)	-0.28	4 (2%)	67 71	39, 55, 80, 136	0
11	K	212/212 (100%)	-0.27	2 (0%)	85 88	35, 54, 79, 97	0
11	Y	212/212 (100%)	-0.24	5 (2%)	62 66	40, 54, 83, 101	0
12	L	222/222 (100%)	-0.04	9 (4%)	41 46	37, 55, 101, 131	0
12	Z	222/222 (100%)	-0.07	10 (4%)	37 42	37, 55, 101, 137	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.41	4 (1%)	73	76	35, 52, 74, 91	0
13	a	233/246 (94%)	-0.40	1 (0%)	93	93	34, 52, 74, 93	0
14	N	196/196 (100%)	-0.39	2 (1%)	84	86	37, 48, 75, 102	0
14	b	196/196 (100%)	-0.38	2 (1%)	84	86	36, 48, 75, 108	0
All	All	6344/6614 (95%)	-0.15	225 (3%)	48	53	33, 57, 101, 183	0

All (225) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	X	1	MET	8.0
9	W	1	SER	7.7
12	L	174	TYR	7.7
2	P	51	VAL	7.6
10	J	1	MET	7.5
12	Z	174	TYR	7.1
12	L	165	ASN	7.0
1	A	249	ALA	6.7
3	Q	50	LEU	6.6
8	V	223	ILE	6.6
1	O	249	ALA	6.5
1	O	2	THR	6.4
3	Q	49	THR	6.3
1	A	2	THR	6.0
2	B	221	ASP	5.8
5	E	202	ASP	5.6
3	Q	206	LYS	5.6
3	Q	238	LYS	5.5
2	B	220	ASN	5.5
12	Z	173	LYS	5.4
1	O	250	LEU	5.4
8	V	224	GLN	5.3
2	P	221	ASP	5.3
8	V	222	ASP	5.3
1	A	1	MET	5.2
8	V	226	GLU	5.2
9	I	1	SER	5.1
3	C	202	GLN	5.1
2	B	51	VAL	5.1
3	Q	239	GLN	5.0
3	Q	240	GLU	4.9
12	Z	162	PRO	4.8

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Mol	Chain	Res	Type	RSRZ
12	Z	163	GLY	4.8
3	C	206	LYS	4.7
1	O	1	MET	4.7
7	U	242	GLN	4.7
8	H	226	GLU	4.7
2	P	219	ALA	4.7
12	L	168	VAL	4.6
5	S	202	ASP	4.6
8	H	222	ASP	4.5
12	Z	165	ASN	4.5
5	E	233	ILE	4.4
8	V	221	CYS	4.3
8	H	224	GLN	4.3
3	Q	236	GLN	4.3
11	Y	212	GLY	4.3
12	Z	168	VAL	4.3
2	P	59	ASP	4.2
3	C	239	GLN	4.2
12	L	163	GLY	4.2
3	C	235	GLU	4.2
8	H	221	CYS	4.1
3	Q	202	GLN	4.1
10	J	194	ASP	4.1
3	C	236	GLN	4.1
7	U	2	GLY	4.1
6	F	202	ASP	4.0
3	C	238	LYS	4.0
2	P	218	GLY	3.9
4	R	125	LEU	3.8
9	I	131	GLU	3.8
6	F	2	THR	3.7
9	W	130	ASP	3.7
11	K	212	GLY	3.7
4	D	242	GLU	3.7
6	T	2	THR	3.7
6	F	215	CYS	3.6
1	O	52	SER	3.6
2	B	219	ALA	3.6
2	P	220	ASN	3.6
13	a	1	THR	3.6
7	G	2	GLY	3.5
10	X	194	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
3	C	50	LEU	3.5
6	T	243	ILE	3.5
8	V	225	GLU	3.4
14	b	195	GLN	3.4
12	L	162	PRO	3.4
6	F	181	GLU	3.4
14	b	105	LYS	3.4
6	F	243	ILE	3.4
12	L	173	LYS	3.3
6	T	180	PRO	3.3
9	W	133	LYS	3.3
9	W	131	GLU	3.3
5	S	173	ARG	3.3
1	A	250	LEU	3.3
3	Q	205	ALA	3.3
3	C	49	THR	3.2
4	R	241	ALA	3.2
12	L	171	PRO	3.2
14	N	195	GLN	3.2
7	U	222	ASP	3.2
3	C	225	GLU	3.2
2	B	218	GLY	3.1
13	M	1	THR	3.1
4	R	54	ASP	3.1
2	P	222	GLY	3.1
3	Q	225	GLU	3.0
4	R	242	GLU	3.0
6	T	182	GLY	3.0
4	R	1	ASP	2.9
6	F	244	ASN	2.9
1	A	54	PRO	2.9
3	C	203	THR	2.9
3	Q	234	ILE	2.9
3	Q	48	SER	2.9
5	S	210	LEU	2.9
6	T	215	CYS	2.9
12	L	156	PHE	2.9
12	Z	171	PRO	2.9
4	R	230	GLU	2.8
9	I	133	LYS	2.8
6	T	230	ASP	2.8
1	A	202	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
4	D	224	ASP	2.8
7	G	68	ARG	2.8
1	A	166	LYS	2.8
14	N	105	LYS	2.7
1	O	201	GLU	2.7
2	P	230	LYS	2.7
12	Z	167	LYS	2.7
6	T	244	ASN	2.7
6	T	178	HIS	2.7
6	T	181	GLU	2.7
3	C	1	GLY	2.7
9	I	130	ASP	2.7
10	X	193	ASP	2.7
6	F	205	GLU	2.7
7	G	3	TYR	2.7
4	D	1	ASP	2.6
13	M	47	ASP	2.6
7	U	3	TYR	2.6
7	G	242	GLN	2.6
13	M	82	ASP	2.6
3	Q	141	ASP	2.5
5	S	233	ILE	2.5
3	Q	187	GLU	2.5
5	E	173	ARG	2.5
5	S	180	LYS	2.5
6	T	201	GLU	2.5
6	T	205	GLU	2.5
7	U	188	GLU	2.5
3	C	216	ASP	2.5
3	Q	204	GLY	2.5
3	Q	229	GLN	2.5
5	E	123	GLY	2.5
5	S	123	GLY	2.5
1	O	248	GLU	2.5
4	R	117	GLU	2.5
3	Q	203	THR	2.5
1	O	4	ARG	2.5
4	D	2	ARG	2.4
4	R	239	GLU	2.4
1	A	228	PRO	2.4
11	K	147	ASP	2.4
7	G	181	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
6	F	178	HIS	2.4
1	A	182	GLU	2.4
5	S	3	ASN	2.4
7	U	181	LYS	2.4
9	I	192	ASP	2.4
3	Q	60	SER	2.4
2	P	240	LYS	2.3
11	Y	208	ASN	2.3
7	U	206	GLY	2.3
7	G	179	LYS	2.3
10	X	195	PHE	2.3
1	A	201	GLU	2.3
12	Z	161	GLU	2.3
3	C	3	ASP	2.3
11	Y	106	ARG	2.3
9	W	160	GLU	2.3
3	Q	47	ARG	2.3
6	F	180	PRO	2.3
3	C	37	LYS	2.2
10	J	24	GLY	2.2
3	C	175	LYS	2.2
2	B	60	THR	2.2
2	P	60	THR	2.2
6	F	201	GLU	2.2
2	B	217	LYS	2.2
3	C	205	ALA	2.2
2	B	93	HIS	2.2
13	M	121	SER	2.2
7	G	188	GLU	2.2
2	B	182	ASP	2.2
3	Q	235	GLU	2.2
8	H	225	GLU	2.2
6	T	204	LYS	2.2
4	D	241	ALA	2.2
1	O	3	ASP	2.2
2	B	201	ASP	2.2
5	S	225	ASP	2.2
7	G	222	ASP	2.2
5	S	203	GLU	2.1
11	Y	202	GLU	2.1
1	O	53	SER	2.1
3	C	60	SER	2.1

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Mol	Chain	Res	Type	RSRZ
8	V	9	ASN	2.1
4	R	217	GLN	2.1
1	A	3	ASP	2.1
2	P	186	ASP	2.1
3	Q	3	ASP	2.1
6	F	193	ALA	2.1
7	G	40	ASP	2.1
12	L	170	LYS	2.1
9	W	192	ASP	2.1
11	Y	209	ASN	2.1
1	O	198	GLU	2.1
5	S	227	GLU	2.1
3	C	180	LYS	2.1
1	A	248	GLU	2.0
12	Z	1	GLN	2.0
1	A	203	GLU	2.0
5	S	201	ARG	2.0
2	B	240	LYS	2.0
6	T	241	LYS	2.0
2	B	59	ASP	2.0
5	E	3	ASN	2.0
4	R	201	GLU	2.0
7	G	241	GLU	2.0
9	I	160	GLU	2.0
9	W	124	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
15	MG	J	201	1/1	0.91	0.32	14.24	53,53,53,53	0
15	MG	K	303	1/1	0.98	0.28	6.47	54,54,54,54	0
17	BO2	b	201	28/28	0.89	0.20	3.09	40,47,53,54	0
17	BO2	Y	301	28/28	0.90	0.19	2.71	45,54,68,72	0
15	MG	Z	301	1/1	0.95	0.21	2.18	62,62,62,62	0
17	BO2	N	201	28/28	0.87	0.19	2.17	34,44,47,49	0
17	BO2	K	301	28/28	0.90	0.19	1.72	35,50,63,65	0
17	BO2	V	301	28/28	0.92	0.21	1.29	46,50,74,76	0
17	BO2	H	301	28/28	0.91	0.20	0.95	43,50,74,77	0
15	MG	I	301	1/1	0.96	0.12	-0.28	63,63,63,63	0
15	MG	G	301	1/1	0.93	0.08	-1.06	54,54,54,54	0
15	MG	K	302	1/1	0.97	0.07	-1.88	49,49,49,49	0
15	MG	N	202	1/1	0.97	0.09	-1.94	40,40,40,40	0
16	CL	N	203	1/1	0.99	0.05	-2.36	45,45,45,45	0
15	MG	Y	302	1/1	0.98	0.03	-2.71	52,52,52,52	0
15	MG	V	302	1/1	0.99	0.04	-3.06	50,50,50,50	0
16	CL	b	202	1/1	0.98	0.04	-3.09	47,47,47,47	0
16	CL	G	302	1/1	1.00	0.09	-	44,44,44,44	0
16	CL	U	301	1/1	0.99	0.13	-	45,45,45,45	0

6.5 Other polymers ⓘ

There are no such residues in this entry.