



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2016 – 11:40 AM EDT

PDB ID : 5LEZ
Title : Human 20S proteasome complex with Oprozomib in Mg-Acetate at 2.2 Angstrom
Authors : Schrader, J.; Henneberg, F.; Mata, R.; Tittmann, K.; Schneider, T.R.; Stark, H.; Bourenkov, G.; Chari, A.
Deposited on : 2016-06-30
Resolution : 2.19 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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.

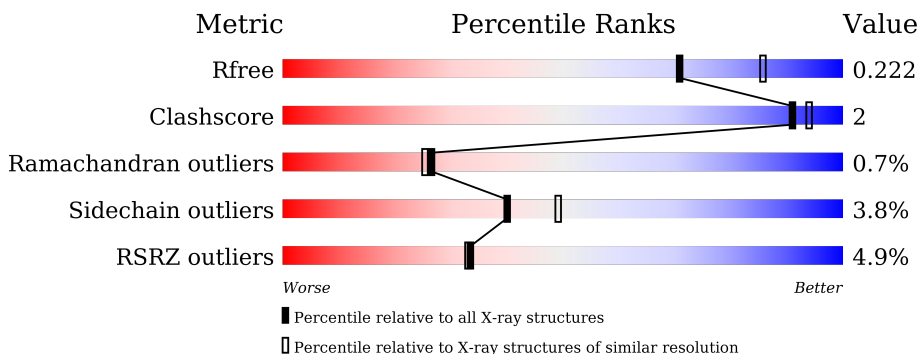
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
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) : rb-20027939

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X-RAY DIFFRACTION

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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	234	<div> <div>2%</div> <div>85%</div> <div>12%</div> <div>• •</div> </div>
1	O	234	<div> <div>13%</div> <div>87%</div> <div>9%</div> <div>• •</div> </div>
2	B	261	<div> <div>7%</div> <div>89%</div> <div>6%</div> <div>5%</div> </div>
2	P	261	<div> <div>11%</div> <div>84%</div> <div>10%</div> <div>• 5%</div> </div>
3	C	248	<div> <div>12%</div> <div>84%</div> <div>8%</div> <div>• •</div> </div>
3	Q	248	<div> <div>17%</div> <div>83%</div> <div>9%</div> <div>• 5%</div> </div>


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Mol	Chain	Length	Quality of chain
4	D	241	
4	R	241	
5	E	263	
5	S	263	
6	F	255	
6	T	255	
7	G	246	
7	U	246	
8	H	234	
8	V	234	
9	I	205	
9	W	205	
10	J	201	
10	X	201	
11	K	204	
11	Y	204	
12	L	213	
12	Z	213	
13	M	219	
13	a	219	
14	N	205	
14	b	205	
15	c	4	
15	d	4	
15	e	4	

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Mol	Chain	Length	Quality of chain
15	f	4	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	K	U	302	-	-	-	X
18	1PE	H	303	-	-	-	X
18	1PE	I	302	-	-	-	X
18	1PE	K	302	-	-	-	X
18	1PE	L	301	-	-	-	X
18	1PE	W	302	-	-	-	X
18	1PE	Y	301	-	-	-	X
18	1PE	a	301	-	-	-	X
19	ACT	f	101	-	-	-	X
7	6V1	U	47	X	-	-	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 52158 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	230	Total	C	N	O	S	0	3	0
			1788	1145	301	336	6			
1	O	230	Total	C	N	O	S	0	0	0
			1741	1111	293	331	6			

- Molecule 2 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	248	Total	C	N	O	S	0	2	0
			1922	1217	331	363	11			
2	P	247	Total	C	N	O	S	0	2	0
			1898	1200	321	366	11			

- Molecule 3 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	237	Total	C	N	O	S	0	2	0
			1798	1121	320	352	5			
3	Q	235	Total	C	N	O	S	0	0	0
			1801	1126	316	354	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	233	Total	C	N	O	S	0	1	0
			1762	1105	290	356	11			
4	R	233	Total	C	N	O	S	0	1	0
			1753	1103	293	346	11			

- Molecule 5 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	234	Total	C	N	O	S	0	1	0
			1822	1144	325	342	11			
5	S	238	Total	C	N	O	S	0	3	0
			1875	1175	340	349	11			

- Molecule 6 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	239	Total	C	N	O	S	0	4	0
			1888	1198	325	353	12			
6	T	240	Total	C	N	O	S	0	1	0
			1856	1178	315	351	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	244	Total	C	N	O	S	0	2	0
			1912	1214	321	364	13			
7	U	238	Total	C	N	O	S	0	1	0
			1815	1147	304	350	14			

- Molecule 8 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	220	Total	C	N	O	S	0	2	0
			1664	1047	284	320	13			
8	V	220	Total	C	N	O	S	0	2	0
			1622	1023	269	318	12			

- 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	3	0
			1613	1028	270	295	20			
9	W	204	Total	C	N	O	S	0	2	0
			1599	1018	267	295	19			

- Molecule 10 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	196	Total	C	N	O	S	0	3	0
			1590	1021	271	288	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	196	Total	C	N	O	S	0	2	0
			1576	1012	267	287	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	200	Total	C	N	O	S	0	0	0
			1551	977	272	293	9			
11	Y	199	Total	C	N	O	S	0	3	0
			1570	991	278	291	10			

- Molecule 12 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	213	Total	C	N	O	S	0	2	0
			1636	1038	277	310	11			
12	Z	213	Total	C	N	O	S	0	1	0
			1642	1041	280	310	11			

- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	216	Total	C	N	O	S	0	1	0
			1692	1067	291	322	12			
13	a	216	Total	C	N	O	S	0	2	0
			1688	1064	291	321	12			

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	202	Total	C	N	O	S	0	1	0
			1519	953	258	295	13			
14	b	203	Total	C	N	O	S	0	1	0
			1524	956	259	296	13			

- Molecule 15 is a protein called bound Oprozomib.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	c	4	Total	C	N	O	S	0	0	0
			37	25	4	7	1			
15	d	4	Total	C	N	O	S	0	0	0
			37	25	4	7	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	e	4	Total	C	N	O	S	0	0	0
			37	25	4	7	1			
15	f	4	Total	C	N	O	S	0	0	0
			37	25	4	7	1			

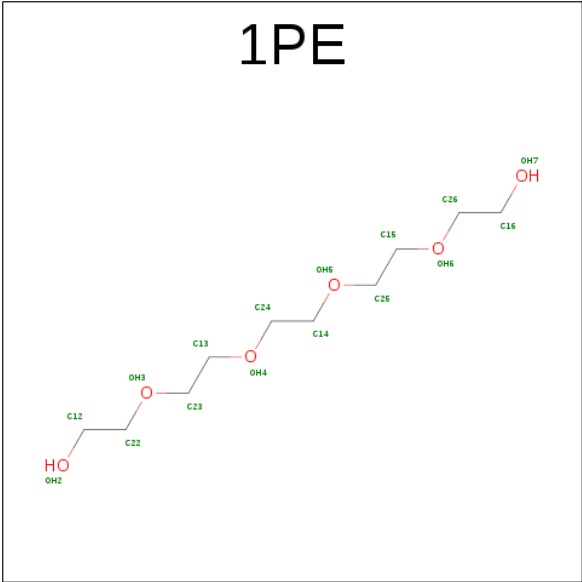
- Molecule 16 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	G	1	Total	K	0	0
			1	1		
16	b	1	Total	K	0	0
			1	1		
16	Z	1	Total	K	0	0
			1	1		
16	N	1	Total	K	0	0
			1	1		
16	U	1	Total	K	0	0
			1	1		
16	L	1	Total	K	0	0
			1	1		

- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

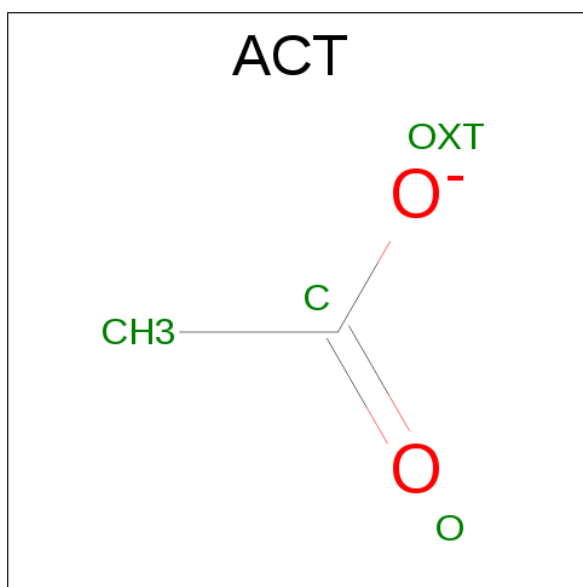
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	J	1	Total	Mg	0	0
			1	1		
17	K	1	Total	Mg	0	0
			1	1		
17	H	2	Total	Mg	0	0
			2	2		
17	I	2	Total	Mg	0	0
			2	2		
17	V	1	Total	Mg	0	0
			1	1		
17	W	1	Total	Mg	0	0
			1	1		
17	X	1	Total	Mg	0	0
			1	1		
17	L	1	Total	Mg	0	0
			1	1		

- Molecule 18 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	H	1	Total	C	O	0	0
			16	10	6		
18	I	1	Total	C	O	0	0
			16	10	6		
18	K	1	Total	C	O	0	0
			16	10	6		
18	L	1	Total	C	O	0	0
			16	10	6		
18	N	1	Total	C	O	0	0
			16	10	6		
18	U	1	Total	C	O	0	0
			16	10	6		
18	W	1	Total	C	O	0	0
			16	10	6		
18	Y	1	Total	C	O	0	0
			16	10	6		
18	a	1	Total	C	O	0	0
			16	10	6		

- Molecule 19 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	c	1	Total	C	O	0	0
			4	2	2		
19	d	1	Total	C	O	0	0
			4	2	2		
19	e	1	Total	C	O	0	0
			4	2	2		
19	f	1	Total	C	O	0	0
			4	2	2		

- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	120	Total	O	0	0
			120	120		
20	B	130	Total	O	0	0
			130	130		
20	C	80	Total	O	0	0
			80	80		
20	D	99	Total	O	0	0
			99	99		
20	E	147	Total	O	0	0
			147	147		
20	F	185	Total	O	0	0
			185	185		
20	G	196	Total	O	0	0
			196	196		
20	H	156	Total	O	0	0
			156	156		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	I	161	Total 161	O 161	0	0
20	J	136	Total 136	O 136	0	0
20	K	106	Total 106	O 106	0	0
20	L	127	Total 127	O 127	0	0
20	M	155	Total 155	O 155	0	0
20	N	160	Total 160	O 160	0	0
20	O	94	Total 94	O 94	0	0
20	P	127	Total 127	O 127	0	0
20	Q	77	Total 77	O 77	0	0
20	R	133	Total 133	O 133	0	0
20	S	132	Total 132	O 132	0	0
20	T	95	Total 95	O 95	0	0
20	U	116	Total 116	O 116	0	0
20	V	114	Total 114	O 114	0	0
20	W	120	Total 120	O 120	0	0
20	X	129	Total 129	O 129	0	0
20	Y	149	Total 149	O 149	0	0
20	Z	168	Total 168	O 168	0	0
20	a	179	Total 179	O 179	0	0
20	b	118	Total 118	O 118	0	0
20	c	2	Total 2	O 2	0	0

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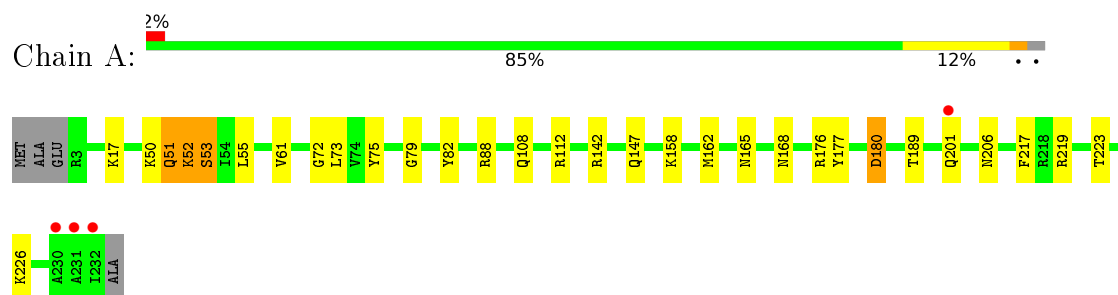
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	d	2	Total 2	O 2	0	0
20	e	3	Total 3	O 3	0	0
20	f	1	Total 1	O 1	0	0

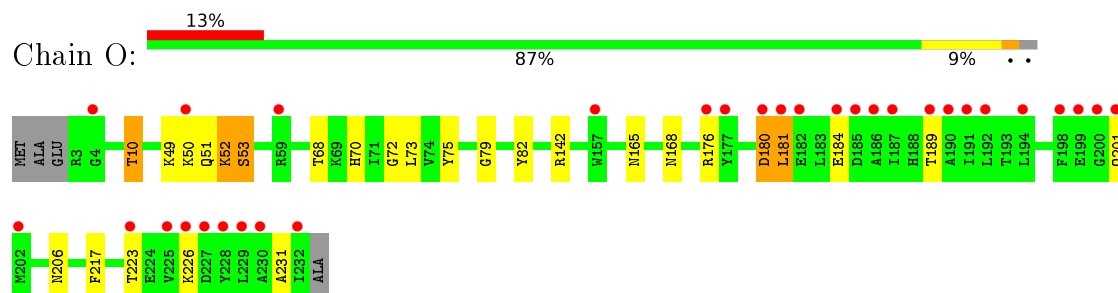
3 Residue-property plots [i](#)

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.

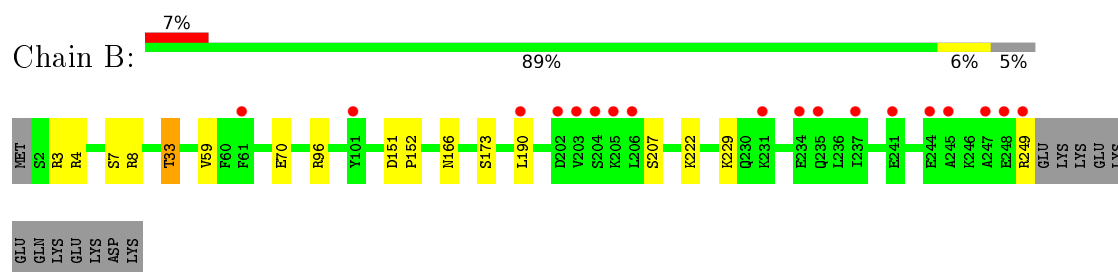
• Molecule 1: Proteasome subunit alpha type-2



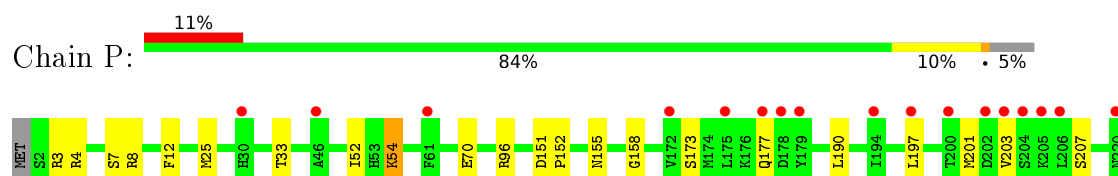
• Molecule 1: Proteasome subunit alpha type-2



• Molecule 2: Proteasome subunit alpha type-4



• Molecule 2: Proteasome subunit alpha type-4





GLU ARG
PRO GLN
ARG LYS
ALA GLN
PRO GLN
ALA GLN
PRO GLN
ASP GLU
PRO GLU
ALA GLU
LYS LYS
ALA ASP
GLU PRO
MET GLU
HIS

• Molecule 5: Proteasome subunit alpha type-1

Chain S: 2% 80% 9% 10%

MET F2 R3 D7 R18 I19 E23 V29 V45 L46 V47 Q60 H65 G71 T78 N86 R89 R101 R122 N152 Y153 F154 R174 E181 L195 D204 F221 E234 G235 L236 E237 E238 PRO GLN ARG LYS ALA GLN PRO
ALA GLN PRO GLU LYS ASP GLU PRO MET HIS

• Molecule 6: Proteasome subunit alpha type-3

Chain F: 1% 86% 7% 6%

MET SER SER ILE GLY THR G6 D17 K28 D43 K51 L52 V53 S62 L81 R85 S86 L87 M117 F131 R169 R187 V190 E203 D206 W215 V227 R232 K240 L243 K244 GLU ASP GLU ASP ASP ASP MET
SER SER ILE GLY THR G6 D17 K28 D43 K51 L52 V53 S62 L81 R85 S86 L87 M117 F131 R169 R187 V190 E203 D206 W215 V227 R232 K240 L243 K244 GLU ASP GLU ASP ASP ASP MET

• Molecule 6: Proteasome subunit alpha type-3

Chain T: 5% 85% 7% 6%

MET SER SER ILE GLY THR G6 D17 M27 K28 D43 L54 S62 N63 L81 R85 S86 L87 M117 F131 R169 Q180 V190 D202 E203 V204 K205 D206 K207 A208 F209 W215 R223 K237 K240 E241 K244 GLU ASP GLU ASP ASP ASP MET
SER ASP ASP ASP ASN MET

• Molecule 7: Proteasome subunit alpha type-6

Chain G: 4% 93% ...

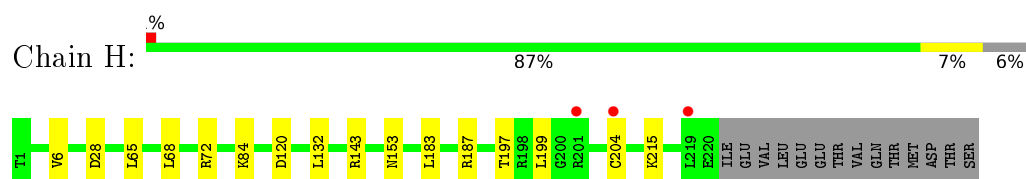
MET S2 R11 I32 I72 I76 G78 D86 S87 R88 N100 E108 R117 C137 M138 I139 L140 V183 K184 K185 K186 F187 D188 W189 T190 L206 S207 L208 D209 P212 E232 R245 ASP
MET S2 R11 I32 I72 I76 G78 D86 S87 R88 N100 E108 R117 C137 M138 I139 L140 V183 K184 K185 K186 F187 D188 W189 T190 L206 S207 L208 D209 P212 E232 R245 ASP

• Molecule 7: Proteasome subunit alpha type-6

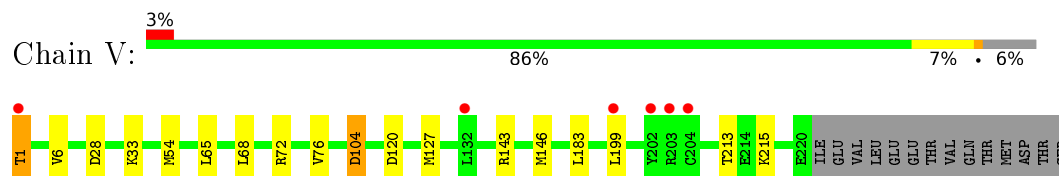
Chain U: 15% 90% 5% ..

MET S2 R3 A7 G36 V56 F57 D58 K59 G78 R88 N100 R117 I118 M138 I139 L140 Y160 F178 K186 PHE ASP TRP THR PHE GLU Q193 T194 V195 E196 T197 A198 I199 T200 C201 L202 S203 T204 V205 L206 S207 L208 D209 F210 K211 P212 S213 E214
V222 E223 L230 T231 E232 T235 D236 A237 E238 L239 V240 A241 L242 A243 E244 R245 ASP
MET S2 R3 A7 G36 V56 F57 D58 K59 G78 R88 N100 R117 I118 M138 I139 L140 Y160 F178 K186 PHE ASP TRP THR PHE GLU Q193 T194 V195 E196 T197 A198 I199 T200 C201 L202 S203 T204 V205 L206 S207 L208 D209 F210 K211 P212 S213 E214

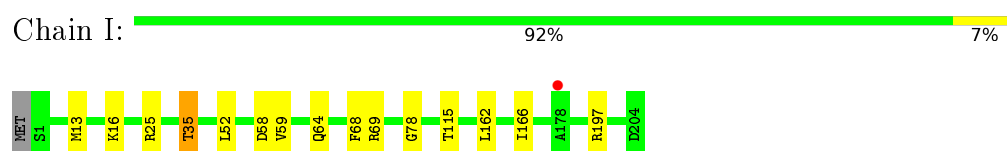
• Molecule 8: Proteasome subunit beta type-7



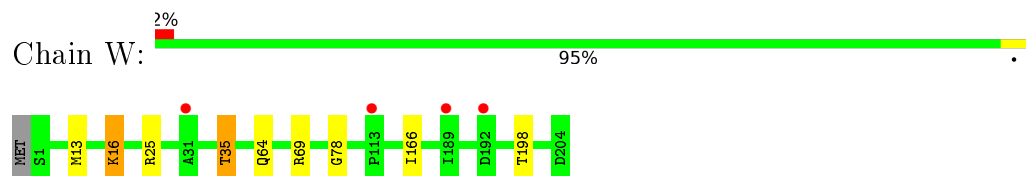
- Molecule 8: Proteasome subunit beta type-7



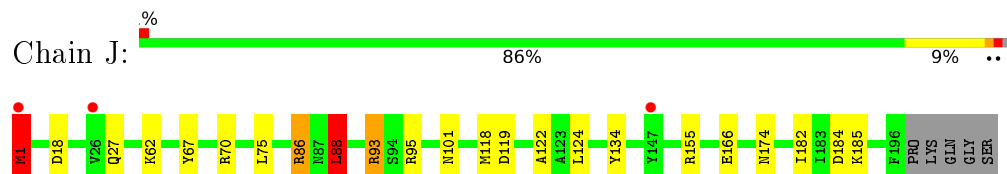
- Molecule 9: Proteasome subunit beta type-3



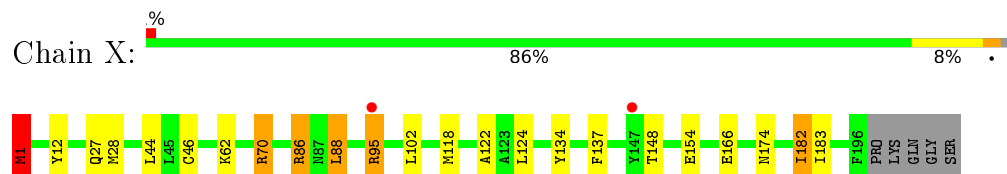
- Molecule 9: Proteasome subunit beta type-3



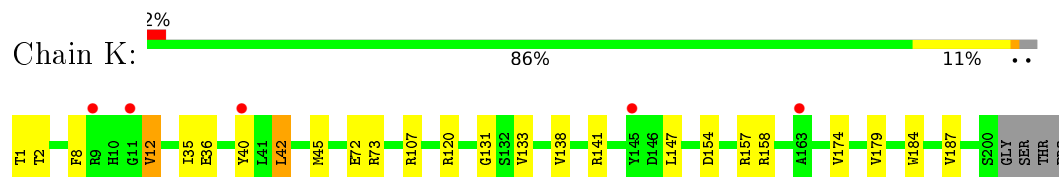
- Molecule 10: Proteasome subunit beta type-2



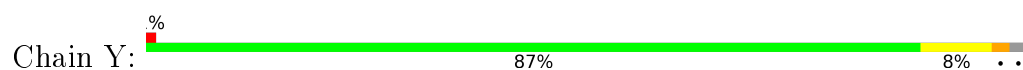
- Molecule 10: Proteasome subunit beta type-2



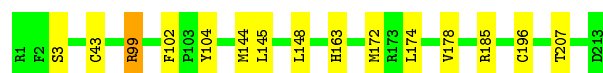
- Molecule 11: Proteasome subunit beta type-5



- Molecule 11: Proteasome subunit beta type-5



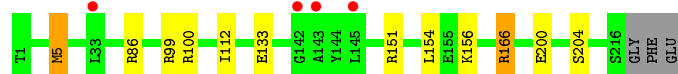
- Molecule 12: Proteasome subunit beta type-1



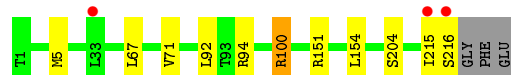
- Molecule 12: Proteasome subunit beta type-1



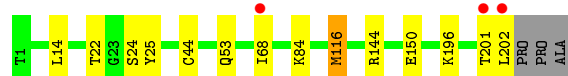
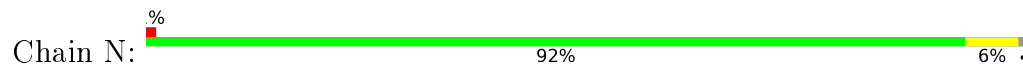
- Molecule 13: Proteasome subunit beta type-4



- Molecule 13: Proteasome subunit beta type-4



- Molecule 14: Proteasome subunit beta type-6



- Molecule 14: Proteasome subunit beta type-6



- Molecule 15: bound Oprozomib

Chain c:  100%

There are no outlier residues recorded for this chain.

- Molecule 15: bound Oprozomib

Chain d:  100%

There are no outlier residues recorded for this chain.

- Molecule 15: bound Oprozomib

Chain e:  100%

There are no outlier residues recorded for this chain.

- Molecule 15: bound Oprozomib

Chain f:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.86Å 203.23Å 315.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	170.81 – 2.19 49.67 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.4 (170.81-2.19) 99.5 (49.67-2.19)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.181 , 0.222 0.185 , 0.222	Depositor DCC
R_{free} test set	18458 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	52158	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 6V9, K, 6V1, 1PE, OAS, YCM, ACT, 6VA

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	0.70	0/1833	0.80	2/2489 (0.1%)
1	O	0.60	0/1778	0.79	1/2419 (0.0%)
2	B	0.73	0/1958	0.87	4/2645 (0.2%)
2	P	0.67	0/1934	0.86	3/2617 (0.1%)
3	C	0.77	1/1818 (0.1%)	0.94	8/2469 (0.3%)
3	Q	0.71	0/1814	0.88	2/2462 (0.1%)
4	D	0.70	0/1789	0.82	4/2424 (0.2%)
4	R	0.82	2/1780 (0.1%)	0.91	5/2408 (0.2%)
5	E	0.71	1/1842 (0.1%)	0.86	2/2493 (0.1%)
5	S	0.71	0/1901	0.89	5/2571 (0.2%)
6	F	0.78	0/1935	0.89	4/2605 (0.2%)
6	T	0.79	1/1894 (0.1%)	0.93	8/2556 (0.3%)
7	G	0.82	3/1909 (0.2%)	0.88	7/2579 (0.3%)
7	U	0.70	0/1804	0.82	2/2441 (0.1%)
8	H	0.81	1/1697 (0.1%)	0.97	5/2299 (0.2%)
8	V	0.68	2/1655 (0.1%)	0.88	4/2251 (0.2%)
9	I	0.76	0/1648	0.96	8/2219 (0.4%)
9	W	0.62	0/1630	0.89	6/2197 (0.3%)
10	J	0.82	0/1613	0.99	5/2180 (0.2%)
10	X	0.74	1/1599 (0.1%)	0.94	4/2163 (0.2%)
11	K	0.73	0/1582	0.97	9/2138 (0.4%)
11	Y	0.85	1/1610 (0.1%)	1.00	9/2172 (0.4%)
12	L	0.67	0/1672	0.85	3/2257 (0.1%)
12	Z	0.84	4/1675 (0.2%)	0.91	3/2257 (0.1%)
13	M	0.79	0/1728	0.93	5/2339 (0.2%)
13	a	0.83	0/1724	0.93	4/2336 (0.2%)
14	N	0.86	2/1548 (0.1%)	0.90	2/2095 (0.1%)
14	b	0.81	0/1554	0.90	4/2104 (0.2%)
All	All	0.75	19/48924 (0.0%)	0.90	128/66185 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying

if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	P	0	3
3	Q	0	2
4	D	0	2
4	R	0	1
5	E	0	1
6	F	0	1
7	U	1	0
9	I	0	1
9	W	0	1
10	J	0	2
10	X	0	2
13	a	0	1
All	All	1	17

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	182	GLU	CD-OE2	8.46	1.34	1.25
7	G	108	GLU	CD-OE1	8.18	1.34	1.25
12	Z	3	SER	CB-OG	7.22	1.51	1.42
10	X	154	GLU	C-O	6.91	1.36	1.23
14	N	24	SER	CB-OG	-6.42	1.33	1.42

The worst 5 of 128 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	Z	99	ARG	NE-CZ-NH2	-11.67	114.46	120.30
10	J	86	ARG	NE-CZ-NH1	10.77	125.68	120.30
9	I	69	ARG	NE-CZ-NH1	10.36	125.48	120.30
4	R	120[A]	ALA	C-N-CA	9.90	146.45	121.70
4	R	120[B]	ALA	C-N-CA	9.90	146.45	121.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	175[A]	GLU	Peptide
4	D	175[B]	GLU	Peptide
5	E	235	GLY	Peptide
6	F	206	ASP	Peptide
9	I	78	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1788	0	1761	12	0
1	O	1741	0	1683	9	0
2	B	1922	0	1913	4	0
2	P	1898	0	1861	11	0
3	C	1798	0	1718	14	0
3	Q	1801	0	1735	14	0
4	D	1762	0	1709	10	0
4	R	1753	0	1726	10	0
5	E	1822	0	1779	11	0
5	S	1875	0	1818	15	0
6	F	1888	0	1882	4	0
6	T	1856	0	1816	4	0
7	G	1912	0	1882	7	0
7	U	1815	0	1748	6	0
8	H	1664	0	1681	6	0
8	V	1622	0	1595	8	0
9	I	1613	0	1646	5	0
9	W	1599	0	1621	4	0
10	J	1590	0	1581	14	0
10	X	1576	0	1561	16	0
11	K	1551	0	1506	9	0
11	Y	1570	0	1547	11	0
12	L	1636	0	1625	7	0
12	Z	1642	0	1635	6	0
13	M	1692	0	1670	4	0
13	a	1688	0	1658	0	0
14	N	1519	0	1493	6	0
14	b	1524	0	1493	0	0
15	c	37	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	d	37	0	6	0	0
15	e	37	0	6	0	0
15	f	37	0	6	0	0
16	G	1	0	0	0	0
16	L	1	0	0	0	0
16	N	1	0	0	0	0
16	U	1	0	0	0	0
16	Z	1	0	0	0	0
16	b	1	0	0	0	0
17	H	2	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	K	1	0	0	0	0
17	L	1	0	0	0	0
17	V	1	0	0	0	0
17	W	1	0	0	0	0
17	X	1	0	0	0	0
18	H	16	0	22	0	0
18	I	16	0	22	0	0
18	K	16	0	22	0	0
18	L	16	0	22	0	0
18	N	16	0	22	0	0
18	U	16	0	22	0	0
18	W	16	0	22	0	0
18	Y	16	0	22	0	0
18	a	16	0	22	0	0
19	c	4	0	3	0	0
19	d	4	0	3	0	0
19	e	4	0	3	0	0
19	f	4	0	3	0	0
20	A	120	0	0	2	0
20	B	130	0	0	1	0
20	C	80	0	0	1	0
20	D	99	0	0	1	0
20	E	147	0	0	3	0
20	F	185	0	0	1	1
20	G	196	0	0	2	1
20	H	156	0	0	1	0
20	I	161	0	0	1	0
20	J	136	0	0	2	0
20	K	106	0	0	1	0
20	L	127	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	M	155	0	0	0	0
20	N	160	0	0	0	0
20	O	94	0	0	1	0
20	P	127	0	0	2	0
20	Q	77	0	0	0	0
20	R	133	0	0	1	0
20	S	132	0	0	5	0
20	T	95	0	0	0	0
20	U	116	0	0	0	0
20	V	114	0	0	1	0
20	W	120	0	0	2	0
20	X	129	0	0	0	0
20	Y	149	0	0	1	0
20	Z	168	0	0	0	0
20	a	179	0	0	0	0
20	b	118	0	0	0	0
20	c	2	0	0	0	0
20	d	2	0	0	0	0
20	e	3	0	0	0	0
20	f	1	0	0	0	0
All	All	52158	0	47577	199	1

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.

The worst 5 of 199 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)
5:E:47:VAL:HG12	5:E:195:LEU:HD22	1.64	0.80
6:F:227:VAL:O	6:F:232[B]:ARG:NH1	2.14	0.80
5:S:18[B]:ARG:HG2	5:S:23:GLU:OE2	1.84	0.78
5:S:47:VAL:HG12	5:S:195:LEU:HD22	1.65	0.77
10:J:1[A]:MET:HE1	10:J:134:TYR:H	1.51	0.74

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:F:465:HOH:O	20:G:566:HOH:O[4_475]	2.06	0.14

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	231/234 (99%)	222 (96%)	4 (2%)	5 (2%)	8	4
1	O	228/234 (97%)	218 (96%)	4 (2%)	6 (3%)	7	3
2	B	248/261 (95%)	240 (97%)	8 (3%)	0	100	100
2	P	247/261 (95%)	233 (94%)	11 (4%)	3 (1%)	16	12
3	C	236/248 (95%)	217 (92%)	14 (6%)	5 (2%)	9	5
3	Q	230/248 (93%)	216 (94%)	8 (4%)	6 (3%)	7	3
4	D	232/241 (96%)	224 (97%)	5 (2%)	3 (1%)	15	11
4	R	232/241 (96%)	224 (97%)	4 (2%)	4 (2%)	11	7
5	E	232/263 (88%)	226 (97%)	5 (2%)	1 (0%)	39	42
5	S	238/263 (90%)	232 (98%)	4 (2%)	2 (1%)	24	22
6	F	241/255 (94%)	235 (98%)	5 (2%)	1 (0%)	39	42
6	T	239/255 (94%)	229 (96%)	6 (2%)	4 (2%)	11	7
7	G	241/246 (98%)	237 (98%)	4 (2%)	0	100	100
7	U	232/246 (94%)	227 (98%)	4 (2%)	1 (0%)	39	42
8	H	220/234 (94%)	217 (99%)	3 (1%)	0	100	100
8	V	220/234 (94%)	217 (99%)	3 (1%)	0	100	100
9	I	205/205 (100%)	202 (98%)	3 (2%)	0	100	100
9	W	204/205 (100%)	200 (98%)	2 (1%)	2 (1%)	19	16
10	J	195/201 (97%)	192 (98%)	3 (2%)	0	100	100
10	X	195/201 (97%)	191 (98%)	4 (2%)	0	100	100
11	K	198/204 (97%)	196 (99%)	2 (1%)	0	100	100
11	Y	200/204 (98%)	197 (98%)	3 (2%)	0	100	100
12	L	213/213 (100%)	211 (99%)	2 (1%)	0	100	100
12	Z	212/213 (100%)	210 (99%)	2 (1%)	0	100	100
13	M	215/219 (98%)	207 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	216/219 (99%)	206 (95%)	10 (5%)	0	100	100
14	N	201/205 (98%)	198 (98%)	3 (2%)	0	100	100
14	b	202/205 (98%)	199 (98%)	3 (2%)	0	100	100
All	All	6203/6458 (96%)	6023 (97%)	137 (2%)	43 (1%)	26	25

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	LYS
1	A	53	SER
3	C	47	LYS
3	C	204	LYS
4	D	176	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	185/191 (97%)	174 (94%)	11 (6%)	24	27
1	O	176/191 (92%)	165 (94%)	11 (6%)	22	24
2	B	199/221 (90%)	190 (96%)	9 (4%)	34	41
2	P	196/221 (89%)	184 (94%)	12 (6%)	23	26
3	C	179/210 (85%)	168 (94%)	11 (6%)	23	26
3	Q	183/210 (87%)	174 (95%)	9 (5%)	31	36
4	D	189/203 (93%)	185 (98%)	4 (2%)	61	74
4	R	187/203 (92%)	186 (100%)	1 (0%)	92	96
5	E	192/223 (86%)	184 (96%)	8 (4%)	36	44
5	S	197/223 (88%)	188 (95%)	9 (5%)	33	40
6	F	199/212 (94%)	189 (95%)	10 (5%)	30	35
6	T	192/212 (91%)	183 (95%)	9 (5%)	32	39
7	G	202/207 (98%)	195 (96%)	7 (4%)	43	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	U	186/207 (90%)	181 (97%)	5 (3%)	52	64
8	H	181/195 (93%)	173 (96%)	8 (4%)	35	42
8	V	172/195 (88%)	165 (96%)	7 (4%)	37	45
9	I	176/174 (101%)	173 (98%)	3 (2%)	68	81
9	W	173/174 (99%)	172 (99%)	1 (1%)	90	95
10	J	166/170 (98%)	158 (95%)	8 (5%)	31	37
10	X	165/170 (97%)	158 (96%)	7 (4%)	36	44
11	K	155/159 (98%)	146 (94%)	9 (6%)	25	28
11	Y	158/159 (99%)	152 (96%)	6 (4%)	40	49
12	L	175/178 (98%)	169 (97%)	6 (3%)	44	54
12	Z	175/178 (98%)	171 (98%)	4 (2%)	58	71
13	M	180/181 (99%)	176 (98%)	4 (2%)	60	72
13	a	178/181 (98%)	171 (96%)	7 (4%)	39	48
14	N	158/159 (99%)	154 (98%)	4 (2%)	55	67
14	b	158/159 (99%)	152 (96%)	6 (4%)	40	49
All	All	5032/5366 (94%)	4836 (96%)	196 (4%)	40	48

5 of 196 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	L	3[A]	SER
1	O	189	THR
12	Z	207	THR
12	L	163	HIS
14	N	68	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
12	L	157	ASN
2	P	40	ASN
13	a	47	ASN
1	O	118	GLN
2	P	146	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

24 non-standard protein/DNA/RNA residues are modelled in this entry.

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$
3	YCM	C	63	3	7,9,10	1.40	2 (28%)	5,10,12	1.27	1 (20%)
5	6V1	E	148	5	11,15,16	1.31	3 (27%)	11,20,22	1.58	2 (18%)
7	YCM	G	137	7	7,9,10	2.21	3 (42%)	5,10,12	6.63	3 (60%)
7	6V1	G	161	7	11,15,16	1.35	3 (27%)	11,20,22	2.34	4 (36%)
7	6V1	G	47	7	11,15,16	1.29	1 (9%)	11,20,22	2.91	2 (18%)
10	6V1	J	91	10	11,15,16	1.56	3 (27%)	11,20,22	4.91	7 (63%)
3	YCM	Q	63	3	7,9,10	1.61	1 (14%)	5,10,12	2.45	3 (60%)
5	6V1	S	148	5	11,15,16	1.39	2 (18%)	11,20,22	2.20	4 (36%)
7	YCM	U	137	7	7,9,10	1.63	2 (28%)	5,10,12	2.47	3 (60%)
7	6V1	U	161	7	11,15,16	1.80	2 (18%)	11,20,22	2.00	2 (18%)
7	6V1	U	47	7	11,15,16	1.16	2 (18%)	11,20,22	3.45	3 (27%)
10	6V1	X	91	10	11,15,16	1.44	3 (27%)	11,20,22	4.81	7 (63%)
15	6V9	c	1	15	6,8,9	0.90	0	2,10,12	4.40	2 (100%)
15	OAS	c	2	15	4,6,9	0.46	0	2,6,11	1.93	1 (50%)
15	OAS	c	3	15	4,6,9	0.58	0	2,6,11	1.87	1 (50%)
15	6V9	d	1	15	6,8,9	1.36	1 (16%)	2,10,12	7.76	2 (100%)
15	OAS	d	2	15	4,6,9	0.42	0	2,6,11	1.95	1 (50%)
15	OAS	d	3	15	4,6,9	0.83	0	2,6,11	1.42	1 (50%)
15	6V9	e	1	15	6,8,9	0.74	0	2,10,12	3.92	2 (100%)
15	OAS	e	2	15	4,6,9	0.47	0	2,6,11	0.99	0
15	OAS	e	3	15	4,6,9	0.43	0	2,6,11	1.77	1 (50%)
15	6V9	f	1	15	6,8,9	1.39	0	2,10,12	7.84	2 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	OAS	f	2	15	4,6,9	0.44	0	2,6,11	1.87	1 (50%)
15	OAS	f	3	15	4,6,9	0.94	0	2,6,11	1.31	0

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
3	YCM	C	63	3	-	0/6/8/10	0/0/0/0
5	6V1	E	148	5	-	0/6/25/27	0/1/1/1
7	YCM	G	137	7	-	0/6/8/10	0/0/0/0
7	6V1	G	161	7	-	0/6/25/27	0/1/1/1
7	6V1	G	47	7	-	0/6/25/27	0/1/1/1
10	6V1	J	91	10	-	0/6/25/27	0/1/1/1
3	YCM	Q	63	3	-	0/6/8/10	0/0/0/0
5	6V1	S	148	5	-	0/6/25/27	0/1/1/1
7	YCM	U	137	7	-	0/6/8/10	0/0/0/0
7	6V1	U	161	7	-	0/6/25/27	0/1/1/1
7	6V1	U	47	7	1/1/5/6	0/6/25/27	0/1/1/1
10	6V1	X	91	10	-	0/6/25/27	0/1/1/1
15	6V9	c	1	15	-	0/0/2/4	0/1/1/1
15	OAS	c	2	15	-	0/3/5/9	0/0/0/0
15	OAS	c	3	15	-	0/3/5/9	0/0/0/0
15	6V9	d	1	15	-	0/0/2/4	0/1/1/1
15	OAS	d	2	15	-	0/3/5/9	0/0/0/0
15	OAS	d	3	15	-	0/3/5/9	0/0/0/0
15	6V9	e	1	15	-	0/0/2/4	0/1/1/1
15	OAS	e	2	15	-	0/3/5/9	0/0/0/0
15	OAS	e	3	15	-	0/3/5/9	0/0/0/0
15	6V9	f	1	15	-	0/0/2/4	0/1/1/1
15	OAS	f	2	15	-	0/3/5/9	0/0/0/0
15	OAS	f	3	15	-	0/3/5/9	0/0/0/0

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	U	161	6V1	C1-SG	-4.48	1.77	1.83
3	Q	63	YCM	CD-SG	-3.60	1.73	1.81
7	G	137	YCM	CB-SG	-3.59	1.74	1.81
10	J	91	6V1	C4-N3	-3.40	1.32	1.38
7	U	137	YCM	CB-SG	-3.20	1.75	1.81

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	f	1	6V9	O1-C4-C3	-10.45	115.72	124.47
15	d	1	6V9	O1-C4-C3	-10.12	116.00	124.47
7	U	47	6V1	C5-C1-C2	-7.21	98.50	103.98
10	X	91	6V1	C6-N3-C4	-5.40	117.50	123.24
10	J	91	6V1	C6-N3-C4	-5.37	117.53	123.24

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	148	6V1	1	0
7	G	137	YCM	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 16 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
18	1PE	H	303	-	15,15,15	0.66	0	14,14,14	0.77	0
18	1PE	I	302	-	15,15,15	0.74	0	14,14,14	0.85	0
18	1PE	K	302	-	15,15,15	0.72	0	14,14,14	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	1PE	L	301	-	15,15,15	0.61	0	14,14,14	0.47	0
18	1PE	N	301	-	15,15,15	0.58	0	14,14,14	0.52	0
18	1PE	U	301	-	15,15,15	0.67	0	14,14,14	0.69	0
18	1PE	W	302	-	15,15,15	0.70	0	14,14,14	0.33	0
18	1PE	Y	301	-	15,15,15	0.65	0	14,14,14	0.63	0
18	1PE	a	301	-	15,15,15	0.61	0	14,14,14	0.39	0
19	ACT	c	101	-	0,3,3	0.00	-	0,3,3	0.00	-
19	ACT	d	101	-	0,3,3	0.00	-	0,3,3	0.00	-
19	ACT	e	101	-	0,3,3	0.00	-	0,3,3	0.00	-
19	ACT	f	101	-	0,3,3	0.00	-	0,3,3	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	1PE	H	303	-	-	0/13/13/13	0/0/0/0
18	1PE	I	302	-	-	0/13/13/13	0/0/0/0
18	1PE	K	302	-	-	0/13/13/13	0/0/0/0
18	1PE	L	301	-	-	0/13/13/13	0/0/0/0
18	1PE	N	301	-	-	0/13/13/13	0/0/0/0
18	1PE	U	301	-	-	0/13/13/13	0/0/0/0
18	1PE	W	302	-	-	0/13/13/13	0/0/0/0
18	1PE	Y	301	-	-	0/13/13/13	0/0/0/0
18	1PE	a	301	-	-	0/13/13/13	0/0/0/0
19	ACT	c	101	-	-	0/0/0/0	0/0/0/0
19	ACT	d	101	-	-	0/0/0/0	0/0/0/0
19	ACT	e	101	-	-	0/0/0/0	0/0/0/0
19	ACT	f	101	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	230/234 (98%)	-0.06	4 (1%) 73 72	42, 62, 99, 120	0
1	O	230/234 (98%)	0.61	31 (13%) 4 4	55, 82, 127, 151	0
2	B	248/261 (95%)	0.30	18 (7%) 18 17	47, 67, 118, 170	0
2	P	247/261 (94%)	0.55	28 (11%) 7 6	53, 80, 137, 171	0
3	C	236/248 (95%)	0.68	30 (12%) 5 4	48, 78, 130, 180	0
3	Q	234/248 (94%)	0.95	43 (18%) 2 2	44, 81, 152, 204	0
4	D	233/241 (96%)	0.28	19 (8%) 14 14	51, 76, 109, 141	0
4	R	233/241 (96%)	-0.03	5 (2%) 67 65	39, 55, 84, 118	0
5	E	233/263 (88%)	0.09	10 (4%) 39 38	40, 56, 99, 130	0
5	S	237/263 (90%)	-0.19	4 (1%) 73 72	41, 58, 94, 125	0
6	F	239/255 (93%)	-0.09	2 (0%) 87 87	39, 51, 77, 98	0
6	T	240/255 (94%)	0.17	14 (5%) 26 26	43, 63, 105, 134	0
7	G	241/246 (97%)	0.26	9 (3%) 45 44	38, 54, 99, 148	0
7	U	235/246 (95%)	0.68	38 (16%) 3 2	53, 74, 111, 148	0
8	H	220/234 (94%)	-0.15	3 (1%) 78 77	34, 48, 82, 112	0
8	V	220/234 (94%)	0.12	6 (2%) 58 57	45, 62, 106, 126	0
9	I	204/205 (99%)	0.04	1 (0%) 91 91	37, 49, 77, 96	0
9	W	204/205 (99%)	0.03	4 (1%) 68 67	48, 66, 98, 109	0
10	J	195/201 (97%)	-0.09	3 (1%) 76 75	38, 53, 74, 91	0
10	X	195/201 (97%)	-0.04	2 (1%) 84 83	44, 56, 77, 95	0
11	K	200/204 (98%)	0.16	5 (2%) 61 60	46, 60, 90, 109	0
11	Y	199/204 (97%)	0.08	2 (1%) 84 83	35, 47, 72, 83	0
12	L	213/213 (100%)	-0.07	0 100 100	43, 65, 91, 114	0
12	Z	213/213 (100%)	-0.03	3 (1%) 78 77	33, 48, 78, 99	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	216/219 (98%)	0.11	4 (1%) 70 68	35, 51, 77, 115	0
13	a	216/219 (98%)	0.03	3 (1%) 78 77	33, 47, 73, 107	0
14	N	202/205 (98%)	0.03	3 (1%) 76 75	35, 44, 70, 117	0
14	b	203/205 (99%)	0.23	10 (4%) 33 33	39, 50, 81, 131	0
15	c	0/4	-	-	-	-
15	d	0/4	-	-	-	-
15	e	0/4	-	-	-	-
15	f	0/4	-	-	-	-
All	All	6216/6474 (96%)	0.18	304 (4%) 33 33	33, 59, 107, 204	0

The worst 5 of 304 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	187	PHE	12.9
3	Q	232	ILE	11.9
14	b	203	PRO	9.3
1	O	232	ILE	9.3
2	P	204	SER	8.6

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
15	OAS	e	3	7/10	0.98	0.13	-	35,35,38,39	0
7	YCM	G	137	10/11	0.92	0.15	-	46,53,68,69	0
15	OAS	e	2	7/10	0.98	0.14	-	34,37,43,48	0
7	6V1	G	47	15/16	0.91	0.16	-	53,79,84,85	0
7	6V1	U	161	15/16	0.91	0.12	-	70,89,97,99	0
15	OAS	d	3	7/10	0.98	0.10	-	42,45,51,52	0
15	6V9	c	1	8/9	0.98	0.09	-	51,52,53,53	0
15	6V9	e	1	8/9	0.99	0.10	-	41,42,44,45	0
10	6V1	J	91	15/16	0.93	0.17	-	43,64,69,69	0
15	OAS	c	3	7/10	0.98	0.14	-	47,48,48,48	0
15	6V9	f	1	8/9	0.92	0.13	-	61,63,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	6V1	E	148	15/16	0.89	0.17	-	47,68,74,76	0
7	6V1	U	47	15/16	0.87	0.33	-	94,131,141,141	0
3	YCM	C	63	10/11	0.94	0.12	-	63,69,85,89	0
5	6V1	S	148	15/16	0.88	0.16	-	44,74,82,83	0
7	6V1	G	161	15/16	0.92	0.17	-	46,69,77,78	0
15	OAS	d	2	7/10	0.95	0.10	-	45,46,47,49	0
15	OAS	c	2	7/10	0.95	0.14	-	49,50,52,54	0
15	6V9	d	1	8/9	0.95	0.12	-	52,55,61,63	0
10	6V1	X	91	15/16	0.92	0.17	-	48,69,76,76	0
3	YCM	Q	63	10/11	0.93	0.15	-	67,72,78,79	0
7	YCM	U	137	10/11	0.84	0.18	-	60,70,87,87	0
15	OAS	f	3	7/10	0.97	0.09	-	52,53,58,60	0
15	OAS	f	2	7/10	0.91	0.11	-	53,56,58,60	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
18	1PE	H	303	16/16	0.83	0.27	12.65	71,82,101,107	0
18	1PE	I	302	16/16	0.70	0.29	9.36	76,88,94,95	0
18	1PE	W	302	16/16	0.71	0.37	7.46	75,93,100,103	0
18	1PE	Y	301	16/16	0.77	0.18	5.22	64,80,88,91	0
16	K	U	302	1/1	0.97	0.21	4.66	62,62,62,62	0
19	ACT	f	101	4/4	0.92	0.18	3.85	59,60,63,67	0
18	1PE	L	301	16/16	0.80	0.34	3.10	80,89,117,117	0
18	1PE	a	301	16/16	0.86	0.23	2.64	77,82,114,116	0
18	1PE	K	302	16/16	0.75	0.19	2.50	78,86,93,94	0
18	1PE	U	301	16/16	0.88	0.17	1.75	57,66,87,89	0
19	ACT	d	101	4/4	0.97	0.16	1.37	54,60,61,65	0
18	1PE	N	301	16/16	0.83	0.13	0.81	51,64,78,79	0
16	K	G	301	1/1	0.97	0.12	0.60	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
16	K	L	302	1/1	0.91	0.09	-1.75	77,77,77,77	0
17	MG	I	301	1/1	0.97	0.09	-2.60	43,43,43,43	0
17	MG	K	301	1/1	0.88	0.07	-3.09	50,50,50,50	0
17	MG	H	302	1/1	0.95	0.07	-3.42	45,45,45,45	0
17	MG	W	301	1/1	0.99	0.03	-4.14	50,50,50,50	0
17	MG	L	303	1/1	0.94	0.04	-4.32	49,49,49,49	0
17	MG	I	303	1/1	0.95	0.09	-4.36	40,40,40,40	0
16	K	b	301	1/1	0.98	0.05	-6.44	60,60,60,60	0
16	K	Z	301	1/1	0.93	0.04	-7.91	67,67,67,67	0
16	K	N	302	1/1	0.97	0.06	-11.27	56,56,56,56	0
17	MG	V	301	1/1	0.91	0.16	-	64,64,64,64	0
19	ACT	e	101	4/4	0.97	0.12	-	47,48,49,49	0
17	MG	X	301	1/1	0.96	0.07	-	65,65,65,65	0
19	ACT	c	101	4/4	0.97	0.12	-	63,65,65,66	0
17	MG	H	301	1/1	0.78	0.17	-	59,59,59,59	0
17	MG	J	301	1/1	0.96	0.11	-	61,61,61,61	0

6.5 Other polymers

There are no such residues in this entry.